



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:53 PM BST

PDB ID : 3ZDX
Title : Integrin alphaIIB beta3 headpiece and RGD peptide complex
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2012-12-03
Resolution : 2.45 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 : 2.13.1
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) : 2.13.1

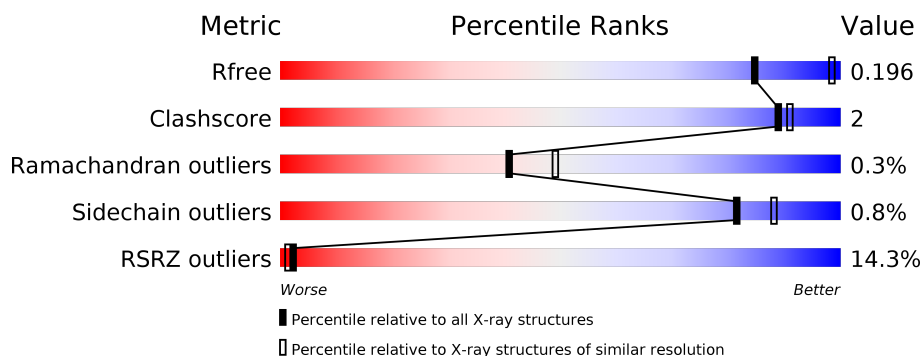
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



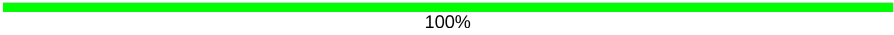
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	
1	C	457	
2	B	472	
2	D	472	
3	E	221	
3	H	221	

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

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
11	CL	B	1468	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 42688 atoms, of which 20255 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	H	N	O	S	0	9	0
			6904	2248	3369	606	673	8			
1	C	453	Total	C	H	N	O	S	0	3	0
			6807	2218	3317	601	663	8			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	6	5	0
			7132	2248	3525	615	710	34			
2	D	469	Total	C	H	N	O	S	10	1	0
			7154	2258	3531	618	713	34			

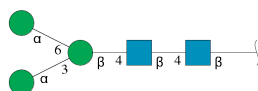
- Molecule 3 is a protein called 10E5 FAB, HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

- Molecule 4 is a protein called 10E5 FAB, LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	5	Total	C	H	N	O	0	0	0
			113	34	52	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	H	N	O	0	0	0
			53	16	25	2	10			
6	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-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	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	C	4	Total	Ca	0	0
			4	4		

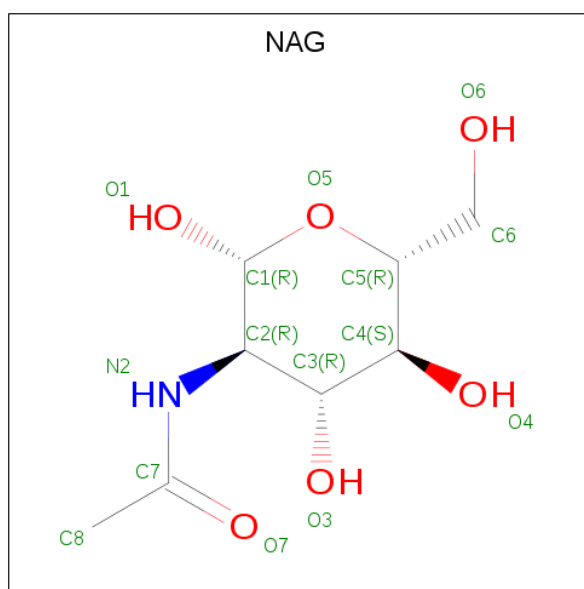
- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Cl 1 1	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	3	Total Mn 3 3	0	0
12	D	3	Total Mn 3 3	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C H N O 27 8 13 1 5	0	0
13	D	1	Total C H N O 27 8 13 1 5	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	527	Total O 527 527	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	221	Total 221	O 221	0	0
14	C	307	Total 307	O 307	0	0
14	D	177	Total 177	O 177	0	0
14	E	11	Total 11	O 11	0	0
14	F	8	Total 8	O 8	0	0
14	H	39	Total 39	O 39	0	0
14	L	34	Total 34	O 34	0	0

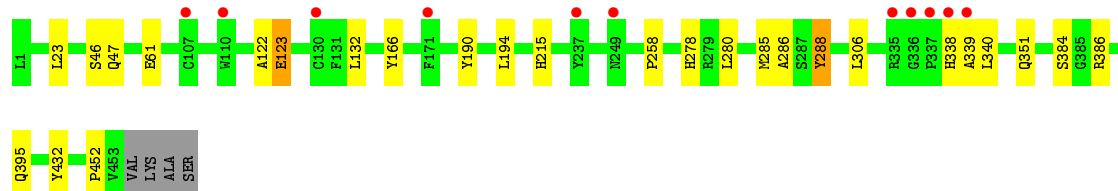
3 Residue-property plots [i](#)

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.

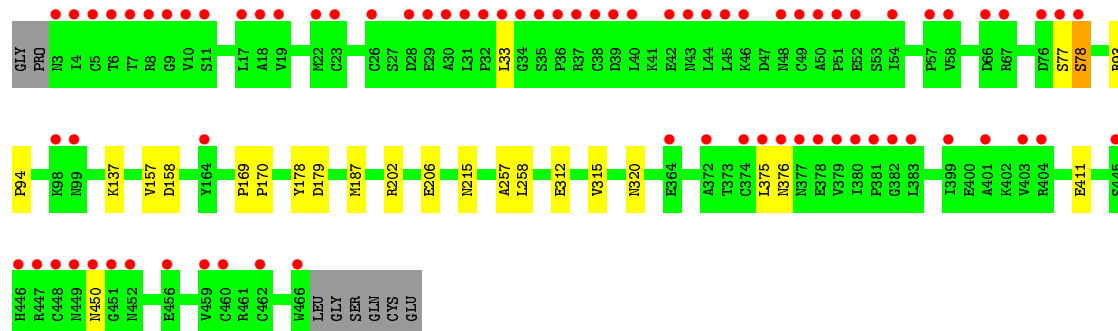
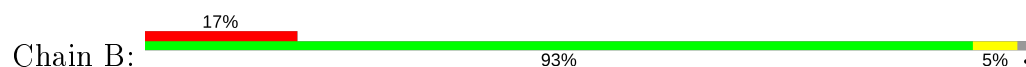
• Molecule 1: INTEGRIN ALPHA-IIB



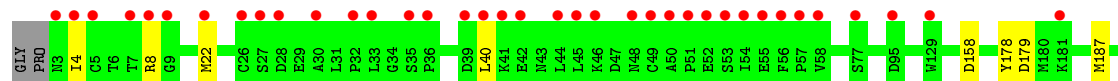
• Molecule 1: INTEGRIN ALPHA-IIB

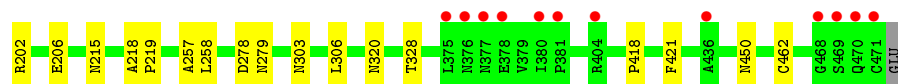


• Molecule 2: INTEGRIN BETA-3

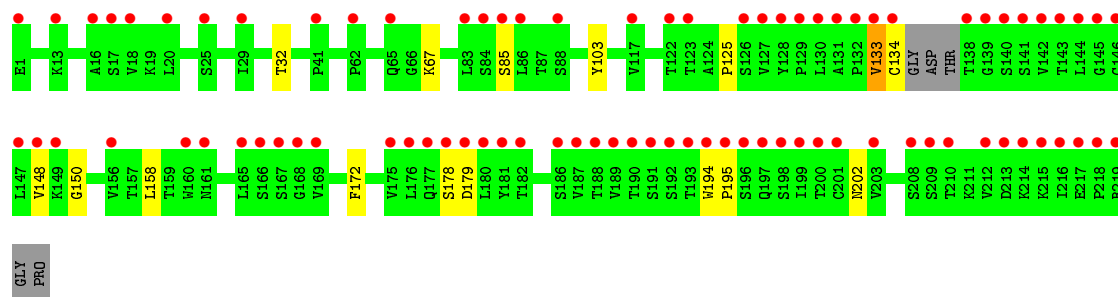
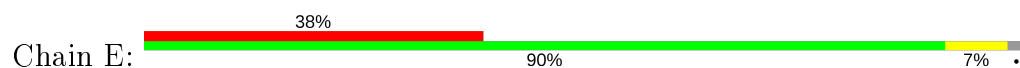


• Molecule 2: INTEGRIN BETA-3

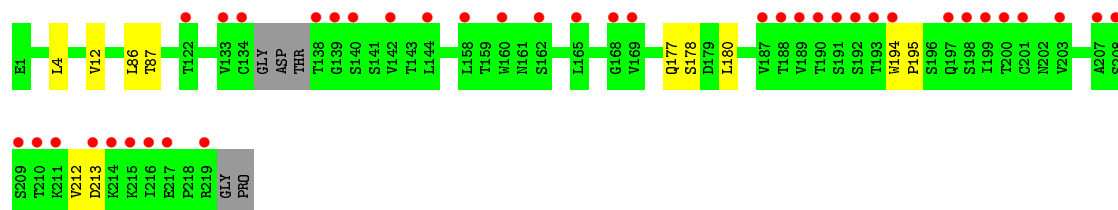




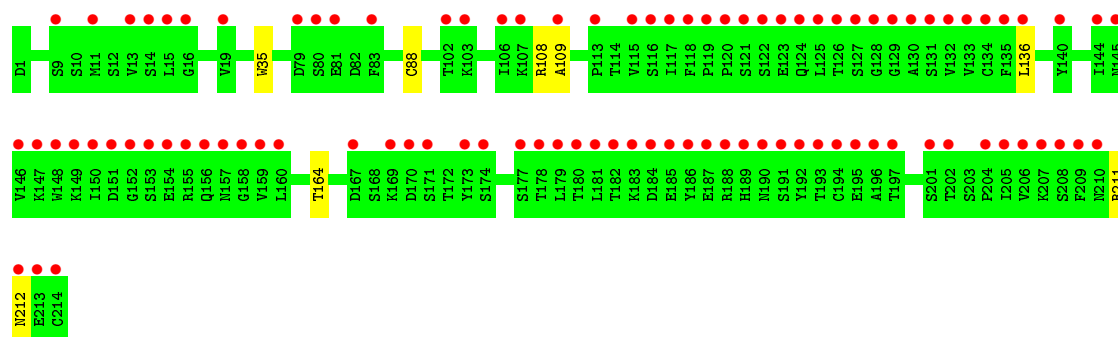
• Molecule 3: 10E5 FAB, HEAVY CHAIN



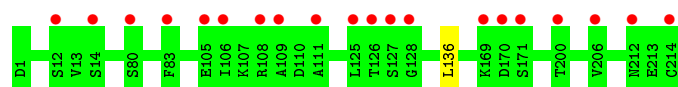
• Molecule 3: 10E5 FAB, HEAVY CHAIN



• Molecule 4: 10E5 FAB, LIGHT CHAIN

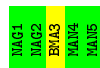


• Molecule 4: 10E5 FAB, LIGHT CHAIN



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

Chain G:  80% 20%



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

Chain I:  100%



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

Chain K:  100%



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	259.71 Å 144.96 Å 104.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.45 48.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.36-2.45) 99.9 (48.36-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.197 0.157 , 0.196	Depositor DCC
R_{free} test set	1008 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42688	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: GOL, BMA, NAG, CL, CA, MN, SO4, 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	A	0.25	0/3659	0.43	0/4987
1	C	0.23	0/3596	0.41	0/4900
2	B	0.22	0/3685	0.40	0/4996
2	D	0.22	0/3694	0.39	0/5009
3	E	0.21	0/1684	0.39	0/2305
3	H	0.22	0/1684	0.40	0/2305
4	F	0.21	0/1673	0.38	0/2269
4	L	0.22	0/1673	0.39	0/2269
All	All	0.23	0/21348	0.40	0/29040

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 [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	3535	3369	3386	13	0
1	C	3490	3317	3328	18	1
2	B	3607	3525	3534	15	0
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1597	1600	6	0
4	F	1637	1550	1553	5	0
4	L	1637	1550	1553	1	0
5	G	61	52	52	0	0
6	I	28	25	25	0	0
6	K	28	25	25	0	0
7	J	50	43	43	0	0
8	A	18	24	24	0	0
8	B	6	8	8	0	0
8	C	12	16	16	1	0
9	A	10	0	0	0	0
9	C	25	0	0	0	0
9	D	10	0	0	0	0
9	L	5	0	0	0	0
10	A	4	0	0	0	0
10	C	4	0	0	0	0
11	B	1	0	0	3	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	B	14	13	13	0	0
13	D	14	13	13	0	0
14	A	527	0	0	5	4
14	B	221	0	0	4	0
14	C	307	0	0	4	3
14	D	177	0	0	0	0
14	E	11	0	0	0	0
14	F	8	0	0	0	0
14	H	39	0	0	0	0
14	L	34	0	0	0	0
All	All	22433	20255	20310	78	4

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 78 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)
11:B:1468:CL:CL	14:B:4039:HOH:O	2.25	0.92
11:B:1468:CL:CL	14:B:4040:HOH:O	2.29	0.86
11:B:1468:CL:CL	14:B:4124:HOH:O	2.32	0.83
1:A:41:ARG:NH2	14:A:4043:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLN:OE1	14:C:4265:HOH:O	2.11	0.69

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4459:HOH:O	14:C:4260:HOH:O[1_554]	1.92	0.28
14:A:4459:HOH:O	14:C:4282:HOH:O[1_554]	1.99	0.21
14:A:4480:HOH:O	14:C:4279:HOH:O[1_554]	2.09	0.11
1:C:386:ARG:NH1	14:A:4485:HOH:O[1_556]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	464/457 (102%)	446 (96%)	17 (4%)	1 (0%)	47	57
1	C	454/457 (99%)	441 (97%)	12 (3%)	1 (0%)	47	57
2	B	467/472 (99%)	444 (95%)	20 (4%)	3 (1%)	25	29
2	D	468/472 (99%)	451 (96%)	17 (4%)	0	100	100
3	E	212/221 (96%)	200 (94%)	10 (5%)	2 (1%)	17	19
3	H	212/221 (96%)	200 (94%)	11 (5%)	1 (0%)	29	34
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	2701/2728 (99%)	2589 (96%)	104 (4%)	8 (0%)	41	49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

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Mol	Chain	Res	Type
2	B	33	LEU
2	B	78	SER
2	B	375	LEU
3	E	133	VAL

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	372/364 (102%)	366 (98%)	6 (2%)	62	74
1	C	364/364 (100%)	359 (99%)	5 (1%)	67	77
2	B	416/417 (100%)	414 (100%)	2 (0%)	88	93
2	D	416/417 (100%)	413 (99%)	3 (1%)	84	90
3	E	187/190 (98%)	186 (100%)	1 (0%)	88	93
3	H	187/190 (98%)	186 (100%)	1 (0%)	88	93
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2318/2318 (100%)	2300 (99%)	18 (1%)	81	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	61	GLU
2	D	303	ASN
2	B	215	ASN
2	B	411	GLU

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

Mol	Chain	Res	Type
2	B	3	ASN

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Mol	Chain	Res	Type
1	C	158	ASN
3	E	202	ASN

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 ⓘ

13 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	0.56	0	17,19,21	0.72	0
5	NAG	G	2	5	14,14,15	0.59	0	17,19,21	0.68	0
5	BMA	G	3	5	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
5	MAN	G	4	5	11,11,12	0.59	0	15,15,17	0.87	0
5	MAN	G	5	5	11,11,12	0.61	0	15,15,17	0.60	0
6	NAG	I	1	2,6	14,14,15	0.58	0	17,19,21	0.70	0
6	NAG	I	2	6	14,14,15	0.55	0	17,19,21	0.64	0
7	NAG	J	1	2,7	14,14,15	0.52	0	17,19,21	0.65	0
7	NAG	J	2	7	14,14,15	0.60	0	17,19,21	0.77	0
7	BMA	J	3	7	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
7	MAN	J	4	7	11,11,12	0.65	0	15,15,17	0.73	0
6	NAG	K	1	2,6	14,14,15	0.63	0	17,19,21	0.87	0
6	NAG	K	2	6	14,14,15	0.54	0	17,19,21	0.62	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	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	3	BMA	C1-C2-C3	2.60	112.86	109.67
5	G	3	BMA	O5-C5-C6	2.40	110.96	107.20

There are no chirality outliers.

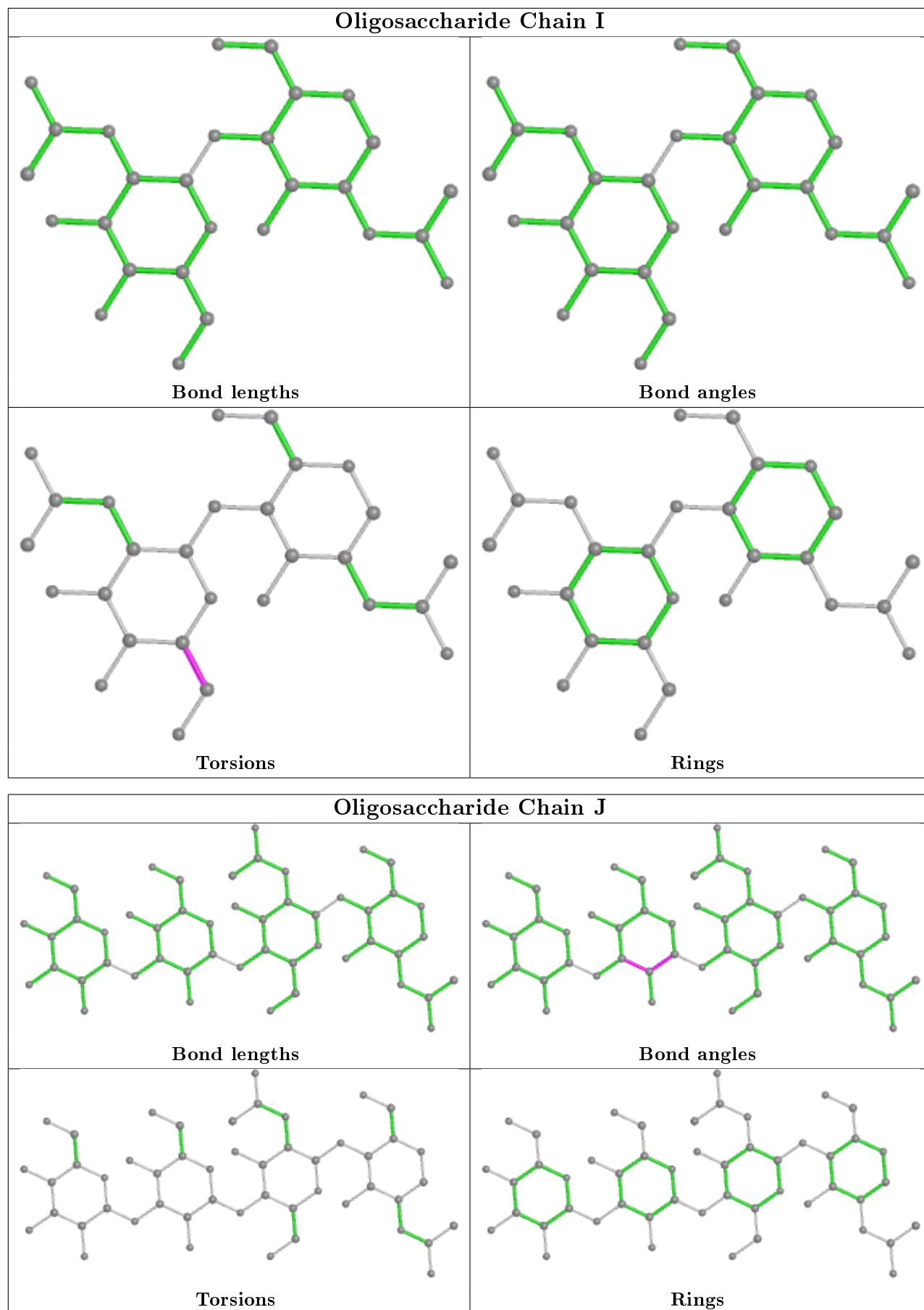
5 of 6 torsion outliers are listed below:

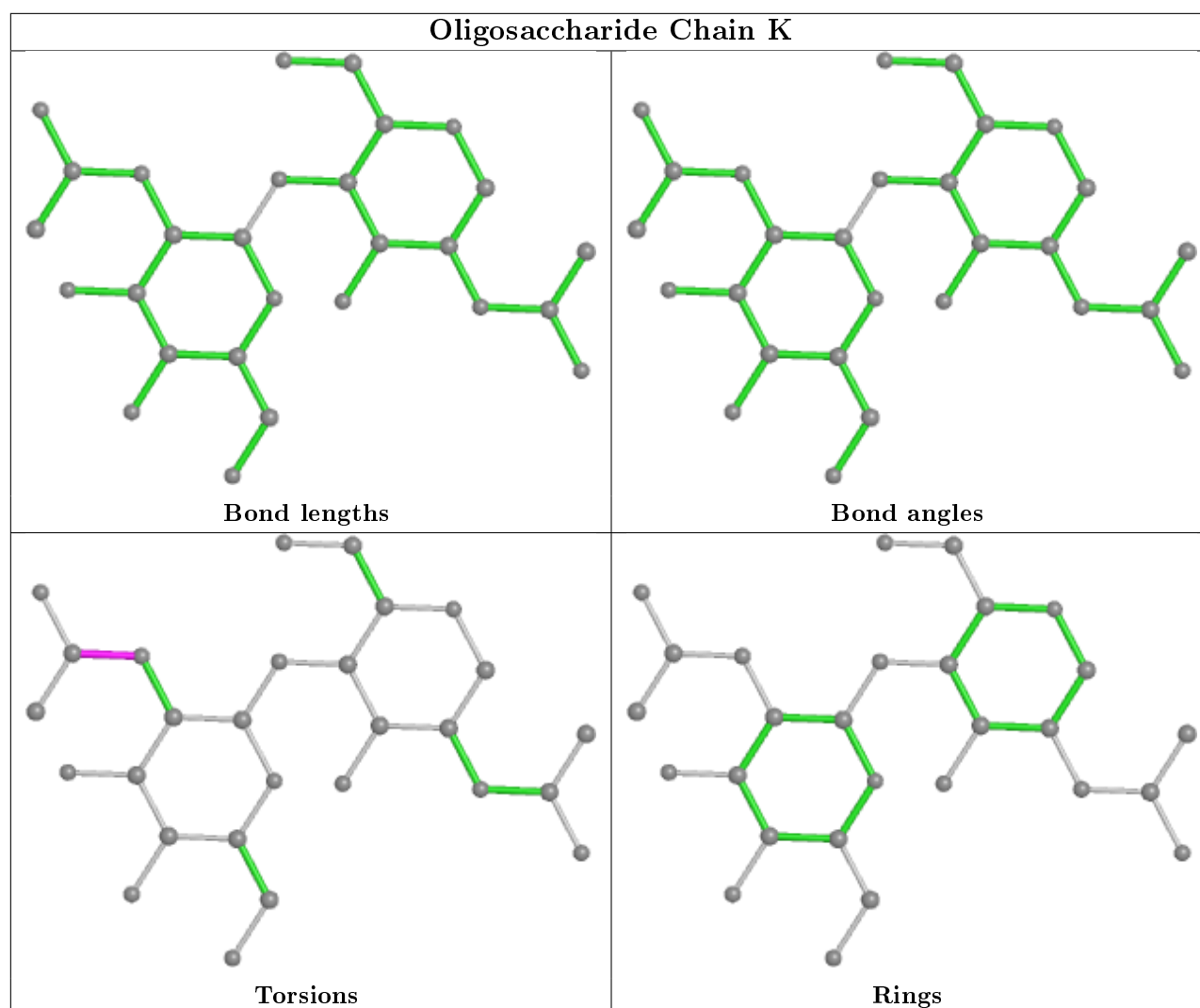
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	C	1456	-	4,4,4	0.15	0	6,6,6	0.05	0
8	GOL	A	1459	-	5,5,5	0.37	0	5,5,5	0.23	0
9	SO4	A	1462	-	4,4,4	0.13	0	6,6,6	0.05	0
9	SO4	D	1472	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	C	1458	-	4,4,4	0.13	0	6,6,6	0.06	0
9	SO4	A	1461	-	4,4,4	0.14	0	6,6,6	0.07	0
8	GOL	C	1454	-	5,5,5	0.36	0	5,5,5	0.29	0
9	SO4	L	1215	-	4,4,4	0.15	0	6,6,6	0.04	0
13	NAG	B	3099	2	14,14,15	0.51	0	17,19,21	0.72	0
13	NAG	D	3099	2	14,14,15	0.52	0	17,19,21	0.61	0
9	SO4	C	1457	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	C	1460	-	4,4,4	0.14	0	6,6,6	0.04	0
8	GOL	A	1458	-	5,5,5	0.38	0	5,5,5	0.26	0
8	GOL	B	1467	-	5,5,5	0.37	0	5,5,5	0.23	0
9	SO4	D	1473	12	4,4,4	0.14	0	6,6,6	0.07	0
8	GOL	C	1455	-	5,5,5	0.36	0	5,5,5	0.23	0
8	GOL	A	1460	-	5,5,5	0.37	0	5,5,5	0.16	0
9	SO4	C	1459	-	4,4,4	0.14	0	6,6,6	0.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	1459	-	-	0/4/4/4	-
8	GOL	C	1454	-	-	2/4/4/4	-
13	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
13	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
8	GOL	A	1460	-	-	2/4/4/4	-
8	GOL	A	1458	-	-	2/4/4/4	-
8	GOL	C	1455	-	-	2/4/4/4	-
8	GOL	B	1467	-	-	2/4/4/4	-

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	C	1454	GOL	O1-C1-C2-C3
8	A	1458	GOL	O1-C1-C2-O2
8	A	1458	GOL	O1-C1-C2-C3
8	A	1460	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	B	1467	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
8	C	1454	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	A	457/457 (100%)	0.37	9 (1%) 65 62	9, 20, 53, 124	1 (0%)
1	C	453/457 (99%)	0.23	11 (2%) 59 54	16, 34, 68, 112	0
2	B	464/472 (98%)	0.97	78 (16%) 1 1	10, 46, 124, 181	2 (0%)
2	D	469/472 (99%)	0.50	49 (10%) 6 4	17, 45, 107, 163	2 (0%)
3	E	216/221 (97%)	2.14	84 (38%) 0 0	40, 103, 180, 201	0
3	H	216/221 (97%)	0.67	39 (18%) 1 0	24, 70, 124, 143	0
4	F	214/214 (100%)	2.20	96 (44%) 0 0	40, 92, 166, 237	0
4	L	214/214 (100%)	0.44	20 (9%) 8 5	28, 56, 89, 173	0
All	All	2703/2728 (99%)	0.79	386 (14%) 2 1	9, 46, 132, 237	5 (0%)

The worst 5 of 386 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	214	CYS	12.9
3	E	216	ILE	12.8
2	B	77	SER	11.9
3	E	199	ILE	11.6
2	D	469	SER	11.6

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

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

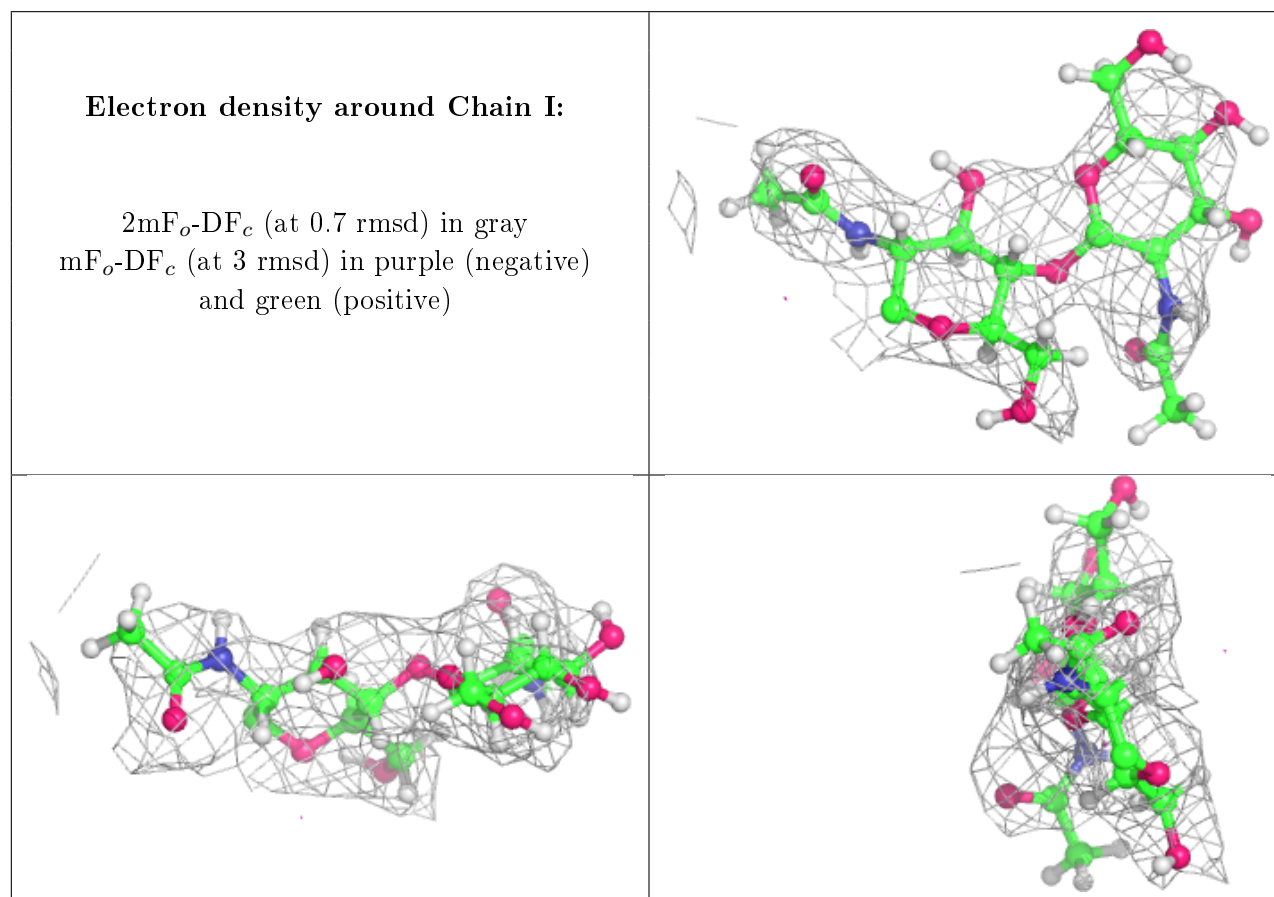
6.3 Carbohydrates ⓘ

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.

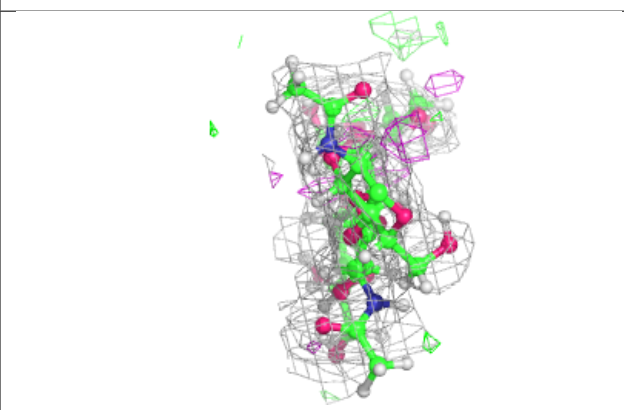
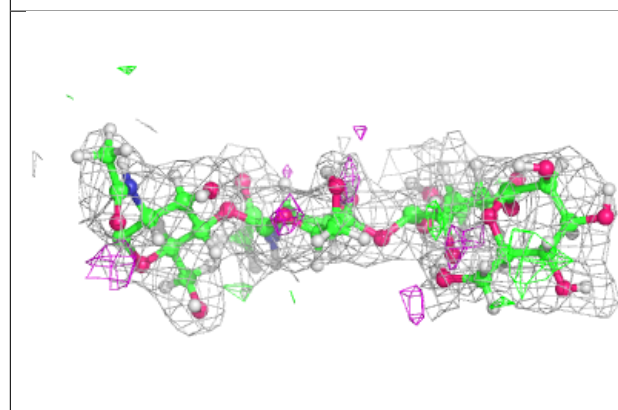
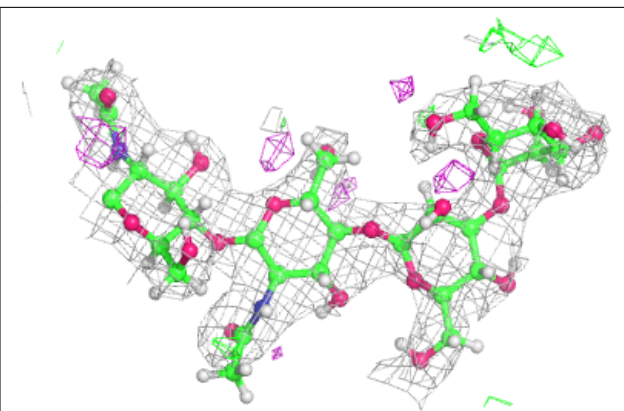
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BMA	J	3	11/12	0.69	0.34	93,132,158,161	0
5	BMA	G	3	11/12	0.75	0.24	81,124,152,153	0
7	MAN	J	4	11/12	0.75	0.22	104,129,153,155	0
5	MAN	G	4	11/12	0.76	0.28	54,111,133,145	0
5	MAN	G	5	11/12	0.80	0.27	108,127,148,152	0
6	NAG	K	2	14/15	0.82	0.50	116,148,185,192	0
6	NAG	I	1	14/15	0.83	0.34	66,98,121,123	0
6	NAG	K	1	14/15	0.84	0.30	55,95,127,136	0
6	NAG	I	2	14/15	0.86	0.39	93,126,151,153	0
7	NAG	J	2	14/15	0.87	0.26	48,77,102,108	0
5	NAG	G	2	14/15	0.92	0.16	47,65,96,99	0
7	NAG	J	1	14/15	0.94	0.14	21,44,61,70	0
5	NAG	G	1	14/15	0.96	0.12	13,28,46,53	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.

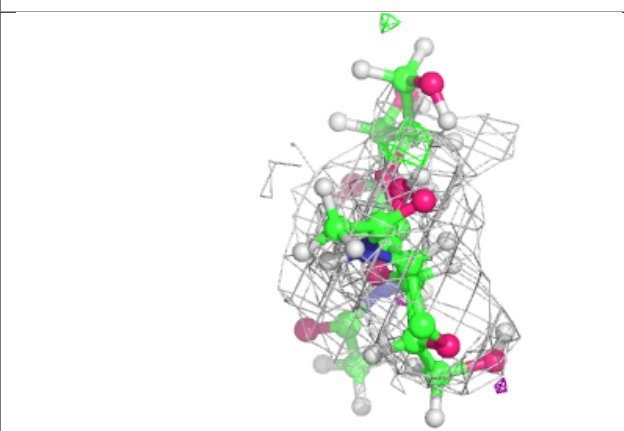
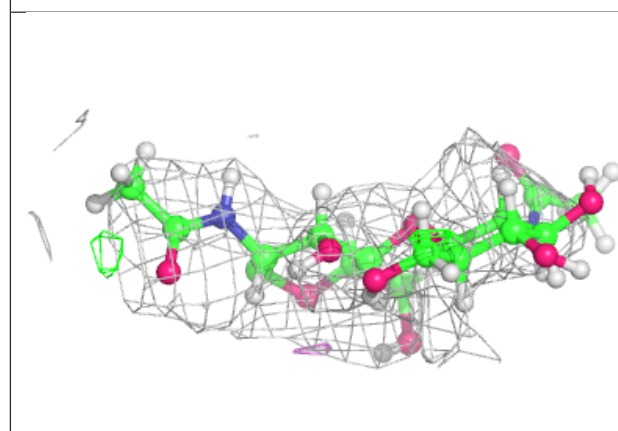
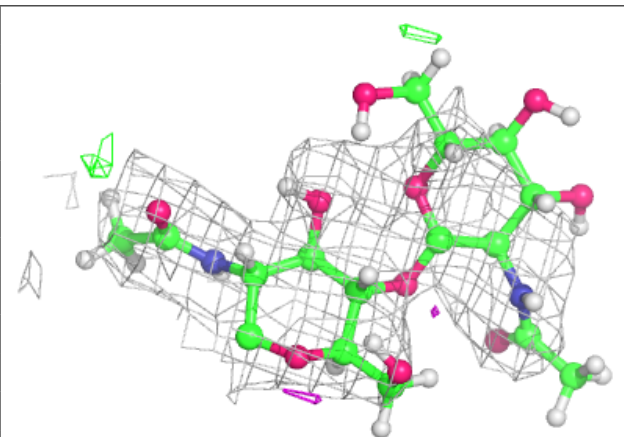


Electron density around Chain J:

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

**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(Å ²)	Q<0.9
9	SO4	C	1460	5/5	0.82	0.25	105,113,126,134	0
13	NAG	B	3099	14/15	0.85	0.37	95,127,149,154	0
9	SO4	D	1472	5/5	0.86	0.28	62,114,118,118	0
8	GOL	A	1460	6/6	0.86	0.19	50,67,81,89	0
8	GOL	C	1455	6/6	0.87	0.26	55,86,104,124	0
13	NAG	D	3099	14/15	0.87	0.30	78,100,120,127	0
9	SO4	C	1457	5/5	0.88	0.19	88,112,116,117	0
9	SO4	L	1215	5/5	0.88	0.24	100,105,109,119	0
8	GOL	A	1459	6/6	0.90	0.28	47,71,81,86	0
9	SO4	C	1459	5/5	0.90	0.23	132,135,136,141	0
8	GOL	C	1454	6/6	0.90	0.19	46,71,85,85	0
8	GOL	B	1467	6/6	0.92	0.20	62,87,101,104	0
9	SO4	A	1462	5/5	0.92	0.19	94,110,116,116	0
9	SO4	C	1458	5/5	0.93	0.24	59,107,112,117	0
9	SO4	C	1456	5/5	0.94	0.20	56,99,110,117	0
8	GOL	A	1458	6/6	0.95	0.20	42,62,82,82	0
9	SO4	A	1461	5/5	0.95	0.19	48,71,91,109	0
10	CA	C	2004	1/1	0.95	0.06	47,47,47,47	0
12	MN	B	2002	1/1	0.97	0.07	41,41,41,41	0
10	CA	A	2004	1/1	0.97	0.05	28,28,28,28	0
10	CA	C	2007	1/1	0.98	0.12	38,38,38,38	0
9	SO4	D	1473	5/5	0.98	0.17	19,55,61,81	0
12	MN	D	2002	1/1	0.98	0.07	43,43,43,43	0
11	CL	B	1468	1/1	0.99	0.21	26,26,26,26	0
12	MN	D	2001	1/1	0.99	0.14	31,31,31,31	0
10	CA	A	2007	1/1	0.99	0.15	14,14,14,14	0
12	MN	D	2003	1/1	0.99	0.13	34,34,34,34	0
12	MN	B	2003	1/1	0.99	0.16	25,25,25,25	0
10	CA	C	2006	1/1	0.99	0.14	33,33,33,33	0
10	CA	A	2006	1/1	0.99	0.20	14,14,14,14	0
10	CA	C	2005	1/1	0.99	0.06	38,38,38,38	0
10	CA	A	2005	1/1	0.99	0.12	15,15,15,15	0
12	MN	B	2001	1/1	1.00	0.20	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.