



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2023 – 11:01 PM EDT

PDB ID : 7U60
Title : Integrin α IIB β 3 complex with cRGDfV
Authors : Zhu, J.; Lin, F.Y.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-03
Resolution : 2.55 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

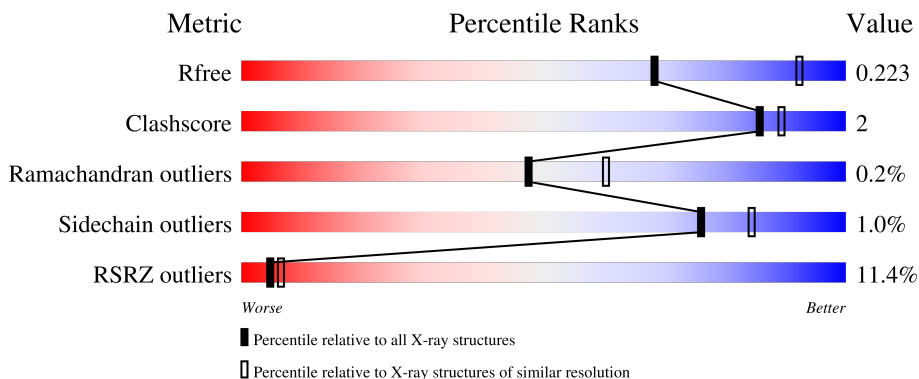
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	455	 94% 6%
1	C	455	 92% 7%
2	B	471	 15% 91% 8%
2	D	471	 7% 93% 7%
3	E	216	 34% 94% 6%

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Mol	Chain	Length	Quality of chain
3	H	216	
4	F	214	
4	L	214	
5	M	5	
5	N	5	
6	G	4	
6	J	4	
7	I	2	
7	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
10	SO4	A	515	-	-	-	X
11	MN	B	2001	-	-	-	X
5	DPN	N	4	-	-	-	X
9	GOL	L	301	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22350 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
			Total	C	N	O	S			
1	A	455	Total	C	N	O	S	0	6	0
			3521	2240	607	666	8			
1	C	453	Total	C	N	O	S	0	3	0
			3492	2219	603	662	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	464	Total	C	N	O	S	4	5	0
			3613	2252	614	714	33			
2	D	469	Total	C	N	O	S	4	2	0
			3626	2260	618	714	34			

- Molecule 3 is a protein called Fab heavy chain.

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

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 a protein called ARG-GLY-ASP-DPN-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	5	Total	C	N	O	0	0	0
			41	26	8	7			
5	N	5	Total	C	N	O	0	0	0
			41	26	8	7			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
6	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 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
7	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 10 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		

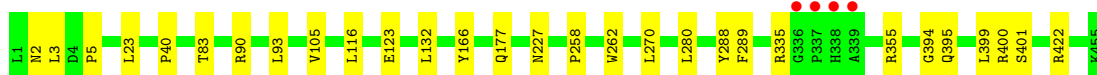
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	396	Total	O	0	0
			396	396		
13	B	181	Total	O	0	0
			181	181		
13	C	246	Total	O	0	0
			246	246		
13	D	192	Total	O	0	0
			192	192		
13	E	20	Total	O	0	0
			20	20		
13	F	22	Total	O	0	0
			22	22		
13	H	35	Total	O	0	0
			35	35		
13	L	53	Total	O	0	0
			53	53		
13	M	3	Total	O	0	0
			3	3		
13	N	6	Total	O	0	0
			6	6		

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.

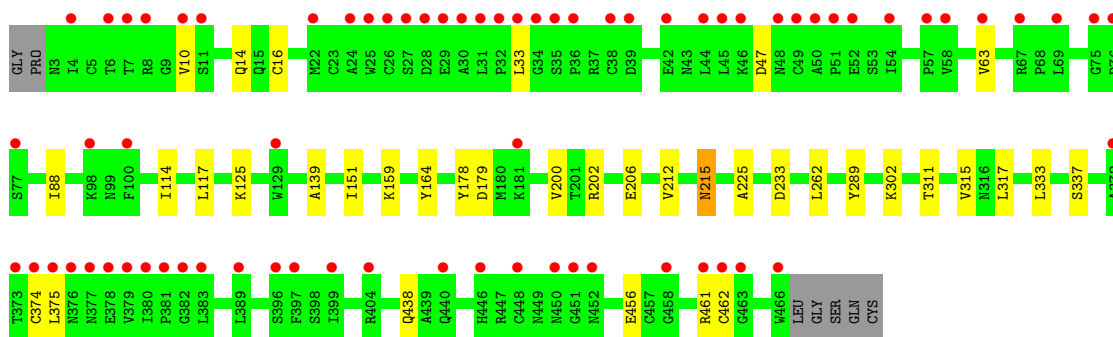
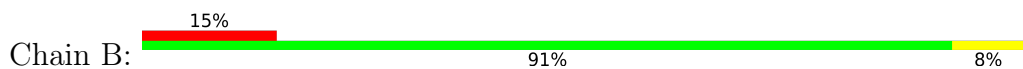
- Molecule 1: Integrin alpha-IIb



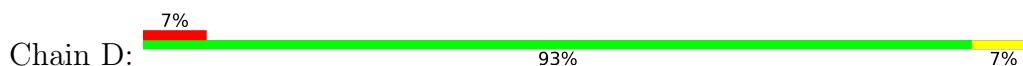
- Molecule 1: Integrin alpha-IIb

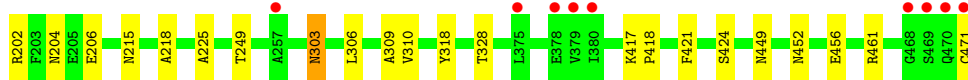
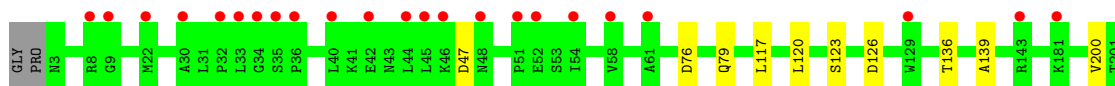


- Molecule 2: Integrin beta-3

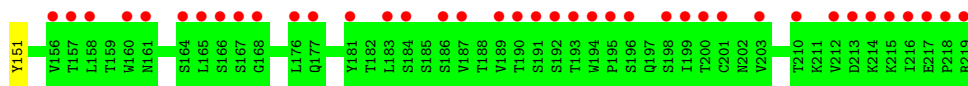


- Molecule 2: Integrin beta-3

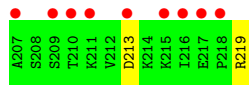
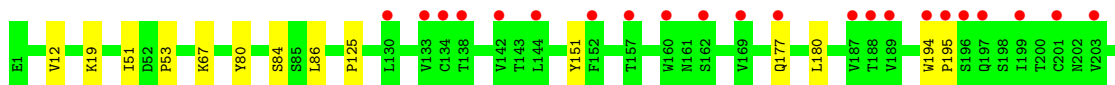
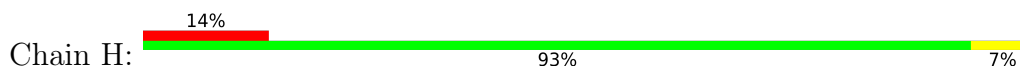




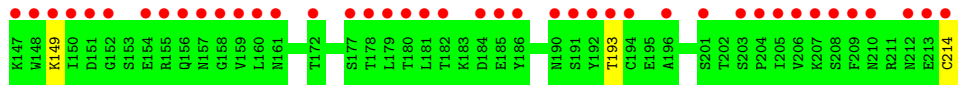
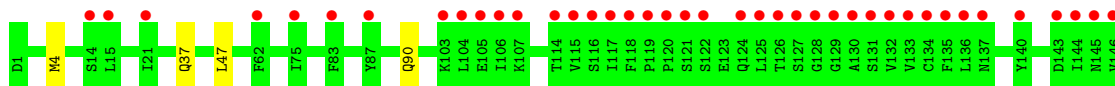
● Molecule 3: Fab heavy chain



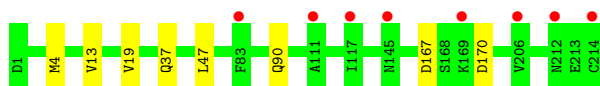
● Molecule 3: Fab heavy chain



● Molecule 4: Fab light chain



● Molecule 4: Fab light chain

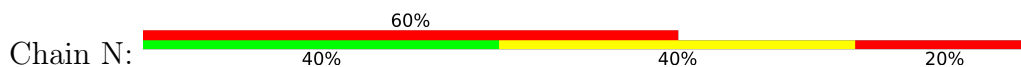


● Molecule 5: ARG-GLY-ASP-DPN-VAL





- Molecule 5: ARG-GLY-ASP-DPN-VAL



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	260.89Å 145.77Å 105.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.55 48.60 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.60-2.55) 98.8 (48.60-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.225 0.188 , 0.223	Depositor DCC
R_{free} test set	1023 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22350	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, NAG, MN, CA, SO4, DPN, 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	0.28	0/3636	0.56	0/4954
1	C	0.27	0/3598	0.55	0/4902
2	B	0.25	0/3692	0.50	0/5006
2	D	0.26	0/3700	0.50	0/5017
3	E	0.24	0/1684	0.48	0/2305
3	H	0.25	0/1684	0.49	0/2305
4	F	0.25	0/1673	0.47	0/2269
4	L	0.25	0/1673	0.50	0/2269
5	M	2.21	2/28 (7.1%)	3.26	2/34 (5.9%)
5	N	2.23	2/28 (7.1%)	3.31	2/34 (5.9%)
All	All	0.28	4/21396 (0.0%)	0.54	4/29095 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1	ARG	NE-CZ	7.38	1.42	1.33
5	M	1	ARG	NE-CZ	7.09	1.42	1.33
5	N	1	ARG	CZ-NH2	5.91	1.40	1.33
5	M	1	ARG	CZ-NH2	5.59	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	ARG	NE-CZ-NH1	15.43	128.02	120.30
5	M	1	ARG	NE-CZ-NH1	14.99	127.80	120.30
5	N	1	ARG	NE-CZ-NH2	-6.19	117.20	120.30
5	M	1	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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	3521	0	3377	16	0
1	C	3492	0	3333	15	0
2	B	3613	0	3528	18	0
2	D	3626	0	3541	18	0
3	E	1642	0	1600	7	0
3	H	1642	0	1600	9	0
4	F	1637	0	1553	3	0
4	L	1637	0	1553	4	0
5	M	41	0	38	1	0
5	N	41	0	37	2	0
6	G	50	0	43	0	0
6	J	50	0	43	0	0
7	I	28	0	25	0	0
7	K	28	0	25	0	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
9	A	42	0	56	4	0
9	C	12	0	16	0	0
9	D	6	0	8	1	0
9	L	6	0	8	0	0
10	A	20	0	0	0	0
10	B	5	0	0	0	0
10	C	10	0	0	0	0
10	L	5	0	0	0	0
11	B	3	0	0	0	0
11	D	3	0	0	0	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
13	A	396	0	0	6	1
13	B	181	0	0	0	0
13	C	246	0	0	3	1
13	D	192	0	0	1	0
13	E	20	0	0	0	0
13	F	22	0	0	0	0
13	H	35	0	0	1	0
13	L	53	0	0	0	0
13	M	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	6	0	0	1	0
All	All	22350	0	20410	90	1

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 90 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)
1:A:400:ARG:HE	9:A:506:GOL:H12	1.60	0.65
3:H:219:ARG:NH2	13:H:301:HOH:O	2.28	0.65
3:E:67:LYS:NZ	3:E:85:SER:O	2.33	0.61
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.84	0.60
2:D:471:CYS:SG	13:D:2227:HOH:O	2.57	0.59

All (1) 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)
13:A:831:HOH:O	13:C:814:HOH:O[1_554]	2.10	0.10

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	459/455 (101%)	444 (97%)	14 (3%)	1 (0%)	47 60
1	C	454/455 (100%)	439 (97%)	14 (3%)	1 (0%)	47 60
2	B	467/471 (99%)	447 (96%)	18 (4%)	2 (0%)	34 46
2	D	469/471 (100%)	451 (96%)	18 (4%)	0	100 100
3	E	212/216 (98%)	201 (95%)	9 (4%)	2 (1%)	17 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
5	M	2/5 (40%)	2 (100%)	0	0	100	100
5	N	2/5 (40%)	2 (100%)	0	0	100	100
All	All	2701/2722 (99%)	2599 (96%)	96 (4%)	6 (0%)	47	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	133	VAL
2	B	33	LEU
2	B	375	LEU
1	A	123	GLU
1	C	123	GLU

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	369/363 (102%)	363 (98%)	6 (2%)	62	77
1	C	364/363 (100%)	358 (98%)	6 (2%)	62	77
2	B	416/416 (100%)	411 (99%)	5 (1%)	71	81
2	D	417/416 (100%)	412 (99%)	5 (1%)	71	81
3	E	187/187 (100%)	187 (100%)	0	100	100
3	H	187/187 (100%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	93
4	L	188/188 (100%)	188 (100%)	0	100	100
5	M	3/3 (100%)	3 (100%)	0	100	100
5	N	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	2322/2314 (100%)	2298 (99%)	24 (1%)	76	84

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

Mol	Chain	Res	Type
1	C	197	GLN
2	D	47	ASP
1	C	288	TYR
2	D	123[A]	SER
2	B	47	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	204	ASN
2	D	438	GLN
2	B	428	GLN
2	B	438	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](#)

2 non-standard protein/DNA/RNA residues 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	DPN	M	4	5	10,11,12	0.61	0	10,13,15	0.83	1 (10%)
5	DPN	N	4	5	10,11,12	0.79	0	10,13,15	1.25	1 (10%)

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	DPN	M	4	5	-	1/5/6/8	0/1/1/1
5	DPN	N	4	5	-	2/5/6/8	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(°)
5	N	4	DPN	CG-CB-CA	3.43	121.03	114.10
5	M	4	DPN	CG-CB-CA	2.06	118.27	114.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	4	DPN	O-C-CA-CB
5	N	4	DPN	C-CA-CB-CG
5	N	4	DPN	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
6	NAG	G	1	6,2	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
6	NAG	G	2	6	14,14,15	0.19	0	17,19,21	0.50	0
6	MAN	G	3	6	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
6	MAN	G	4	6	11,11,12	0.68	0	15,15,17	1.13	2 (13%)
7	NAG	I	1	7,2	14,14,15	0.32	0	17,19,21	0.34	0
7	NAG	I	2	7	14,14,15	0.21	0	17,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	J	1	6,2	14,14,15	0.42	0	17,19,21	0.48	0
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.53	0
6	MAN	J	3	6	11,11,12	0.88	0	15,15,17	0.88	1 (6%)
6	MAN	J	4	6	11,11,12	0.90	0	15,15,17	0.94	1 (6%)
7	NAG	K	1	7,2	14,14,15	0.35	0	17,19,21	0.41	0
7	NAG	K	2	7	14,14,15	0.25	0	17,19,21	0.45	0

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

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	4	MAN	C1-O5-C5	3.08	116.36	112.19
6	G	3	MAN	C1-O5-C5	2.72	115.88	112.19
6	G	4	MAN	O2-C2-C3	-2.34	105.46	110.14
6	G	3	MAN	O2-C2-C3	-2.31	105.52	110.14
6	J	4	MAN	O2-C2-C3	-2.14	105.85	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

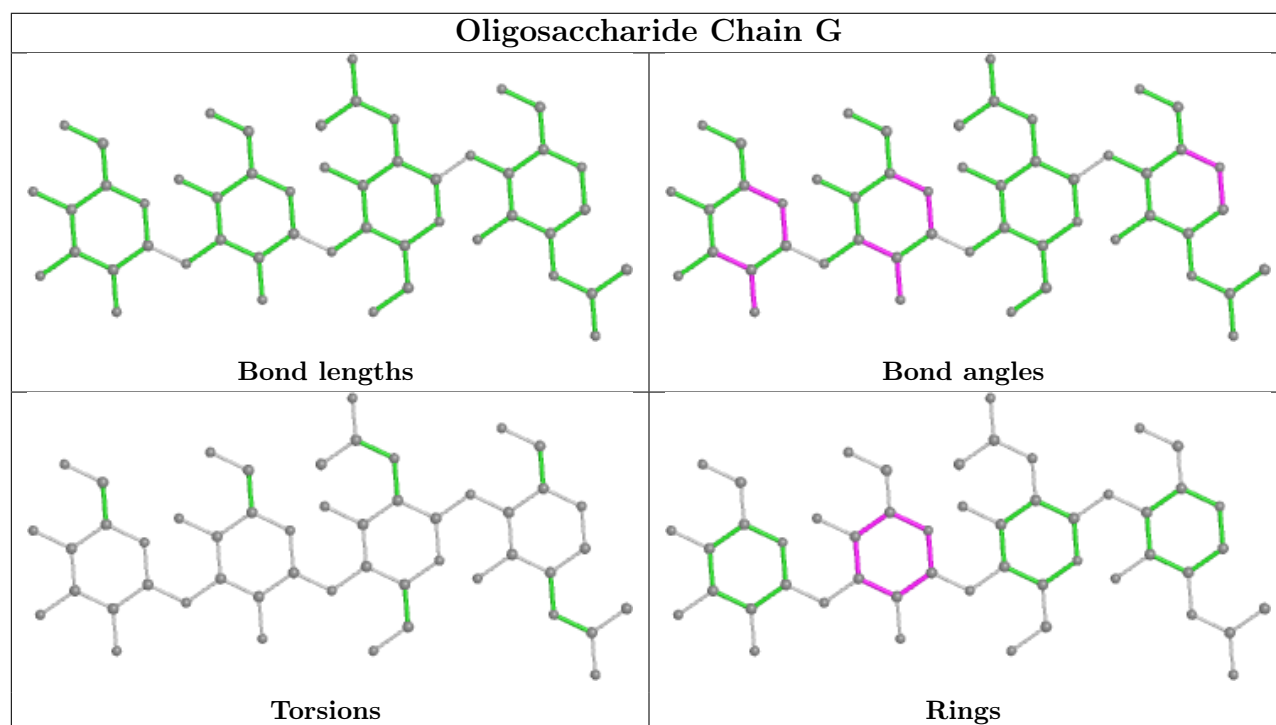
Mol	Chain	Res	Type	Atoms
6	J	3	MAN	O5-C5-C6-O6
6	J	3	MAN	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6

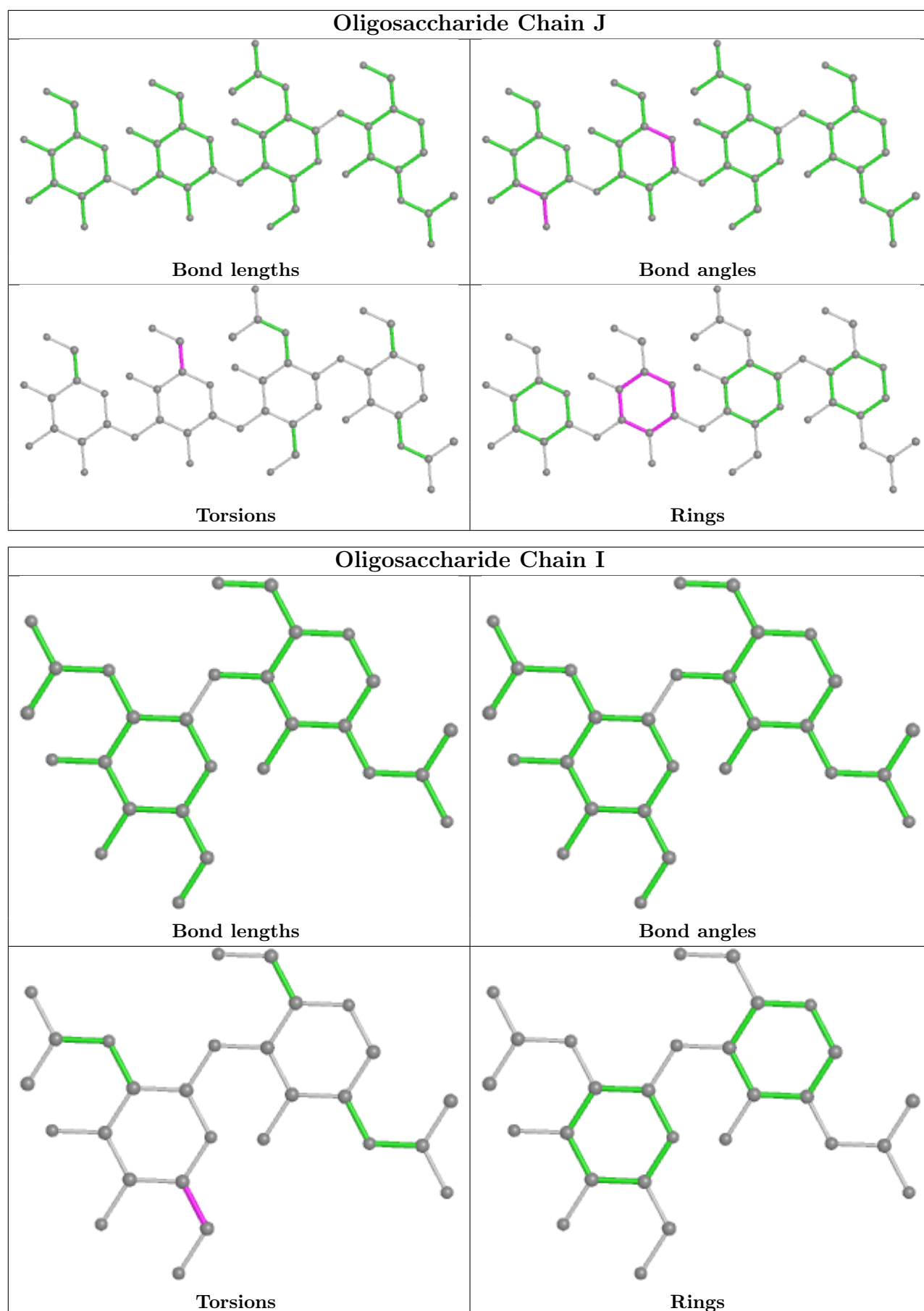
All (2) ring outliers are listed below:

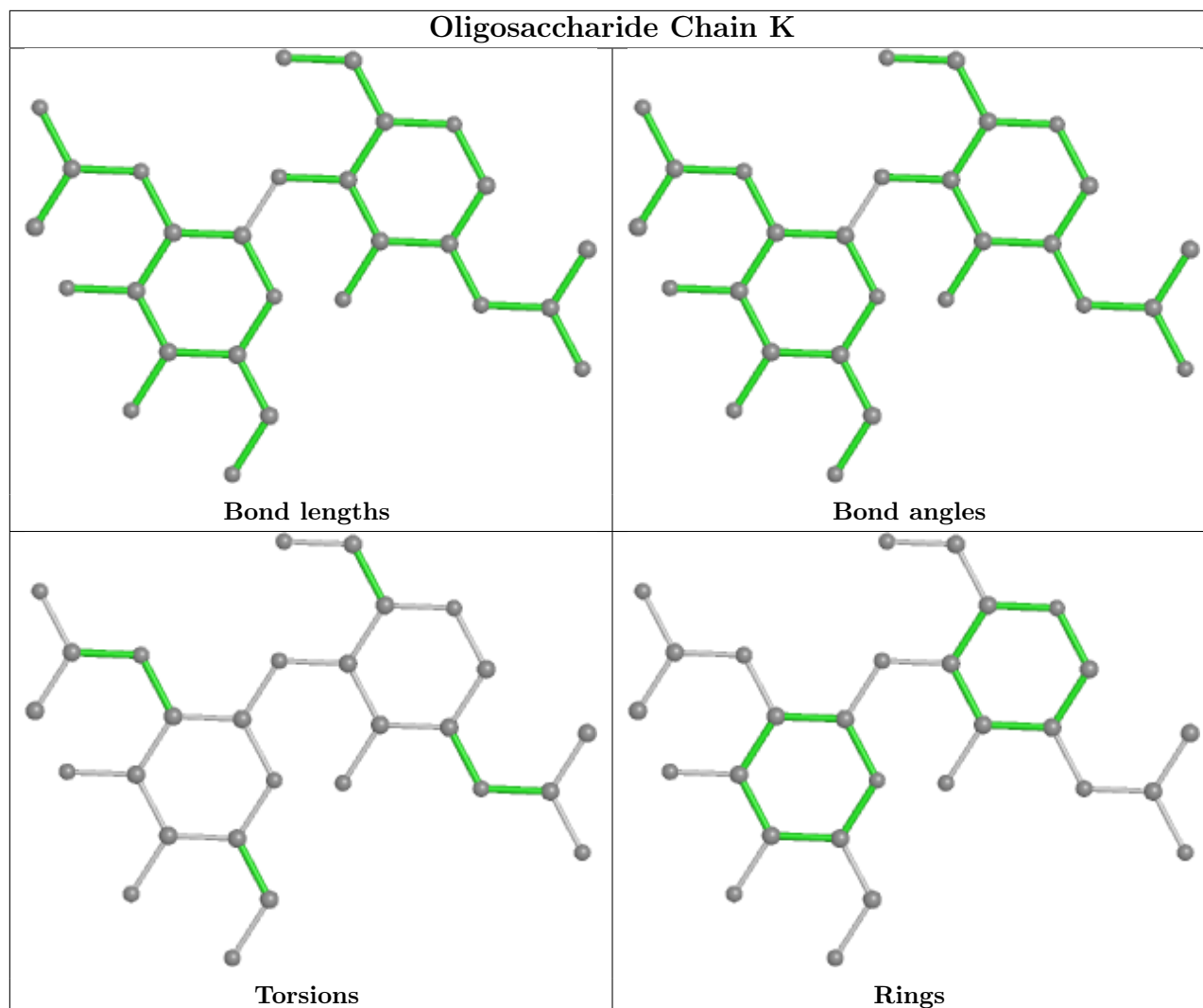
Mol	Chain	Res	Type	Atoms
6	G	3	MAN	C1-C2-C3-C4-C5-O5
6	J	3	MAN	C1-C2-C3-C4-C5-O5

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 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	$\# Z > 2$
12	NAG	B	2004	2	14,14,15	0.36	0	17,19,21	0.55	0
10	SO4	A	513	-	4,4,4	0.14	0	6,6,6	0.05	0
9	GOL	D	2005	-	5,5,5	0.96	0	5,5,5	0.87	0
9	GOL	A	506	-	5,5,5	0.95	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	A	508	-	5,5,5	0.89	0	5,5,5	0.98	0
9	GOL	A	507	-	5,5,5	0.86	0	5,5,5	1.05	0
9	GOL	A	509	-	5,5,5	0.89	0	5,5,5	1.04	0
9	GOL	A	511	-	5,5,5	0.91	0	5,5,5	0.97	0
10	SO4	C	508	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.05	0
9	GOL	A	505	-	5,5,5	0.86	0	5,5,5	1.01	0
10	SO4	A	512	-	4,4,4	0.14	0	6,6,6	0.04	0
9	GOL	L	301	-	5,5,5	0.90	0	5,5,5	0.99	0
9	GOL	C	505	-	5,5,5	0.92	0	5,5,5	0.97	0
9	GOL	C	506	-	5,5,5	0.88	0	5,5,5	1.01	0
10	SO4	B	2005	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	A	514	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	A	515	-	4,4,4	0.14	0	6,6,6	0.05	0
12	NAG	D	2004	2	14,14,15	0.38	0	17,19,21	0.50	0
9	GOL	A	510	-	5,5,5	0.87	0	5,5,5	1.02	0
10	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.06	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
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
9	GOL	C	505	-	-	3/4/4/4	-
12	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
9	GOL	C	506	-	-	2/4/4/4	-
9	GOL	A	505	-	-	2/4/4/4	-
9	GOL	D	2005	-	-	2/4/4/4	-
9	GOL	A	506	-	-	0/4/4/4	-
9	GOL	A	508	-	-	0/4/4/4	-
9	GOL	A	507	-	-	3/4/4/4	-
9	GOL	A	510	-	-	3/4/4/4	-
9	GOL	L	301	-	-	2/4/4/4	-
9	GOL	A	509	-	-	2/4/4/4	-
9	GOL	A	511	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	505	GOL	O1-C1-C2-O2
9	A	505	GOL	O1-C1-C2-C3
9	A	507	GOL	O1-C1-C2-C3
9	A	509	GOL	O1-C1-C2-C3
9	A	510	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	2005	GOL	1	0
9	A	506	GOL	2	0
9	A	511	GOL	1	0
9	A	510	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	134:CYS	C	138:THR	N	8.32
1	H	134:CYS	C	138:THR	N	6.44

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	455/455 (100%)	0.11	4 (0%) 84 88	17, 27, 50, 110	0
1	C	453/455 (99%)	0.09	3 (0%) 87 90	22, 42, 70, 111	0
2	B	464/471 (98%)	0.78	72 (15%) 2 2	18, 57, 133, 175	2 (0%)
2	D	469/471 (99%)	0.37	32 (6%) 17 20	23, 52, 107, 139	2 (0%)
3	E	216/216 (100%)	1.85	74 (34%) 0 0	50, 105, 166, 186	0
3	H	216/216 (100%)	0.56	31 (14%) 2 3	31, 77, 128, 146	0
4	F	214/214 (100%)	1.77	82 (38%) 0 0	53, 100, 163, 226	0
4	L	214/214 (100%)	0.33	8 (3%) 41 48	36, 64, 90, 143	0
5	M	4/5 (80%)	0.33	0 100 100	48, 49, 57, 79	0
5	N	4/5 (80%)	4.38	3 (75%) 0 0	90, 95, 97, 104	0
All	All	2709/2722 (99%)	0.60	309 (11%) 5 6	17, 53, 135, 226	4 (0%)

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	214	CYS	12.2
3	E	199	ILE	9.8
2	B	33	LEU	9.5
2	B	77	SER	9.2
5	N	5	VAL	9.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DPN	N	4	11/12	0.67	0.60	105,108,112,112	0
5	DPN	M	4	11/12	0.82	0.23	61,65,71,77	0

6.3 Carbohydrates [i](#)

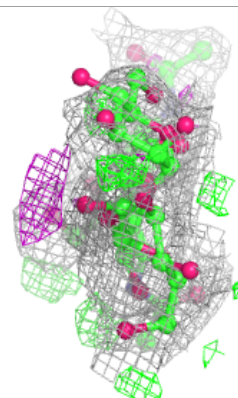
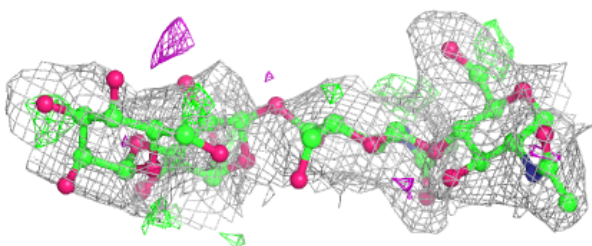
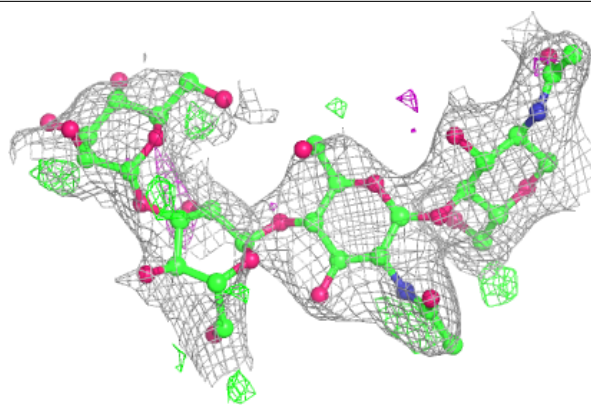
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	J	3	11/12	0.67	0.21	103,113,124,125	0
6	MAN	G	3	11/12	0.75	0.27	96,103,108,109	0
7	NAG	K	2	14/15	0.76	0.37	111,116,122,124	0
7	NAG	I	1	14/15	0.77	0.33	74,84,93,99	0
6	MAN	G	4	11/12	0.79	0.32	109,111,113,114	0
7	NAG	K	1	14/15	0.80	0.29	67,80,94,104	0
7	NAG	I	2	14/15	0.83	0.38	106,112,115,118	0
6	NAG	J	2	14/15	0.86	0.25	76,82,93,98	0
6	MAN	J	4	11/12	0.87	0.19	124,128,131,132	0
6	NAG	G	2	14/15	0.90	0.19	65,71,94,99	0
6	NAG	J	1	14/15	0.96	0.14	28,46,56,70	0
6	NAG	G	1	14/15	0.96	0.12	25,38,41,57	0

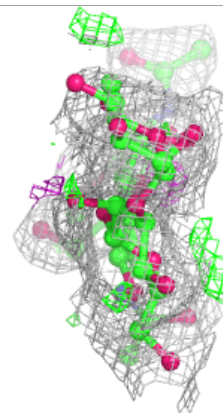
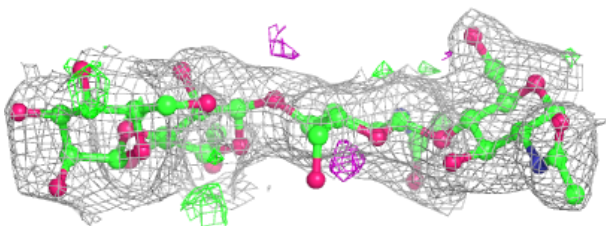
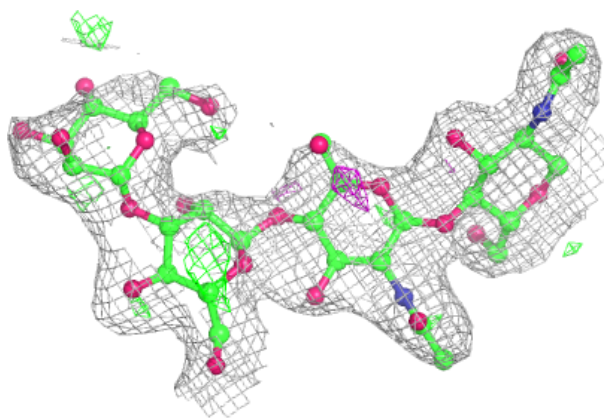
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

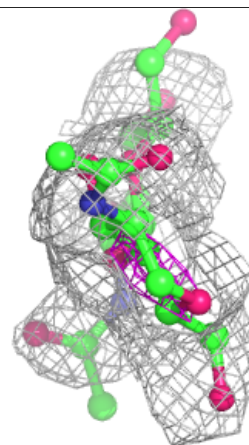
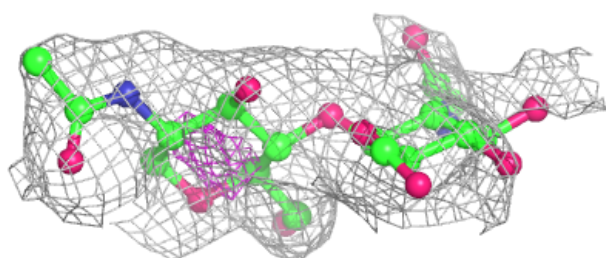
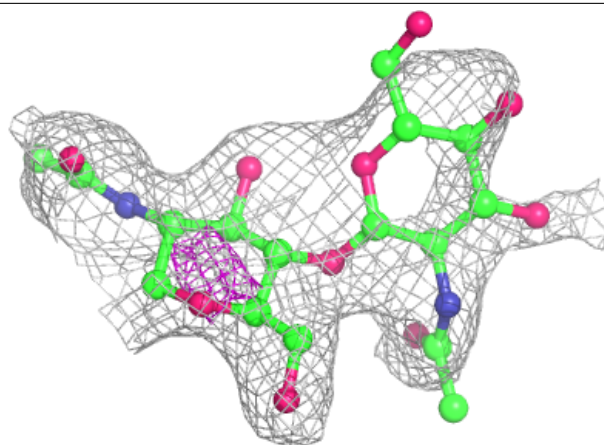
**Electron density around Chain J:**

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

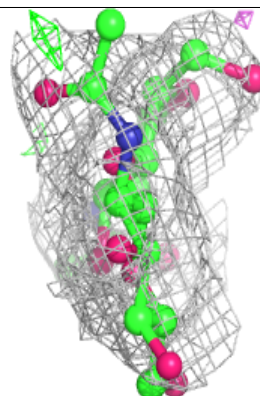
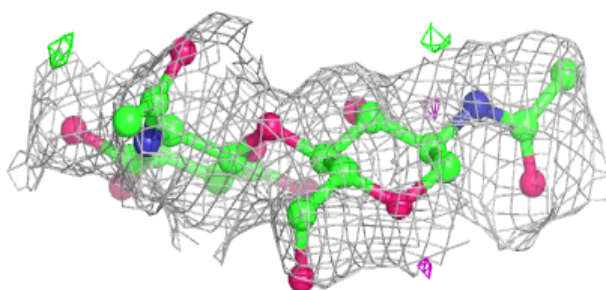
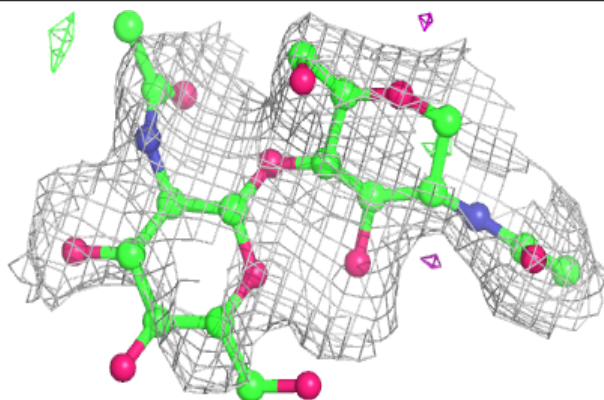


Electron density around Chain I:

$2mF_o-DF_c$ (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 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
11	MN	D	2002	1/1	0.40	0.15	94,94,94,94	0
11	MN	B	2001	1/1	0.49	0.45	87,87,87,87	0
9	GOL	C	506	6/6	0.73	0.32	99,100,104,107	0
11	MN	B	2002	1/1	0.74	0.14	159,159,159,159	0
10	SO4	B	2005	5/5	0.74	0.33	149,150,151,151	0
8	CA	C	501	1/1	0.75	0.06	63,63,63,63	0
9	GOL	L	301	6/6	0.76	0.42	111,112,113,113	0
10	SO4	A	515	5/5	0.77	0.45	172,172,174,174	0
12	NAG	B	2004	14/15	0.77	0.40	80,92,102,104	0
10	SO4	A	512	5/5	0.82	0.25	133,135,136,138	0
9	GOL	C	505	6/6	0.83	0.29	73,79,84,85	0
11	MN	D	2001	1/1	0.84	0.14	46,46,46,46	0
9	GOL	D	2005	6/6	0.85	0.31	78,90,97,99	0
9	GOL	A	511	6/6	0.85	0.24	70,73,76,82	0
12	NAG	D	2004	14/15	0.85	0.34	73,82,87,88	0
9	GOL	A	508	6/6	0.86	0.27	41,51,60,64	0
8	CA	C	504	1/1	0.86	0.09	48,48,48,48	0
9	GOL	A	506	6/6	0.86	0.18	52,56,65,69	0
9	GOL	A	510	6/6	0.87	0.19	44,63,70,75	0
10	SO4	L	302	5/5	0.88	0.20	115,115,115,118	0
10	SO4	C	507	5/5	0.90	0.23	117,121,122,125	0
10	SO4	C	508	5/5	0.90	0.23	115,117,117,122	0
9	GOL	A	509	6/6	0.90	0.26	57,73,76,77	0
10	SO4	A	513	5/5	0.91	0.22	90,101,105,108	0
9	GOL	A	507	6/6	0.92	0.19	45,54,79,86	0
8	CA	A	501	1/1	0.92	0.10	32,32,32,32	0
10	SO4	A	514	5/5	0.93	0.19	104,105,106,106	0
11	MN	D	2003	1/1	0.93	0.12	43,43,43,43	0
8	CA	C	502	1/1	0.94	0.08	46,46,46,46	0
8	CA	A	502	1/1	0.95	0.08	26,26,26,26	0
9	GOL	A	505	6/6	0.96	0.18	29,34,49,60	0
8	CA	C	503	1/1	0.96	0.08	40,40,40,40	0
11	MN	B	2003	1/1	0.97	0.06	26,26,26,26	0
8	CA	A	504	1/1	0.99	0.07	20,20,20,20	0
8	CA	A	503	1/1	0.99	0.16	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.