



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:38 AM UTC

PDB ID : 3ZE2 / pdb_00003ze2
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 : 2.35 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:

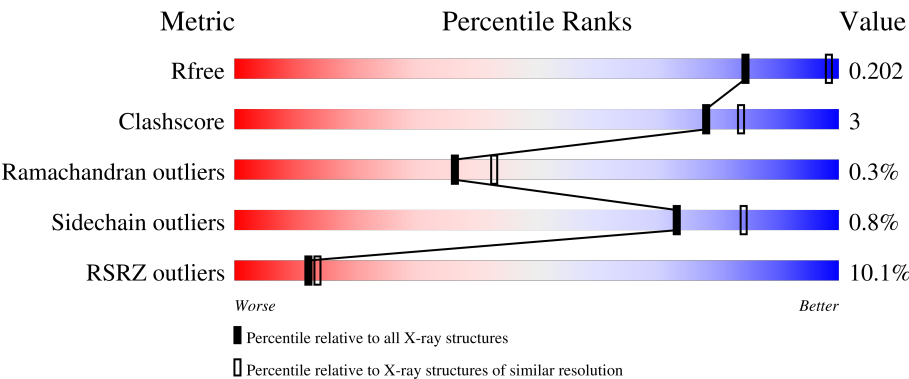
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	93%6%
1	C	457	94%5%
2	B	472	89%10%
2	D	472	74%22%
3	E	221	92%5%

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

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41569 atoms, of which 19764 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	H	N	O	S	2	5	0
			6845	2228	3341	600	668	8			
1	C	453	Total	C	H	N	O	S	1	6	0
			6840	2227	3337	602	666	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	469	Total	C	H	N	O	S	0	7	0
			7218	2275	3569	619	721	34			
2	D	367	Total	C	H	N	O	S	0	6	0
			5806	1834	2896	487	570	19			

- 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			

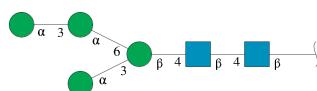
- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	2	0
			3222	1028	1569	273	343	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			111	32	52	15	12			
5	J	6	Total	C	H	N	O	0	0	0
			74	22	34	9	9			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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
6	G	6	Total	C	H	N	O	0	0	0
			133	40	61	2	30			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



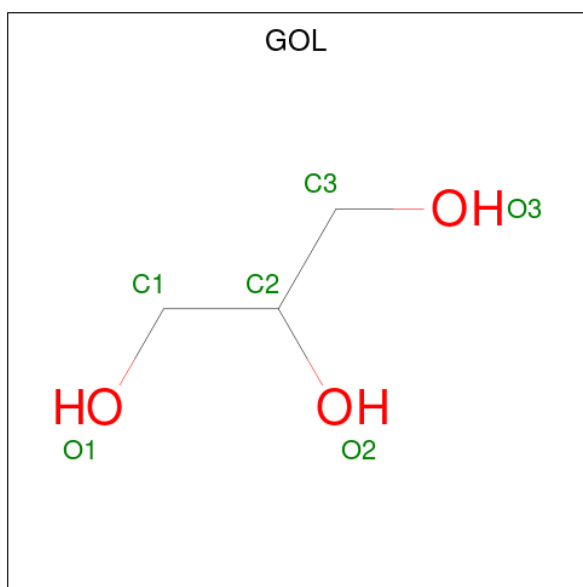
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 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.



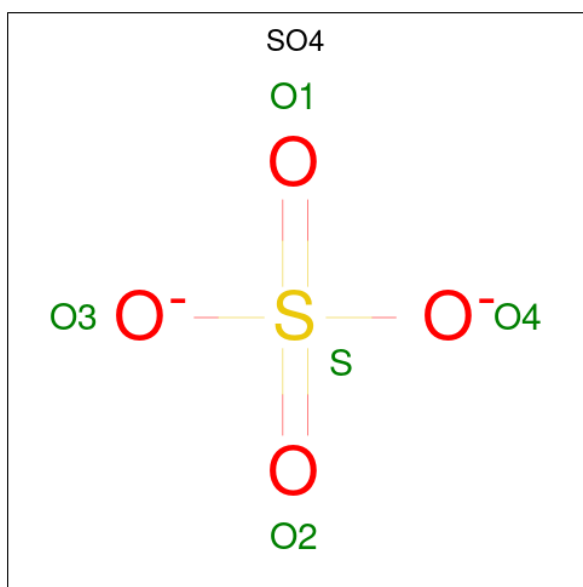
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	C	1	Total	C	H	O	0	0
			14	3	8	3		
9	C	1	Total	C	H	O	0	0
			14	3	8	3		
9	C	1	Total	C	H	O	0	0
			14	3	8	3		
9	C	1	Total	C	H	O	0	0
			14	3	8	3		
9	E	1	Total	C	H	O	0	0
			14	3	8	3		
9	F	1	Total	C	H	O	0	0
			14	3	8	3		
9	F	1	Total	C	H	O	0	0
			14	3	8	3		
9	J	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

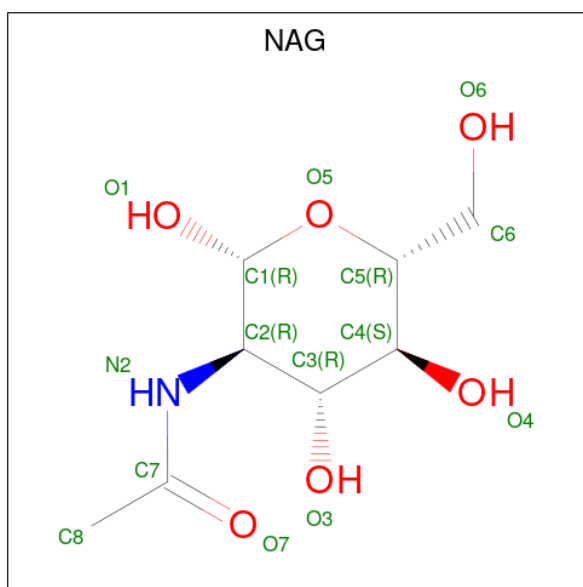
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

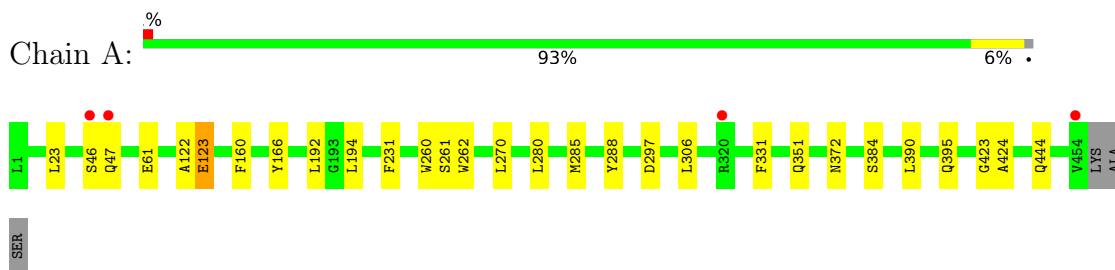
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	483	Total	O	0	0
			483	483		
14	B	211	Total	O	0	0
			211	211		
14	C	283	Total	O	0	0
			283	283		
14	D	107	Total	O	0	0
			107	107		
14	E	129	Total	O	0	0
			129	129		
14	F	68	Total	O	0	0
			68	68		
14	H	18	Total	O	0	0
			18	18		
14	I	2	Total	O	0	0
			2	2		
14	J	2	Total	O	0	0
			2	2		
14	L	15	Total	O	0	0
			15	15		

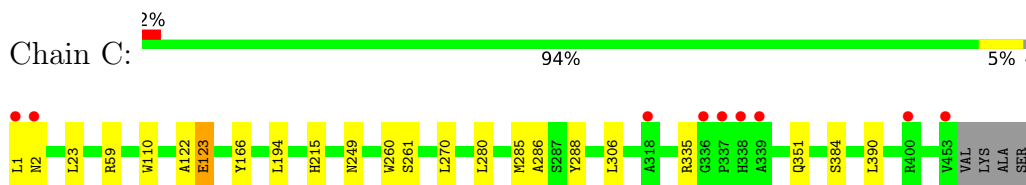
3 Residue-property plots

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.

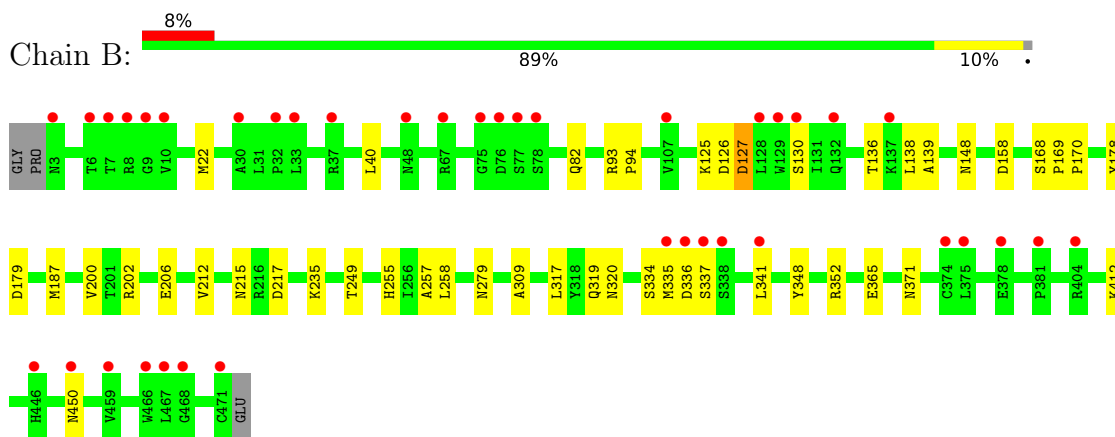
• Molecule 1: INTEGRIN ALPHA-IIB



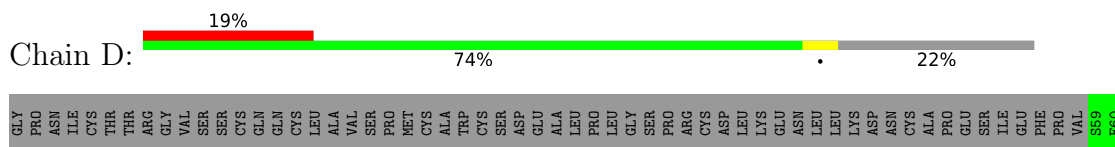
• Molecule 1: INTEGRIN ALPHA-IIB

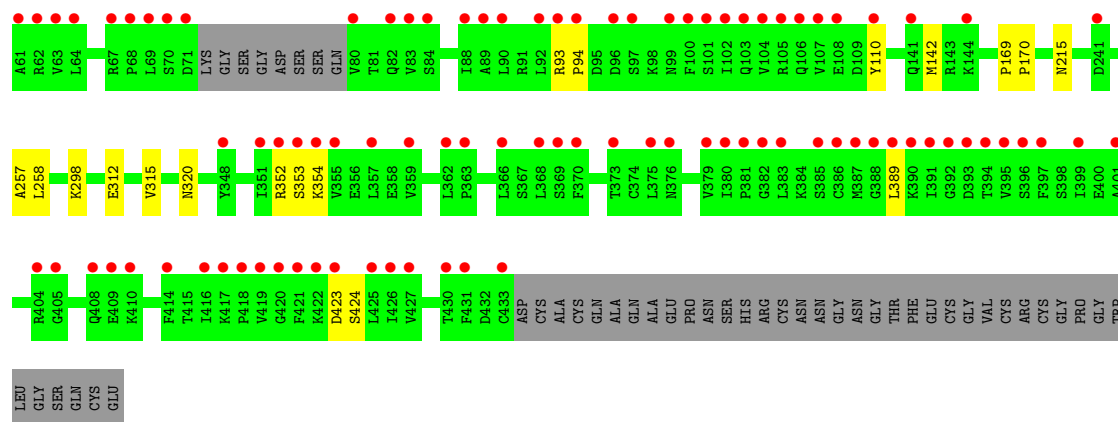


• Molecule 2: INTEGRIN BETA-3

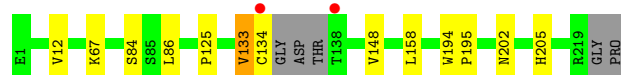


• Molecule 2: INTEGRIN BETA-3

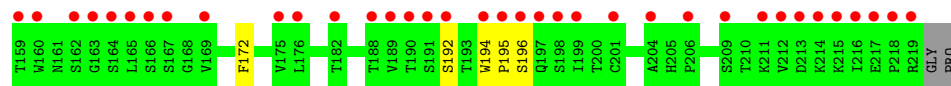
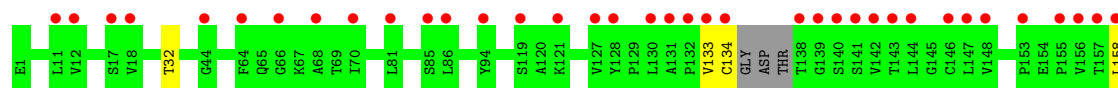




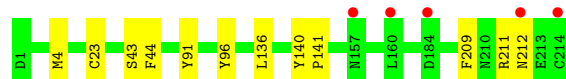
• Molecule 3: 10E5 FAB HEAVY CHAIN



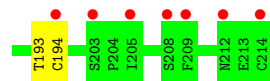
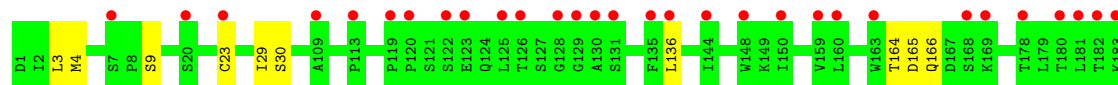
• Molecule 3: 10E5 FAB HEAVY CHAIN



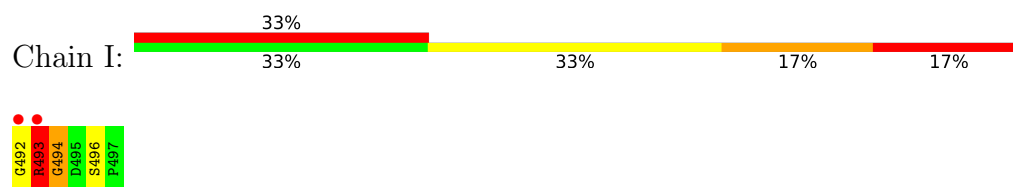
• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 5: RGD PEPTIDE



- Molecule 5: RGD PEPTIDE



There are no outlier residues recorded for this chain.

- Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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



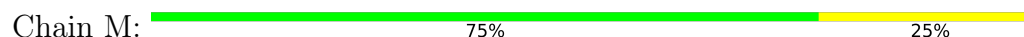


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: 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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	233.21Å 143.56Å 104.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.02 – 2.35 54.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.02-2.35) 100.0 (54.02-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.204 0.174 , 0.202	Depositor DCC
R_{free} test set	1017 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.0	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	0.95	EDS
Total number of atoms	41569	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, GOL, CA, NAG, SO4, MN

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	0.29	0/3612	0.65	0/4923
1	C	0.27	0/3615	0.64	0/4927
2	B	0.27	0/3737	0.64	0/5066
2	D	0.26	0/2976	0.64	0/4031
3	E	0.27	0/1684	0.62	2/2305 (0.1%)
3	H	0.26	0/1684	0.61	0/2305
4	F	0.25	0/1692	0.59	0/2294
4	L	0.24	0/1673	0.57	0/2269
5	I	0.22	0/59	0.58	0/76
5	J	0.32	0/40	0.57	0/52
All	All	0.27	0/20772	0.63	2/28248 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	205	HIS	CA-C-N	5.04	124.48	119.24
3	E	205	HIS	C-N-CA	5.04	124.48	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3504	3341	3348	20	0
1	C	3503	3337	3345	20	0
2	B	3649	3569	3575	31	0
2	D	2910	2896	2900	11	0
3	E	1642	1597	1600	6	0
3	H	1642	1597	1600	6	0
4	F	1653	1569	1571	8	0
4	L	1637	1550	1553	7	0
5	I	59	52	51	7	0
5	J	40	34	34	0	0
6	G	72	61	61	0	0
7	K	28	25	25	2	0
8	M	50	43	43	0	0
9	A	12	16	16	0	0
9	C	24	32	32	1	0
9	E	6	8	8	0	0
9	F	12	16	16	0	0
9	J	6	8	8	0	0
10	A	10	0	0	1	0
11	A	4	0	0	0	0
11	C	4	0	0	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	C	14	13	13	0	0
14	A	483	0	0	6	1
14	B	211	0	0	6	0
14	C	283	0	0	6	1
14	D	107	0	0	1	0
14	E	129	0	0	0	0
14	F	68	0	0	0	0
14	H	18	0	0	0	0
14	I	2	0	0	0	0
14	J	2	0	0	0	0
14	L	15	0	0	1	0
All	All	21805	19764	19799	111	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 3.

The worst 5 of 111 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)
14:A:3238:HOH:O	5:I:492[B]:GLY:N	2.03	0.90
14:A:3222:HOH:O	5:I:493[A]:ARG:NH2	2.17	0.78
1:C:384:SER:OG	14:C:3243:HOH:O	2.05	0.74
1:A:384:SER:OG	14:A:3430:HOH:O	2.06	0.73
10:A:1457:SO4:O3	14:A:3482:HOH:O	2.09	0.70

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)
14:A:3480:HOH:O	14:C:3252:HOH:O[1_554]	2.18	0.02

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	457/457 (100%)	445 (97%)	11 (2%)	1 (0%)	43	52
1	C	457/457 (100%)	440 (96%)	16 (4%)	1 (0%)	43	52
2	B	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	43	52
2	D	369/472 (78%)	355 (96%)	13 (4%)	1 (0%)	36	43
3	E	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	24	27
3	H	212/221 (96%)	200 (94%)	12 (6%)	0	100	100
4	F	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	I	6/6 (100%)	2 (33%)	0	4 (67%)	0	0
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2617/2740 (96%)	2514 (96%)	94 (4%)	9 (0%)	36	43

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	D	142	MET
1	C	123	GLU
5	I	493[A]	ARG
5	I	493[B]	ARG

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%)	361 (98%)	6 (2%)	55	70
1	C	367/364 (101%)	363 (99%)	4 (1%)	65	79
2	B	422/417 (101%)	419 (99%)	3 (1%)	76	86
2	D	336/417 (81%)	335 (100%)	1 (0%)	86	92
3	E	187/190 (98%)	186 (100%)	1 (0%)	81	89
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	190/188 (101%)	190 (100%)	0	100	100
4	L	188/188 (100%)	187 (100%)	1 (0%)	81	89
5	I	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	4 (100%)	0	100	100
All	All	2253/2326 (97%)	2235 (99%)	18 (1%)	73	84

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

Mol	Chain	Res	Type
3	E	202	ASN
4	L	3	LEU
5	I	493[B]	ARG
2	B	215	ASN
2	D	215	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	157	ASN
3	E	170	HIS
1	C	197	GLN
2	D	316	ASN
2	B	450	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 ⓘ

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	2,6	14,14,15	0.61	0	17,19,21	0.62	0
6	NAG	G	2	6	14,14,15	0.55	0	17,19,21	0.76	0
6	BMA	G	3	6	11,11,12	0.62	0	15,15,17	0.63	0
6	MAN	G	4	6	11,11,12	0.63	0	15,15,17	0.62	0
6	MAN	G	5	6	11,11,12	0.63	0	15,15,17	0.53	0
6	MAN	G	6	6	11,11,12	0.63	0	15,15,17	0.55	0
7	NAG	K	1	7	14,14,15	0.51	0	17,19,21	0.75	0
7	NAG	K	2	7	14,14,15	0.54	0	17,19,21	0.56	0
8	NAG	M	1	2,8	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
8	NAG	M	2	8	14,14,15	0.61	0	17,19,21	0.84	0
8	BMA	M	3	8	11,11,12	0.62	0	15,15,17	0.63	0
8	MAN	M	4	8	11,11,12	0.60	0	15,15,17	0.57	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	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
8	NAG	M	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1	NAG	C1-O5-C5	2.13	115.05	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

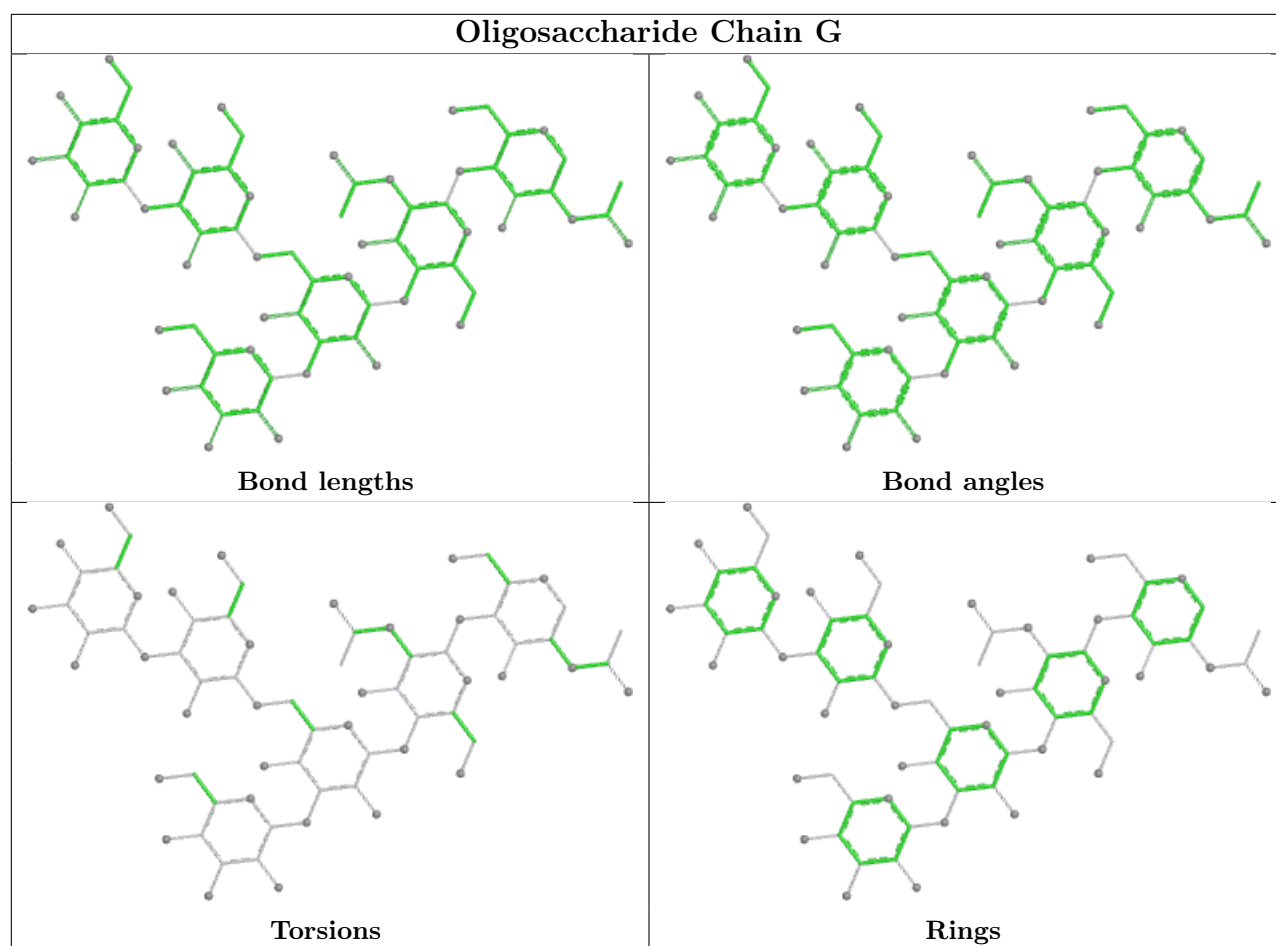
Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
8	M	3	BMA	O5-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
7	K	2	NAG	C8-C7-N2-C2

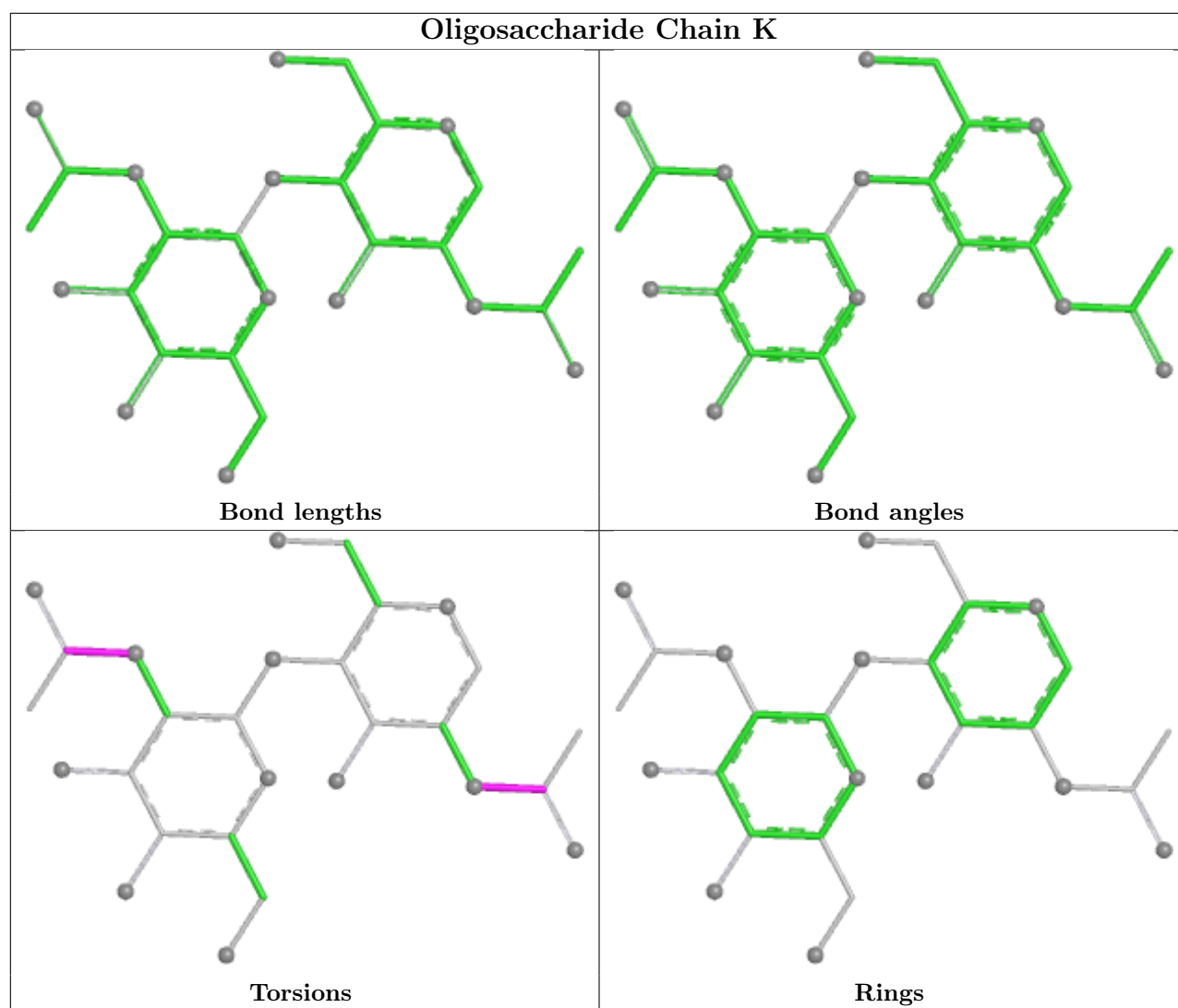
There are no ring outliers.

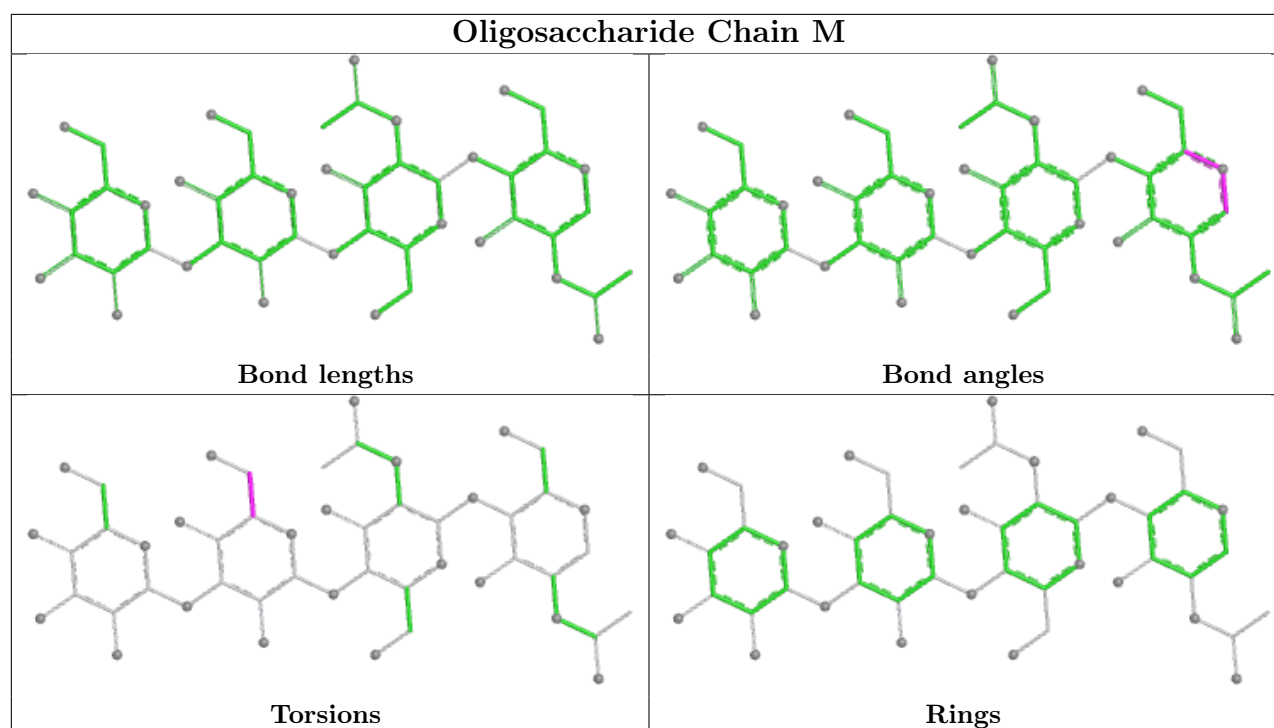
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	2	NAG	1	0
7	K	1	NAG	2	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 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	GOL	C	1456	-	5,5,5	0.37	0	5,5,5	0.33	0
9	GOL	A	1456	-	5,5,5	0.38	0	5,5,5	0.20	0
9	GOL	F	1216	-	5,5,5	0.36	0	5,5,5	0.27	0
9	GOL	C	1455	-	5,5,5	0.37	0	5,5,5	0.27	0
10	SO4	A	1457	-	4,4,4	0.23	0	6,6,6	0.13	0
9	GOL	C	1454	-	5,5,5	0.38	0	5,5,5	0.31	0
10	SO4	A	1458	-	4,4,4	0.24	0	6,6,6	0.06	0
9	GOL	E	1220	-	5,5,5	0.39	0	5,5,5	0.24	0
9	GOL	J	1498	-	5,5,5	0.37	0	5,5,5	0.29	0
9	GOL	C	1457	-	5,5,5	0.38	0	5,5,5	0.19	0
9	GOL	A	1455	-	5,5,5	0.39	0	5,5,5	0.11	0
9	GOL	F	1215	-	5,5,5	0.40	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	C	2015	1	14,14,15	0.54	0	17,19,21	0.75	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	C	1456	-	-	2/4/4/4	-
9	GOL	A	1456	-	-	2/4/4/4	-
9	GOL	F	1216	-	-	2/4/4/4	-
9	GOL	C	1455	-	-	2/4/4/4	-
9	GOL	C	1454	-	-	2/4/4/4	-
9	GOL	E	1220	-	-	4/4/4/4	-
9	GOL	J	1498	-	-	1/4/4/4	-
9	GOL	C	1457	-	-	2/4/4/4	-
9	GOL	A	1455	-	-	3/4/4/4	-
9	GOL	F	1215	-	-	2/4/4/4	-
13	NAG	C	2015	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1455	GOL	O1-C1-C2-C3
9	C	1456	GOL	O1-C1-C2-C3
9	C	1457	GOL	O1-C1-C2-C3
9	E	1220	GOL	C1-C2-C3-O3
9	F	1215	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1457	SO4	1	0
9	C	1457	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%)	-0.63	4 (0%) 81 84	13, 28, 58, 131	9 (1%)
1	C	453/457 (99%)	-0.32	9 (1%) 65 70	19, 41, 79, 144	7 (1%)
2	B	469/472 (99%)	0.34	39 (8%) 17 19	14, 48, 126, 216	134 (28%)
2	D	367/472 (77%)	0.90	92 (25%) 1 1	20, 56, 188, 236	82 (22%)
3	E	216/221 (97%)	-0.21	2 (0%) 81 84	28, 46, 78, 111	0
3	H	216/221 (97%)	1.49	73 (33%) 1 0	52, 117, 175, 232	0
4	F	214/214 (100%)	0.02	5 (2%) 61 66	25, 52, 95, 200	4 (1%)
4	L	214/214 (100%)	1.29	37 (17%) 4 4	64, 124, 223, 260	1 (0%)
5	I	6/6 (100%)	1.29	2 (33%) 1 0	15, 28, 42, 54	3 (50%)
5	J	6/6 (100%)	-0.04	0 100 100	33, 40, 74, 83	0
All	All	2615/2740 (95%)	0.24	263 (10%) 12 14	13, 48, 164, 260	240 (9%)

The worst 5 of 263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	THR	7.9
2	D	419	VAL	7.2
1	A	454	VAL	6.9
2	B	129	TRP	6.8
2	B	337[A]	SER	6.3

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 ⓘ

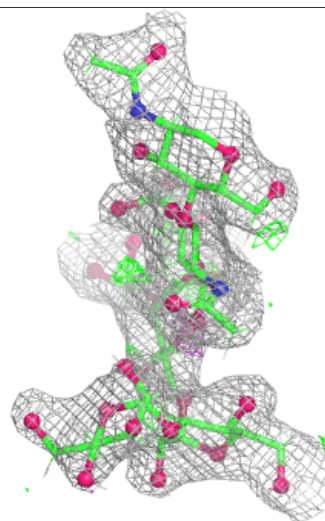
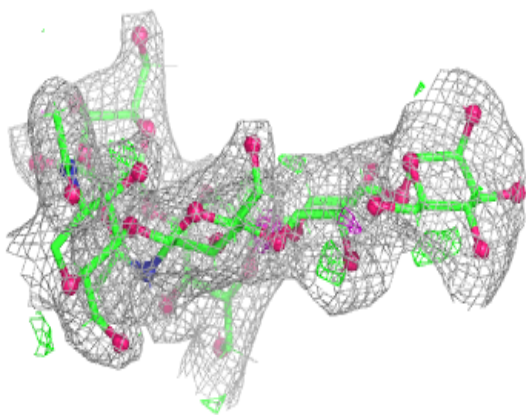
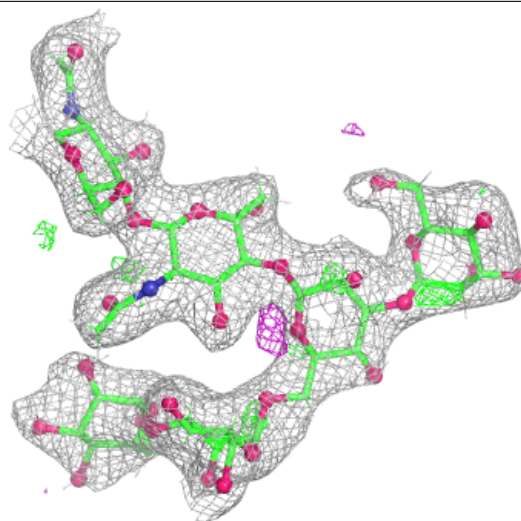
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	G	1	14/15	-	-	16,30,47,55	0
6	NAG	G	2	14/15	-	-	34,48,64,68	0
6	BMA	G	3	11/12	-	-	58,74,92,95	0
6	MAN	G	4	11/12	-	-	65,72,87,89	0
6	MAN	G	5	11/12	-	-	73,78,93,95	0
6	MAN	G	6	11/12	-	-	71,78,92,95	0
8	BMA	M	3	11/12	0.37	0.15	103,113,135,136	0
8	MAN	M	4	11/12	0.63	0.18	106,115,138,138	0
8	NAG	M	2	14/15	0.79	0.15	66,86,99,105	0
8	NAG	M	1	14/15	0.91	0.09	41,55,74,79	0
7	NAG	K	2	14/15	0.94	0.08	112,122,145,150	0
7	NAG	K	1	14/15	0.97	0.05	77,95,114,119	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.

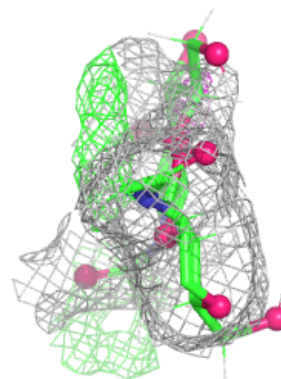
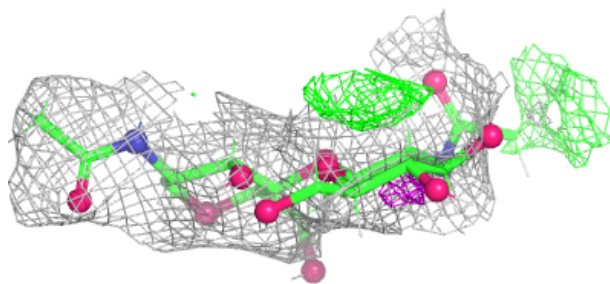
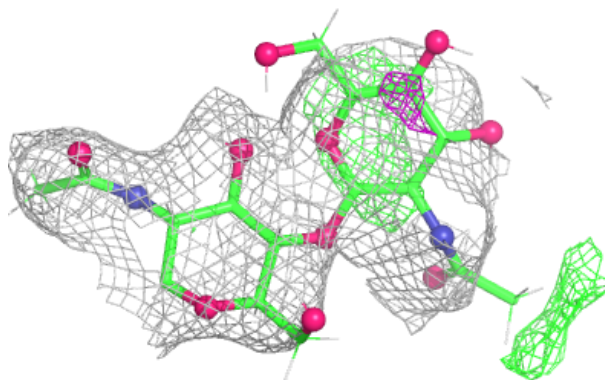
Electron density around Chain G:

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

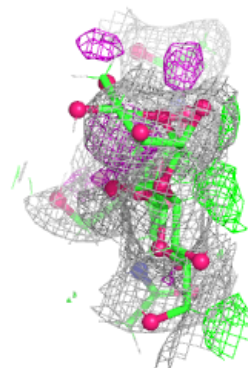
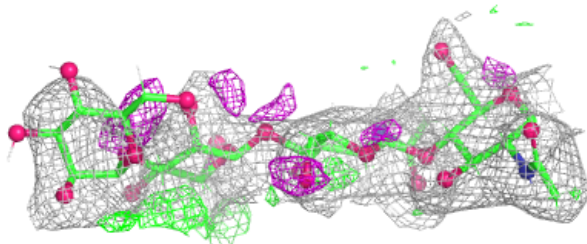
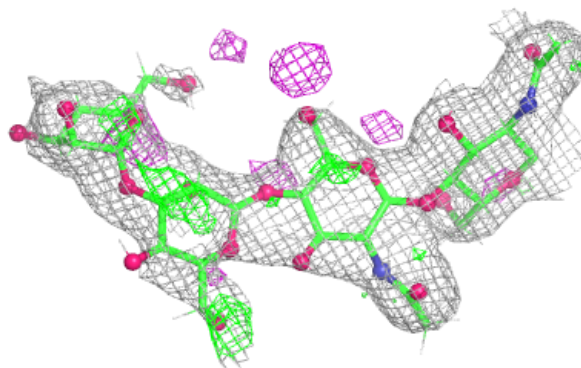


Electron density around Chain K:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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
13	NAG	C	2015	14/15	0.49	0.17	86,102,119,129	0
10	SO4	A	1458	5/5	0.77	0.18	95,97,98,102	0
9	GOL	C	1455	6/6	0.80	0.24	85,102,105,107	0
9	GOL	C	1457	6/6	0.82	0.22	65,78,87,92	0
9	GOL	C	1454	6/6	0.82	0.30	86,104,110,114	0
9	GOL	A	1456	6/6	0.82	0.23	64,84,100,103	0
9	GOL	A	1455	6/6	0.84	0.21	56,67,77,79	0
9	GOL	F	1215	6/6	0.84	0.19	70,84,86,86	0
9	GOL	F	1216	6/6	0.85	0.15	58,70,80,83	0
9	GOL	J	1498	6/6	0.85	0.20	68,82,86,88	0
9	GOL	E	1220	6/6	0.87	0.15	67,81,85,85	0
10	SO4	A	1457	5/5	0.87	0.15	72,79,82,82	0
9	GOL	C	1456	6/6	0.91	0.15	62,79,89,95	0
11	CA	A	2006	1/1	0.99	0.01	19,19,19,19	0
11	CA	C	2005	1/1	0.99	0.05	46,46,46,46	0
11	CA	C	2006	1/1	0.99	0.03	42,42,42,42	0
11	CA	C	2007	1/1	0.99	0.04	41,41,41,41	0
12	MN	B	2002	1/1	0.99	0.04	52,52,52,52	0
12	MN	B	2003	1/1	0.99	0.03	28,28,28,28	0
11	CA	A	2004	1/1	0.99	0.01	27,27,27,27	0
12	MN	B	2001	1/1	1.00	0.04	23,23,23,23	0
11	CA	A	2005	1/1	1.00	0.02	23,23,23,23	0
11	CA	A	2007	1/1	1.00	0.02	23,23,23,23	0
12	MN	D	2001	1/1	1.00	0.03	25,25,25,25	0
12	MN	D	2002	1/1	1.00	0.01	30,30,30,30	0
12	MN	D	2003	1/1	1.00	0.05	33,33,33,33	0
11	CA	C	2004	1/1	1.00	0.02	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.