



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:31 PM UTC

PDB ID : 9ROB / pdb_00009rob
Title : Crystal structure of human CD22 Ig domains 1-3 in complex with modified sialoside 1B
Authors : Ereno-Orbea, J.; Sicard, T.; Julien, J.-P.
Deposited on : 2025-06-20
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

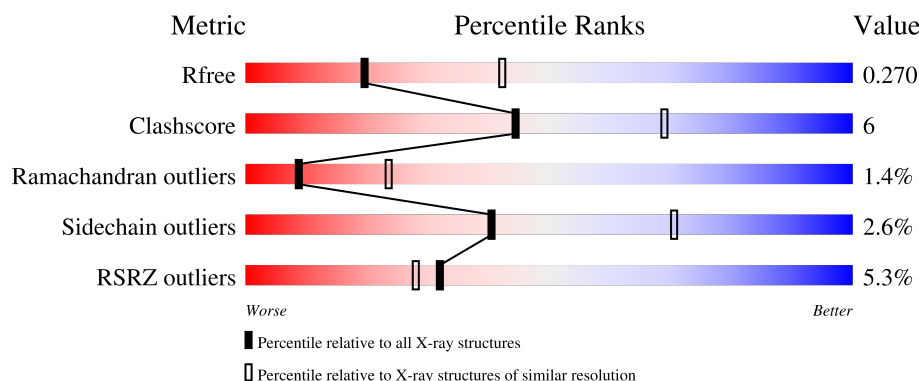
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	324	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	B	324	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
2	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	H	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4979 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 B-cell receptor CD22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2374	1503	402	456	13			
1	B	301	Total	C	N	O	S	0	0	0
			2402	1521	407	461	13			

There are 36 discrepancies between the modelled and reference sequences:

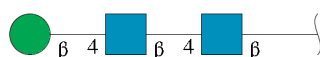
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	-	expression tag	UNP P20273
A	18	THR	-	expression tag	UNP P20273
A	19	GLY	-	expression tag	UNP P20273
A	67	ALA	ASN	engineered mutation	UNP P20273
A	112	ALA	ASN	engineered mutation	UNP P20273
A	135	ALA	ASN	engineered mutation	UNP P20273
A	164	ALA	ASN	engineered mutation	UNP P20273
A	231	ALA	ASN	engineered mutation	UNP P20273
A	331	GLY	-	expression tag	UNP P20273
A	332	GLY	-	expression tag	UNP P20273
A	333	THR	-	expression tag	UNP P20273
A	334	LYS	-	expression tag	UNP P20273
A	335	HIS	-	expression tag	UNP P20273
A	336	HIS	-	expression tag	UNP P20273
A	337	HIS	-	expression tag	UNP P20273
A	338	HIS	-	expression tag	UNP P20273
A	339	HIS	-	expression tag	UNP P20273
A	340	HIS	-	expression tag	UNP P20273
B	17	GLU	-	expression tag	UNP P20273
B	18	THR	-	expression tag	UNP P20273
B	19	GLY	-	expression tag	UNP P20273
B	67	ALA	ASN	engineered mutation	UNP P20273
B	112	ALA	ASN	engineered mutation	UNP P20273
B	135	ALA	ASN	engineered mutation	UNP P20273
B	164	ALA	ASN	engineered mutation	UNP P20273

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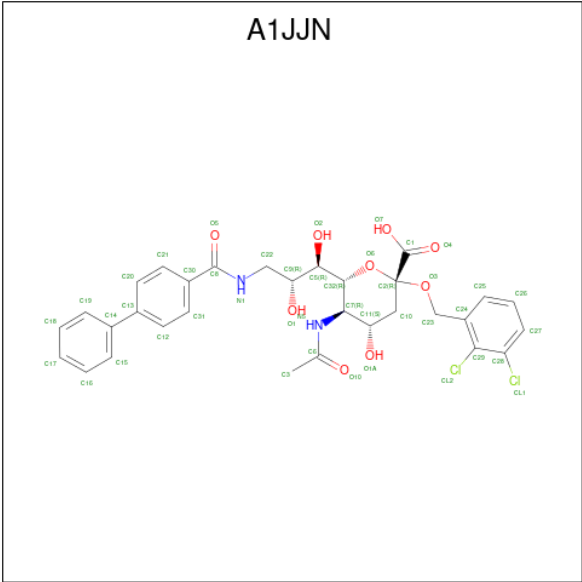
Chain	Residue	Modelled	Actual	Comment	Reference
B	231	ALA	ASN	engineered mutation	UNP P20273
B	331	GLY	-	expression tag	UNP P20273
B	332	GLY	-	expression tag	UNP P20273
B	333	THR	-	expression tag	UNP P20273
B	334	LYS	-	expression tag	UNP P20273
B	335	HIS	-	expression tag	UNP P20273
B	336	HIS	-	expression tag	UNP P20273
B	337	HIS	-	expression tag	UNP P20273
B	338	HIS	-	expression tag	UNP P20273
B	339	HIS	-	expression tag	UNP P20273
B	340	HIS	-	expression tag	UNP P20273

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



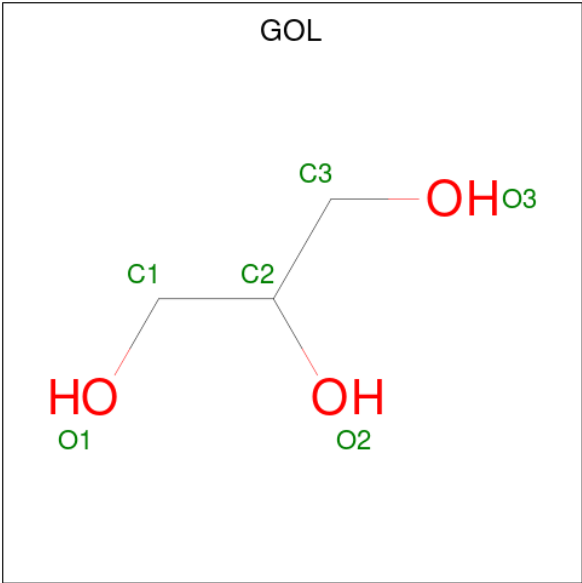
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is (2R,4S,5R,6R)-5-acetamido-2-[[2,3-bis(chloranyl)phenyl]methoxy]-6-[(1R,2R)-1,2-bis(oxidanyl)-3-[(4-phenylphenyl)carbonylamino]propyl]-4-oxidanyl-oxane-2-carboxylic acid (CCD ID: A1JJN) (formula: C₃₁H₃₂Cl₂N₂O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			44	31	2	2	9		
3	B	1	Total	C	Cl	N	O	0	0
			44	31	2	2	9		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

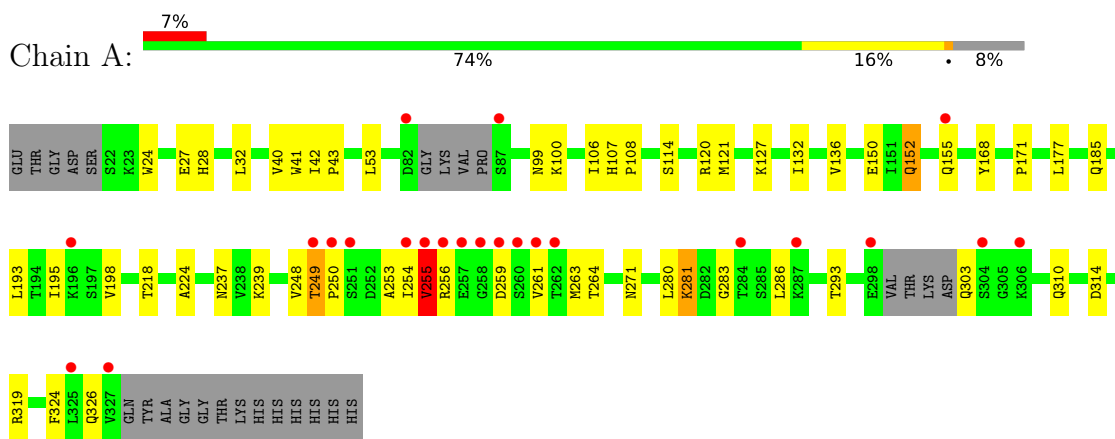
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	11	Total	O	0	0
			11	11		

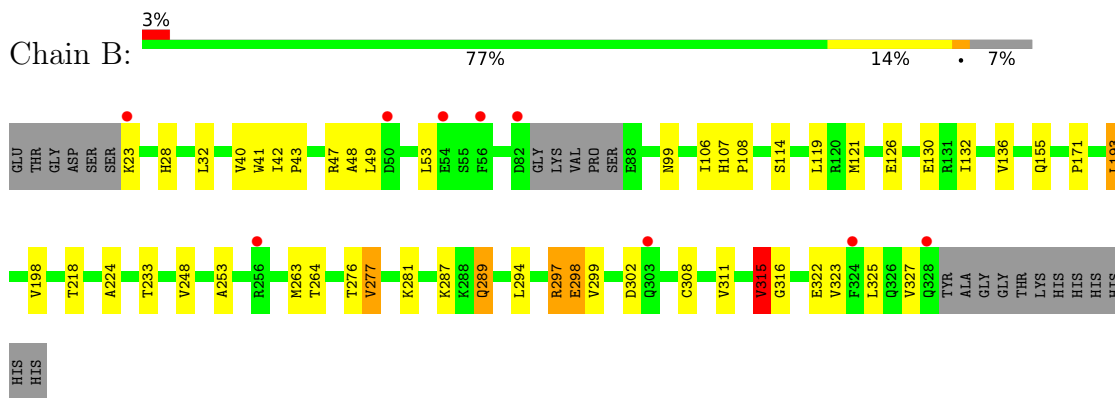
3 Residue-property plots [i](#)

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.

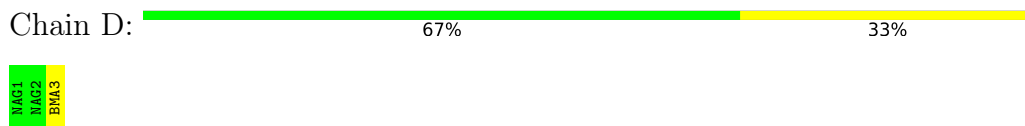
- Molecule 1: B-cell receptor CD22



- Molecule 1: B-cell receptor CD22

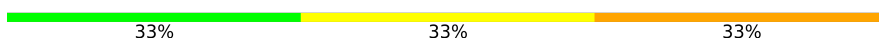


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.62Å 111.10Å 164.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.01 – 2.70 41.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.01-2.70) 99.8 (41.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.69Å)	Xtriage
Refinement program	PHENIX v1.13	Depositor
R, R_{free}	0.221 , 0.267 0.227 , 0.270	Depositor DCC
R_{free} test set	1171 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4979	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0658e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, GOL, A1JJN, BMA

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	0.10	0/2430	0.32	0/3296
1	B	0.09	0/2459	0.29	0/3337
All	All	0.09	0/4889	0.31	0/6633

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2374	0	2319	32	0
1	B	2402	0	2351	24	0
2	D	39	0	34	0	0
2	H	39	0	34	2	0
3	A	44	0	0	0	0
3	B	44	0	0	1	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
5	A	8	0	0	1	0
5	B	11	0	0	0	0
All	All	4979	0	4762	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (58) 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:248:VAL:HG22	1:A:250:PRO:HD2	1.54	0.88
1:A:255:VAL:HG23	1:A:259:ASP:H	1.52	0.74
1:B:248:VAL:HG21	1:B:323:VAL:HG11	1.70	0.72
1:A:253:ALA:HB1	1:A:326:GLN:H	1.59	0.68
1:B:281:LYS:NZ	1:B:302:ASP:O	2.28	0.67
1:A:254:ILE:O	1:A:256:ARG:N	2.30	0.65
1:A:32:LEU:HD22	1:A:42:ILE:HG12	1.81	0.62
1:A:264:THR:HG22	1:A:293:THR:HG22	1.82	0.62
1:B:53:LEU:HD11	1:B:121:MET:HE3	1.82	0.60
1:B:253:ALA:HB1	1:B:325:LEU:HA	1.83	0.60
1:B:47:ARG:NH1	1:B:48:ALA:O	2.34	0.60
1:A:281:LYS:HB2	1:A:286:LEU:HD11	1.84	0.59
1:B:23:LYS:HG2	1:B:49:LEU:HD12	1.86	0.58
2:H:2:NAG:H83	2:H:2:NAG:H3	1.86	0.56
1:A:248:VAL:HG23	1:A:263:MET:HG2	1.87	0.56
1:B:40:VAL:HG12	1:B:106:ILE:HB	1.88	0.55
1:A:53:LEU:HD11	1:A:121:MET:HE3	1.90	0.54
1:A:114:SER:HB2	1:A:136:VAL:HB	1.91	0.53
1:B:308:CYS:SG	1:B:322:GLU:HG2	2.50	0.52
1:B:32:LEU:HD22	1:B:42:ILE:HG12	1.92	0.52
1:A:255:VAL:HG13	1:A:256:ARG:H	1.76	0.51
1:B:114:SER:HB2	1:B:136:VAL:HB	1.92	0.51
1:B:119:LEU:HB2	1:B:130:GLU:HB3	1.94	0.50
1:A:250:PRO:HD3	1:A:261:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:HG13	1:B:311:VAL:HG22	1.93	0.49
1:B:315:VAL:HG12	1:B:316:GLY:H	1.78	0.49
1:A:28:HIS:CE1	1:A:132:ILE:HG12	2.48	0.48
1:A:150:GLU:OE2	1:A:239:LYS:NZ	2.40	0.48
1:B:218:THR:HG23	1:B:233:THR:HG22	1.96	0.47
1:A:120:ARG:NH2	1:A:127:LYS:HD3	2.30	0.47
1:A:168:TYR:CZ	1:A:193:LEU:HD23	2.50	0.46
1:B:28:HIS:CE1	1:B:132:ILE:HG12	2.50	0.46
1:A:237:ASN:OD1	1:A:271:ASN:ND2	2.41	0.46
1:B:289:GLN:HG2	1:B:294:LEU:HD13	1.97	0.46
1:B:248:VAL:HG22	1:B:263:MET:HG2	1.97	0.46
1:B:126:GLU:OE1	3:B:2102:A1JJN:O1A	2.33	0.46
1:A:177:LEU:HB2	1:A:218:THR:HB	1.97	0.46
1:A:107:HIS:HA	1:A:108:PRO:HA	1.85	0.45
1:B:297:ARG:O	1:B:299:VAL:N	2.50	0.45
1:A:324:PHE:HD2	1:A:326:GLN:HE21	1.64	0.45
1:A:152:GLN:HG2	1:A:155:GLN:HG3	1.99	0.44
1:A:310:GLN:HB2	1:A:319:ARG:HD3	1.99	0.44
1:A:41:TRP:O	1:A:43:PRO:HD3	2.18	0.44
1:A:40:VAL:HG12	1:A:106:ILE:HB	1.99	0.44
1:A:99:ASN:OD1	1:A:99:ASN:N	2.51	0.44
2:H:1:NAG:H61	2:H:2:NAG:C7	2.48	0.44
1:A:100:LYS:NZ	5:A:501:HOH:O	2.50	0.44
1:B:41:TRP:O	1:B:43:PRO:HD3	2.18	0.43
1:A:24:TRP:HZ3	1:A:121:MET:HE2	1.84	0.43
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.77	0.42
1:B:107:HIS:HA	1:B:108:PRO:HA	1.87	0.42
1:B:193:LEU:HD12	1:B:198:VAL:HG22	2.01	0.42
1:A:193:LEU:HD12	1:A:198:VAL:HG22	2.02	0.42
1:A:171:PRO:HG2	1:A:224:ALA:HB2	2.02	0.41
1:A:27:GLU:HB3	1:A:195:ILE:HD12	2.02	0.41
1:A:281:LYS:NZ	1:A:303:GLN:HA	2.35	0.41
1:B:171:PRO:HG2	1:B:224:ALA:HB2	2.03	0.40
1:A:185:GLN:OE1	1:A:185:GLN:N	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/324 (90%)	263 (90%)	26 (9%)	3 (1%)	12	32
1	B	297/324 (92%)	274 (92%)	18 (6%)	5 (2%)	7	19
All	All	589/648 (91%)	537 (91%)	44 (8%)	8 (1%)	9	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	287	LYS
1	B	298	GLU
1	B	297	ARG
1	A	281	LYS
1	A	283	GLY
1	B	99	ASN
1	B	315	VAL

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	271/292 (93%)	266 (98%)	5 (2%)	51	78
1	B	274/292 (94%)	265 (97%)	9 (3%)	33	63
All	All	545/584 (93%)	531 (97%)	14 (3%)	40	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	249	THR
1	A	255	VAL
1	A	280	LEU
1	A	314	ASP
1	B	155	GLN
1	B	193	LEU
1	B	264	THR
1	B	276	THR
1	B	277	VAL
1	B	289	GLN
1	B	298	GLU
1	B	315	VAL
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	222	GLN
1	B	99	ASN
1	B	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.44	0	17,19,21	0.60	0
2	NAG	D	2	2	14,14,15	0.36	0	17,19,21	0.57	0
2	BMA	D	3	2	11,11,12	0.55	0	15,15,17	0.92	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.31	0	17,19,21	0.49	0
2	NAG	H	2	2	14,14,15	0.48	0	17,19,21	1.37	2 (11%)
2	BMA	H	3	2	11,11,12	0.54	0	15,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C2-N2-C7	4.49	128.92	122.90
2	D	3	BMA	C1-O5-C5	2.31	115.28	112.19
2	H	2	NAG	C1-C2-N2	2.29	114.04	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	3	BMA	C4-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C1-C2-N2-C7

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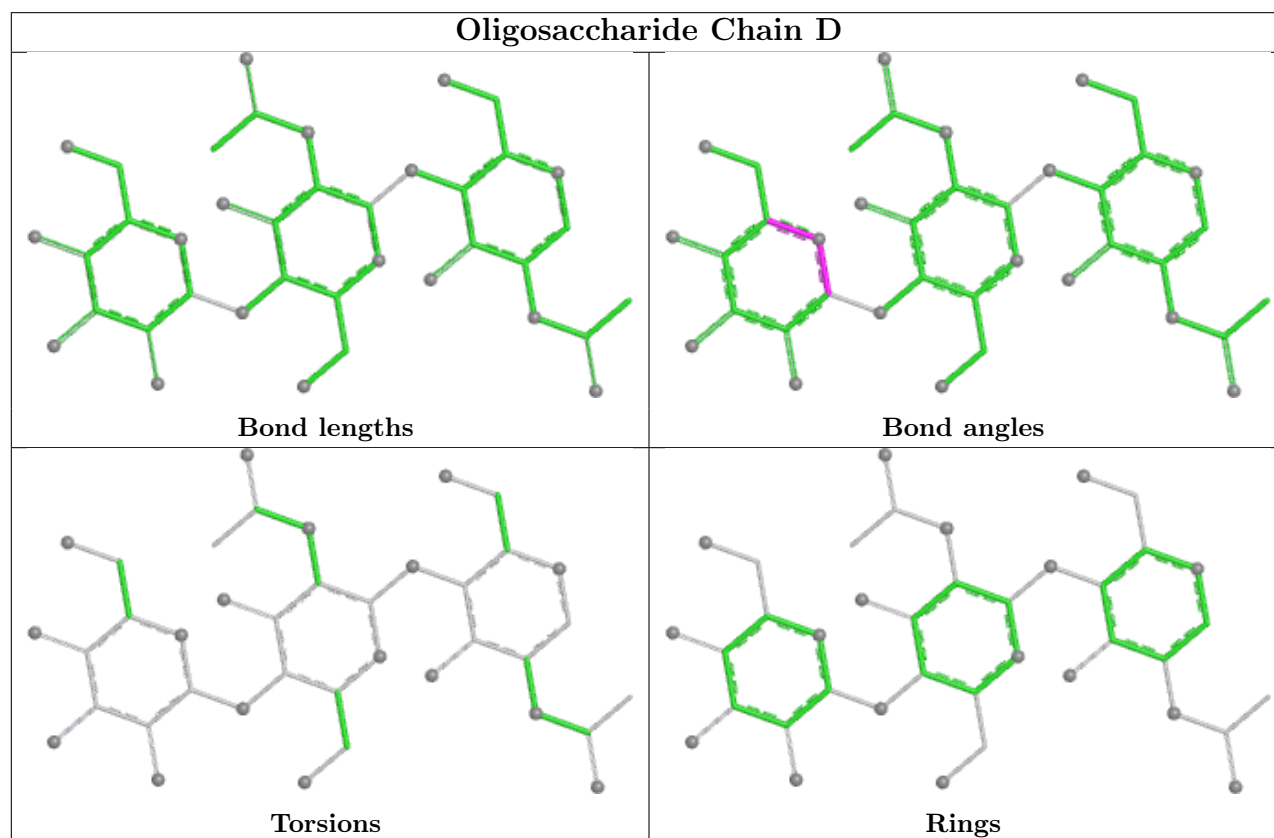
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7

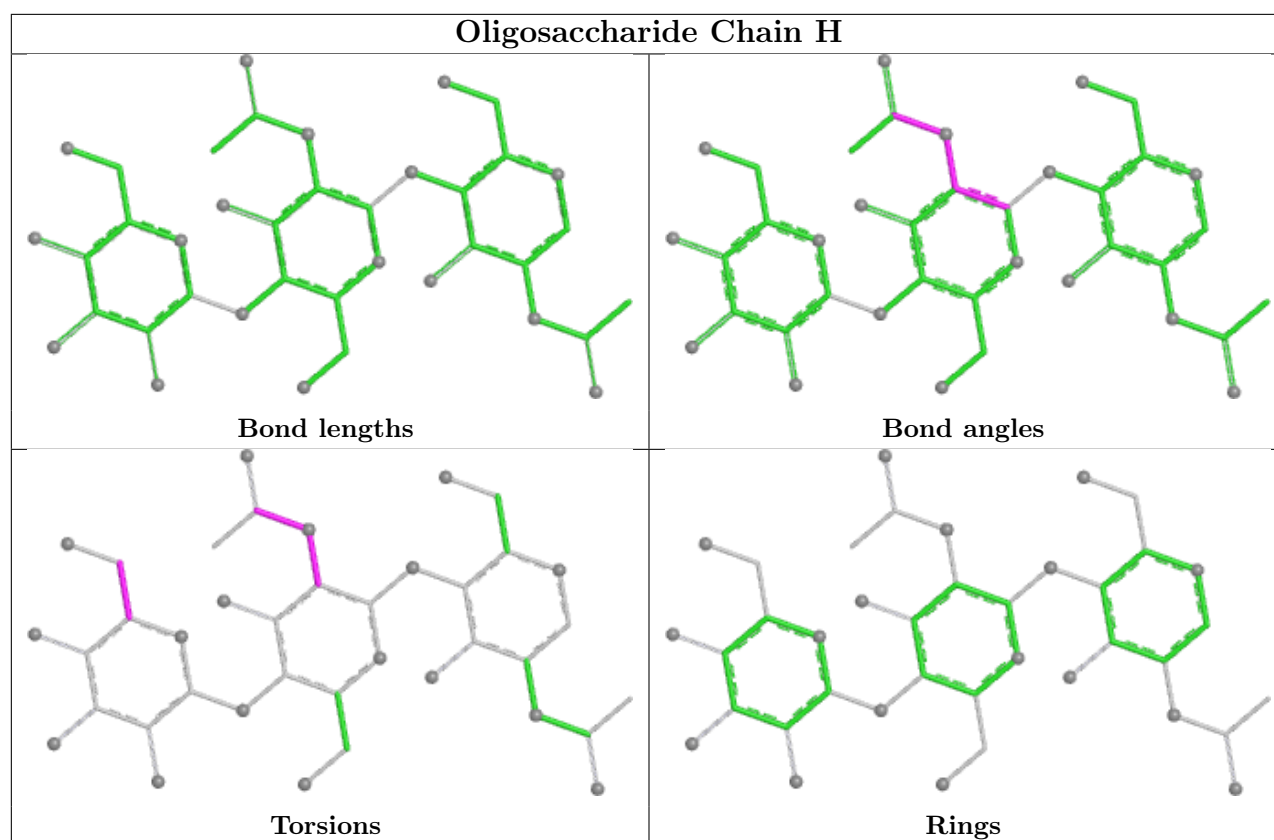
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	H	2	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](#)

5 ligands 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	$\# Z > 2$
4	GOL	A	402	-	5,5,5	0.91	0	5,5,5	1.09	0
3	A1JJN	A	401	-	47,47,47	0.30	0	63,67,67	0.67	2 (3%)
4	GOL	B	2103	-	5,5,5	0.92	0	5,5,5	1.09	0
4	GOL	B	2101	-	5,5,5	0.70	0	5,5,5	1.17	0
3	A1JJN	B	2102	-	47,47,47	0.30	0	63,67,67	0.66	3 (4%)

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
4	GOL	A	402	-	-	0/4/4/4	-
3	A1JJN	A	401	-	-	3/37/55/55	0/4/4/4
4	GOL	B	2103	-	-	2/4/4/4	-
4	GOL	B	2101	-	-	1/4/4/4	-
3	A1JJN	B	2102	-	-	2/37/55/55	0/4/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	A1JJN	O6-C32-C7	-3.23	106.89	109.84
3	B	2102	A1JJN	C2-O6-C32	2.72	120.76	114.36
3	A	401	A1JJN	O4-C1-C2	-2.64	115.85	123.79
3	B	2102	A1JJN	O4-C1-C2	-2.61	115.92	123.79
3	B	2102	A1JJN	O3-C23-C24	-2.09	105.86	109.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1JJN	O7-C1-C2-O3
3	B	2102	A1JJN	O7-C1-C2-O3
4	B	2103	GOL	C1-C2-C3-O3
4	B	2103	GOL	O2-C2-C3-O3
3	B	2102	A1JJN	O3-C23-C24-C29
3	A	401	A1JJN	O4-C1-C2-O3
4	B	2101	GOL	O2-C2-C3-O3
3	A	401	A1JJN	C10-C2-O3-C23

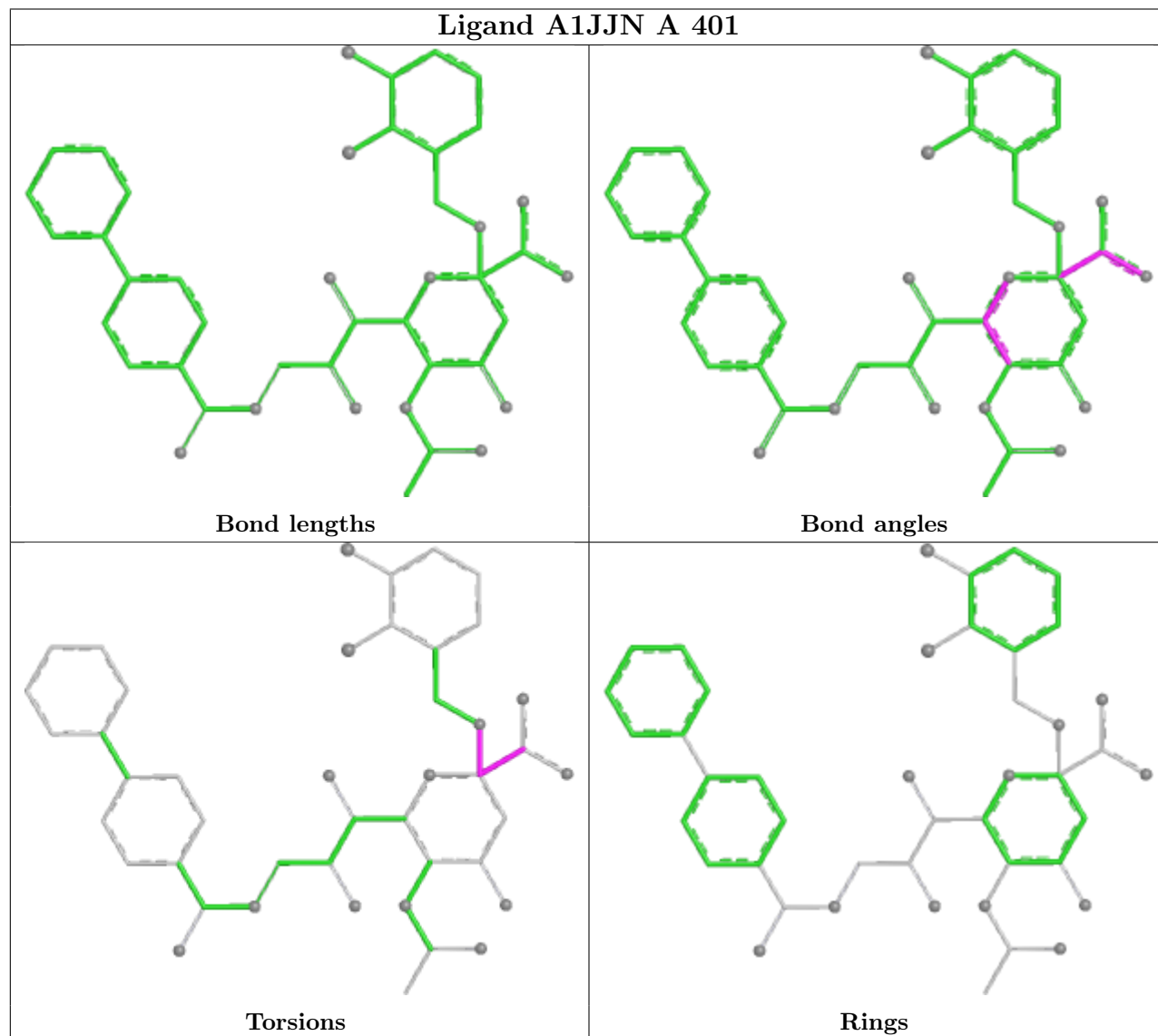
There are no ring outliers.

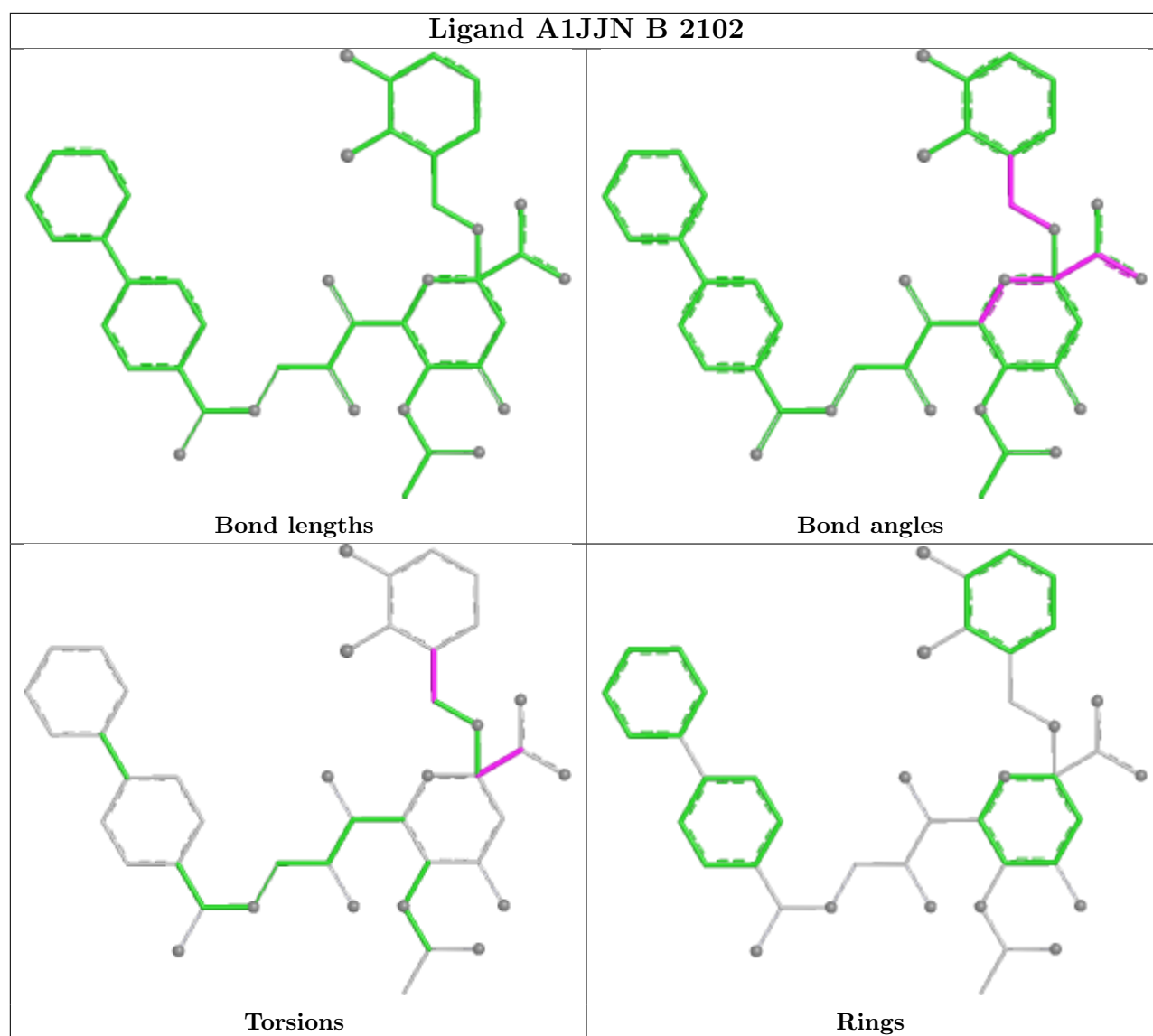
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2102	A1JJN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	298/324 (91%)	0.32	23 (7%)	19 17	35, 57, 102, 143	0
1	B	301/324 (92%)	0.36	9 (2%)	52 49	40, 58, 89, 108	0
All	All	599/648 (92%)	0.34	32 (5%)	32 28	35, 58, 95, 143	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	VAL	5.7
1	A	254	ILE	3.8
1	A	250	PRO	3.5
1	B	56	PHE	3.3
1	A	260	SER	3.2
1	B	82	ASP	3.1
1	A	255	VAL	3.1
1	A	196	LYS	2.9
1	A	256	ARG	2.7
1	A	82	ASP	2.7
1	B	54	GLU	2.6
1	A	249	THR	2.6
1	A	287	LYS	2.6
1	A	298	GLU	2.6
1	A	259	ASP	2.5
1	A	257	GLU	2.5
1	B	23	LYS	2.5
1	A	87	SER	2.5
1	A	251	SER	2.4
1	A	325	LEU	2.3
1	A	258	GLY	2.3
1	A	304	SER	2.2
1	A	306	LYS	2.2
1	A	262	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	155	GLN	2.1
1	B	50	ASP	2.1
1	B	303	GLN	2.0
1	B	256	ARG	2.0
1	B	324	PHE	2.0
1	A	284	THR	2.0
1	B	328	GLN	2.0
1	A	261	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

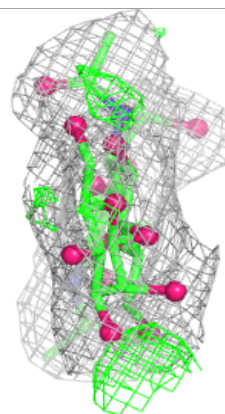
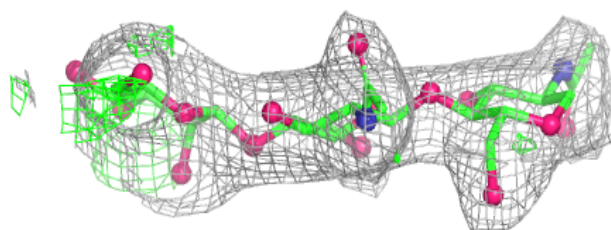
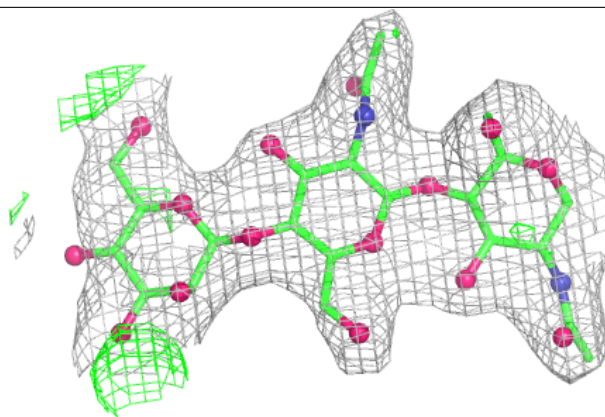
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.76	0.12	38,54,57,66	0
2	BMA	D	3	11/12	0.77	0.12	44,59,70,81	0
2	NAG	D	1	14/15	0.92	0.10	45,52,57,58	0
2	NAG	H	1	14/15	-	-	61,66,72,74	0
2	NAG	H	2	14/15	-	-	63,70,82,85	0
2	BMA	H	3	11/12	-	-	63,68,73,81	0

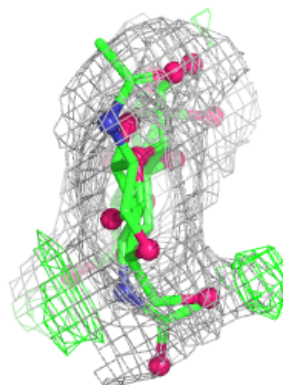
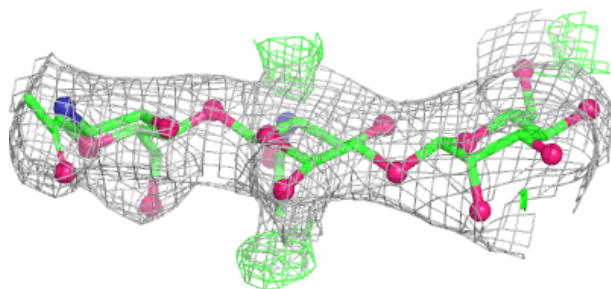
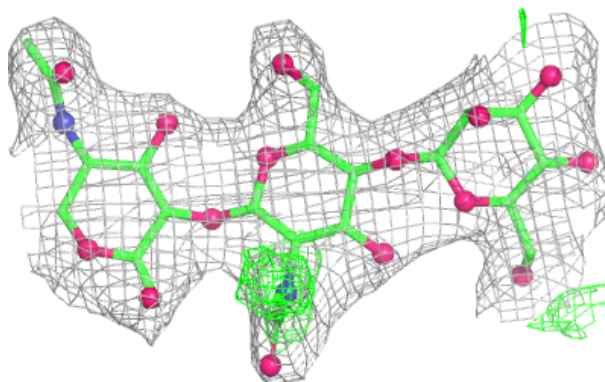
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

**Electron density around Chain H:**

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



6.4 Ligands [i](#)

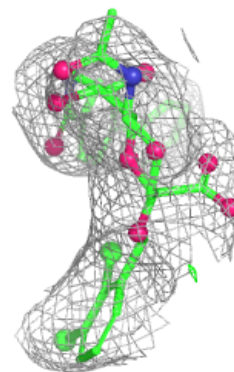
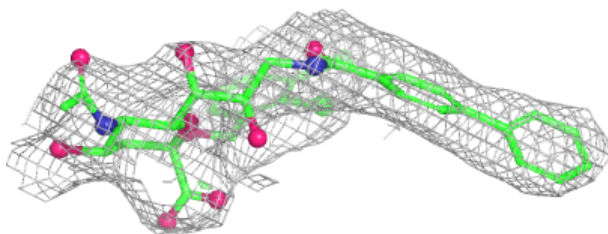
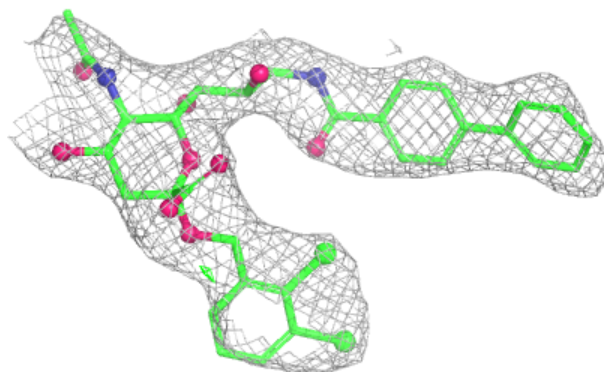
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

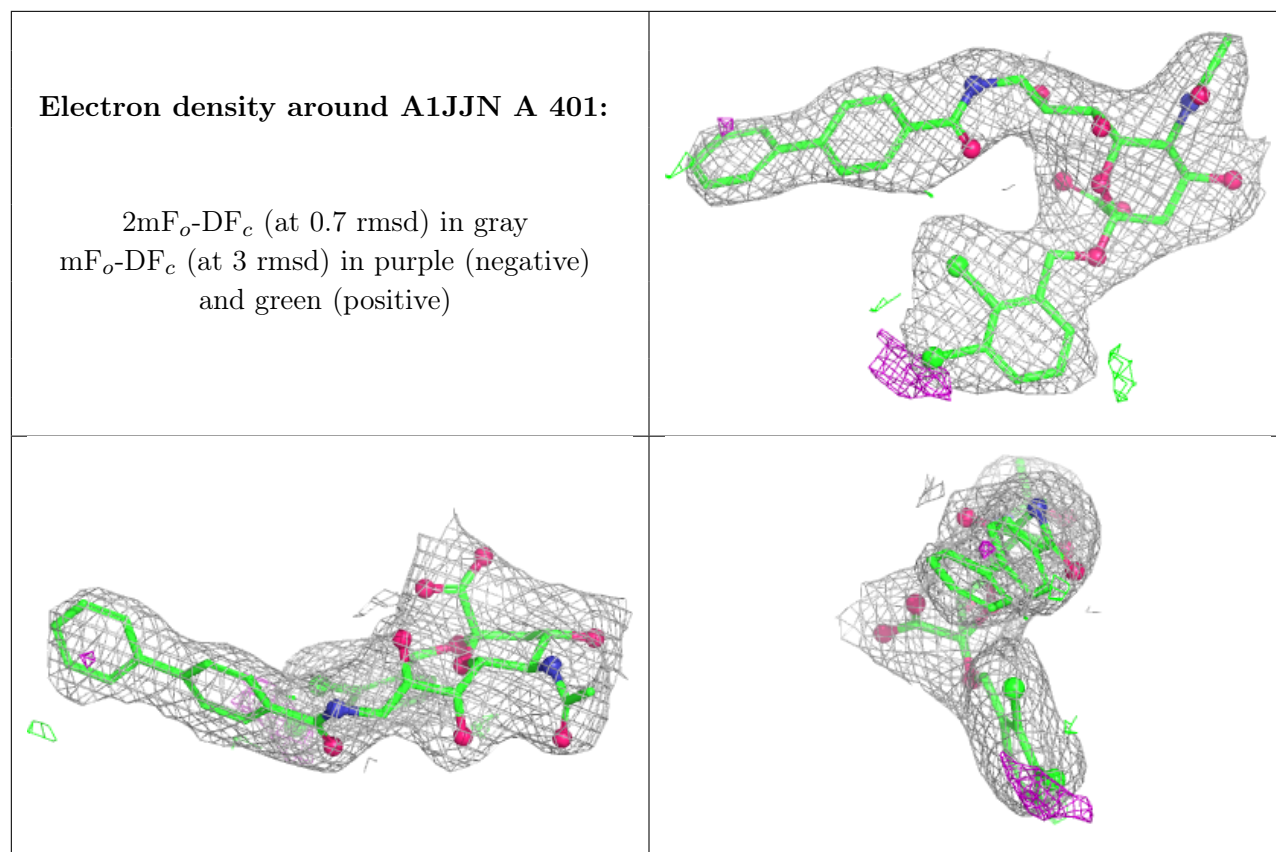
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	2103	6/6	0.54	0.16	84,86,91,92	0
4	GOL	B	2101	6/6	0.82	0.14	48,54,65,73	0
4	GOL	A	402	6/6	0.86	0.12	44,48,54,60	0
3	A1JJN	B	2102	44/44	0.87	0.12	57,81,97,103	0
3	A1JJN	A	401	44/44	0.90	0.11	46,54,62,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1JJN B 2102:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.