



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:32 AM BST

PDB ID : 3O5W
Title : Binding of kinetin in the active site of mistletoe lectin I
Authors : Malecki, P.H.; Meyer, A.; Rypniewski, W.; Szymanski, M.; Barciszewski, J.; Betzel, C.
Deposited on : 2010-07-28
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

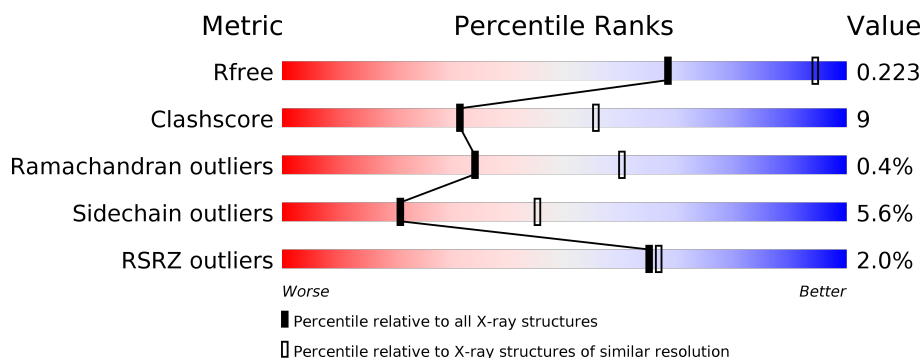
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>...</div> </div> </div>
2	B	263	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>
3	E	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
4	D	3	<div> <div></div> <div>33%</div> <div>67%</div> </div>

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
3	NAG	E	1	X	-	-	-
3	NAG	E	2	-	-	-	X
4	NAG	D	3	-	-	-	X
7	GOL	B	1	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4413 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 Beta-galactoside-specific lectin 1 chain A isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1921	1216	332	369	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	GLU	SEE REMARK 999	UNP P81446
A	19	SER	ARG	SEE REMARK 999	UNP P81446
A	36	ASN	GLU	SEE REMARK 999	UNP P81446
A	45	VAL	ILE	SEE REMARK 999	UNP P81446
A	49	GLU	ASP	SEE REMARK 999	UNP P81446
A	50	GLY	ALA	SEE REMARK 999	UNP P81446
A	61	ALA	GLU	SEE REMARK 999	UNP P81446
A	90	SER	ARG	SEE REMARK 999	UNP P81446
A	94	ALA	ARG	SEE REMARK 999	UNP P81446
A	100	ASP	LEU	SEE REMARK 999	UNP P81446
A	208	HIS	GLN	SEE REMARK 999	UNP P81446
A	219	ALA	ARG	SEE REMARK 999	UNP P81446
A	223	ALA	PRO	SEE REMARK 999	UNP P81446
A	227	ILE	PHE	SEE REMARK 999	UNP P81446

- Molecule 2 is a protein called Beta-galactoside-specific lectin 1 chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2001	1241	354	393	13			

There are 7 discrepancies between the modelled and reference sequences:

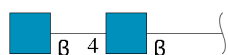
Chain	Residue	Modelled	Actual	Comment	Reference
B	268	THR	CYS	SEE REMARK 999	UNP P81446
B	301	LYS	ARG	SEE REMARK 999	UNP P81446

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Chain	Residue	Modelled	Actual	Comment	Reference
B	337	ILE	LEU	SEE REMARK 999	UNP P81446
B	414	ALA	ILE	SEE REMARK 999	UNP P81446
B	436	SER	ASP	SEE REMARK 999	UNP P81446
B	489	SER	LYS	SEE REMARK 999	UNP P81446
B	491	GLN	ARG	SEE REMARK 999	UNP P81446

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
4	D	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



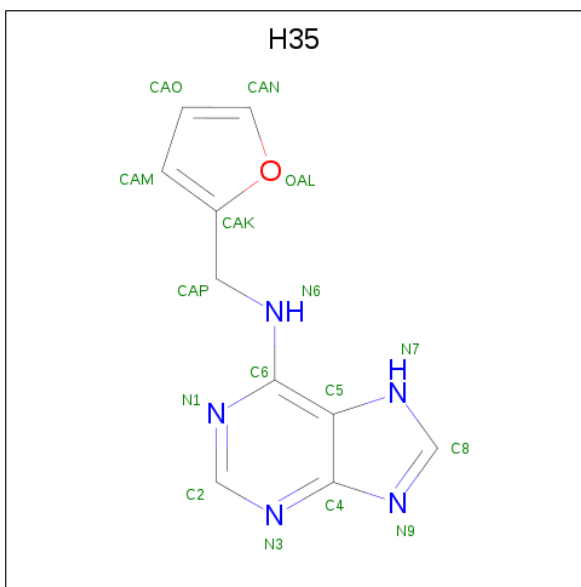
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is N-(FURAN-2-YLMETHYL)-7H-PURIN-6-AMINE (three-letter code: H35) (formula: C₁₀H₉N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			16	10	5	1		

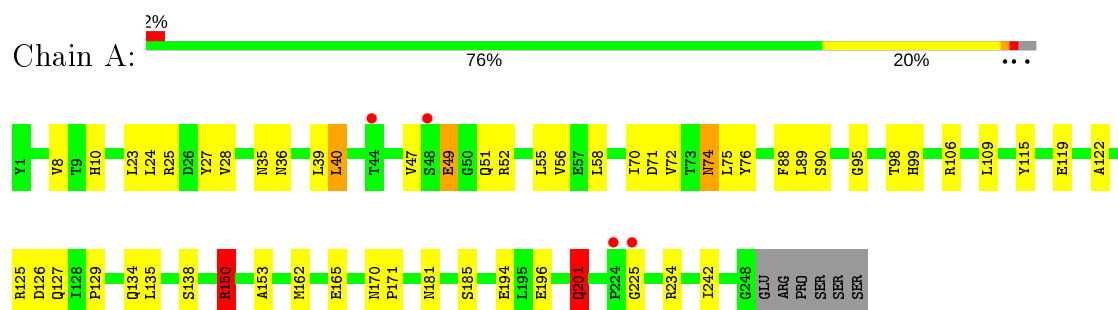
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	128	Total	O	0	0
			128	128		
9	B	182	Total	O	0	0
			182	182		

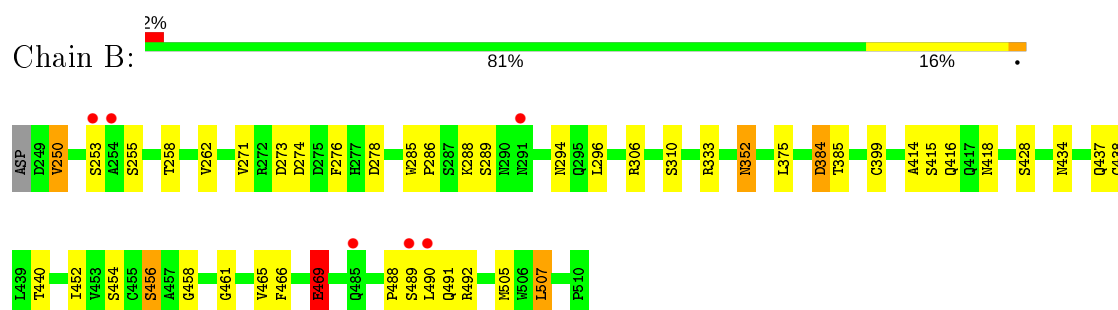
3 Residue-property plots [i](#)

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.

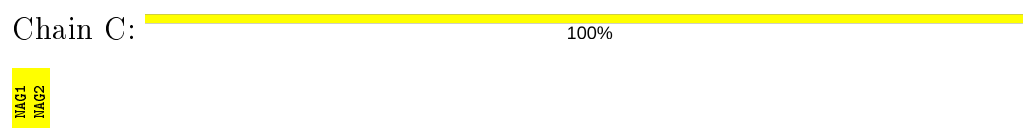
- Molecule 1: Beta-galactoside-specific lectin 1 chain A isoform 1



- Molecule 2: Beta-galactoside-specific lectin 1 chain B



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



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



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

Chain D:  33% 67%

 MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.57Å 107.57Å 310.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-2.70) 99.5 (19.97-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.174 , 0.226 0.173 , 0.223	Depositor DCC
R_{free} test set	1517 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4413	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: GOL, SO4, NAG, H35

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	0.98	0/1961	0.94	3/2674 (0.1%)
2	B	1.02	5/2041 (0.2%)	0.95	1/2783 (0.0%)
All	All	1.00	5/4002 (0.1%)	0.94	4/5457 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	469	GLU	CB-CG	7.09	1.65	1.52
2	B	469	GLU	CG-CD	6.41	1.61	1.51
2	B	438	CYS	CB-SG	-6.10	1.71	1.82
2	B	399	CYS	CB-SG	-6.09	1.71	1.82
2	B	434	ASN	CB-CG	5.12	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	384	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	201	GLN	CB-CA-C	5.09	120.57	110.40
1	A	27	TYR	CA-CB-CG	-5.08	103.76	113.40

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	1921	0	1891	42	0
2	B	2001	0	1935	28	0
3	C	28	0	25	0	0
3	E	28	0	25	1	0
4	D	42	0	37	1	0
5	A	5	0	0	0	0
6	A	14	0	13	1	0
7	A	24	0	32	3	0
7	B	24	0	32	8	0
8	A	16	0	9	5	0
9	A	128	0	0	7	1
9	B	182	0	0	2	0
All	All	4413	0	3999	73	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 9.

All (73) 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)
2:B:488:PRO:O	2:B:491:GLN:HG3	1.55	1.04
1:A:181:ASN:HB3	9:A:346:HOH:O	1.65	0.97
7:B:800:GOL:H12	9:B:548:HOH:O	1.72	0.88
1:A:49:GLU:HG3	1:A:51:GLN:H	1.44	0.83
9:A:348:HOH:O	7:B:1:GOL:H31	1.85	0.75
2:B:469:GLU:HG2	9:B:120:HOH:O	1.91	0.71
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.55	0.71
4:D:2:NAG:O3	4:D:3:NAG:H61	1.92	0.69
1:A:115:TYR:HB3	8:A:255:H35:H6	1.57	0.67
2:B:466:PHE:HB2	7:B:1:GOL:H32	1.78	0.65
2:B:489:SER:HA	2:B:491:GLN:HE21	1.63	0.63
1:A:74:ASN:HD22	1:A:76:TYR:H	1.45	0.62
2:B:262:VAL:CG2	2:B:385:THR:HG22	2.33	0.59
7:A:256:GOL:O3	7:B:1:GOL:H2	2.02	0.59
1:A:47:VAL:HG12	1:A:99:HIS:HD2	1.68	0.58
1:A:115:TYR:HA	1:A:119:GLU:OE1	2.04	0.57
1:A:74:ASN:ND2	1:A:76:TYR:H	2.02	0.57
2:B:375:LEU:HD12	2:B:458:GLY:HA2	1.87	0.56
1:A:8:VAL:O	1:A:8:VAL:HG23	2.05	0.56
1:A:165:GLU:OE1	1:A:196:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD13	1:A:242:ILE:HG12	1.89	0.54
2:B:416:GLN:HG2	2:B:418:ASN:OD1	2.08	0.54
1:A:234:ARG:HH21	7:A:256:GOL:H32	1.73	0.54
1:A:126:ASP:OD1	1:A:127:GLN:HG3	2.09	0.53
1:A:39:LEU:HD11	2:B:250:VAL:HG22	1.91	0.53
2:B:375:LEU:HD21	2:B:428:SER:HB3	1.90	0.52
1:A:171:PRO:HA	2:B:507:LEU:HD11	1.90	0.52
2:B:271:VAL:HB	2:B:294:ASN:HB2	1.92	0.52
1:A:234:ARG:HB3	7:A:256:GOL:H12	1.92	0.51
1:A:10:HIS:HE1	9:A:355:HOH:O	1.93	0.51
2:B:278:ASP:H	7:B:511:GOL:H32	1.77	0.50
1:A:71:ASP:HB3	1:A:74:ASN:HD21	1.77	0.50
2:B:288:LYS:HE2	7:B:800:GOL:O1	2.11	0.50
1:A:196:GLU:OE1	8:A:255:H35:HAM	2.12	0.50
1:A:74:ASN:HD22	1:A:74:ASN:C	2.16	0.49
1:A:35:ASN:O	1:A:36:ASN:HB2	2.12	0.49
2:B:466:PHE:H	7:B:1:GOL:H32	1.78	0.48
2:B:285:TRP:CD1	2:B:286:PRO:HD2	2.48	0.48
2:B:306:ARG:HA	2:B:310:SER:O	2.13	0.48
1:A:165:GLU:CD	1:A:196:GLU:HG2	2.35	0.47
1:A:24:LEU:O	1:A:28:VAL:HG22	2.15	0.47
2:B:465:VAL:HA	7:B:1:GOL:O2	2.15	0.47
1:A:201:GLN:HB2	9:A:304:HOH:O	2.13	0.47
1:A:194:GLU:HG2	9:A:347:HOH:O	2.15	0.46
2:B:384:ASP:OD1	2:B:384:ASP:C	2.55	0.46
1:A:76:TYR:CE1	8:A:255:H35:N9	2.85	0.45
6:A:601:NAG:H62	9:A:333:HOH:O	2.15	0.45
2:B:437:GLN:HE21	2:B:452:ILE:HG22	1.82	0.45
2:B:352:ASN:HA	2:B:352:ASN:HD22	1.61	0.45
1:A:95:GLY:HA2	9:A:388:HOH:O	2.16	0.45
1:A:135:LEU:HG	1:A:162:MET:HE2	1.98	0.44
1:A:89:LEU:HD12	1:A:109:LEU:HD12	1.98	0.44
1:A:115:TYR:CB	8:A:255:H35:H6	2.27	0.44
1:A:88:PHE:HE2	1:A:106:ARG:HG2	1.82	0.44
1:A:115:TYR:HB3	8:A:255:H35:N6	2.30	0.44
2:B:273:ASP:O	2:B:274:ASP:HB2	2.17	0.44
2:B:454:SER:OG	2:B:456:SER:HB2	2.18	0.43
2:B:333:ARG:HH11	2:B:333:ARG:HG3	1.83	0.43
2:B:490:LEU:O	2:B:491:GLN:HB2	2.17	0.43
2:B:414:ALA:O	2:B:415:SER:HB2	2.19	0.42
2:B:276:PHE:CE2	3:E:1:NAG:H82	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:CE2	1:A:106:ARG:HG2	2.53	0.42
1:A:135:LEU:CD1	1:A:162:MET:HE3	2.51	0.41
2:B:258:THR:HG22	2:B:296:LEU:HB3	2.03	0.41
1:A:71:ASP:HB3	1:A:74:ASN:ND2	2.36	0.41
1:A:129:PRO:O	1:A:134:GLN:HG2	2.20	0.41
1:A:52:ARG:O	1:A:72:VAL:HG22	2.21	0.40
1:A:56:VAL:HG12	1:A:58:LEU:HD13	2.03	0.40
1:A:135:LEU:HD11	1:A:162:MET:HE3	2.03	0.40
1:A:135:LEU:HG	1:A:162:MET:CE	2.51	0.40
1:A:122:ALA:HB2	1:A:153:ALA:HB1	2.03	0.40
1:A:170:ASN:N	1:A:171:PRO:CD	2.85	0.40
2:B:440:THR:HA	2:B:461:GLY:O	2.21	0.40

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)
9:A:379:HOH:O	9:A:379:HOH:O[12_564]	1.68	0.52

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	246/254 (97%)	233 (95%)	12 (5%)	1 (0%)	34	60
2	B	260/263 (99%)	247 (95%)	12 (5%)	1 (0%)	34	60
All	All	506/517 (98%)	480 (95%)	24 (5%)	2 (0%)	34	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	253	SER

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Mol	Chain	Res	Type
1	A	225	GLY

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	209/215 (97%)	194 (93%)	15 (7%)	14	34
2	B	221/222 (100%)	212 (96%)	9 (4%)	30	59
All	All	430/437 (98%)	406 (94%)	24 (6%)	21	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	ARG
1	A	40	LEU
1	A	49	GLU
1	A	55	LEU
1	A	70	ILE
1	A	74	ASN
1	A	75	LEU
1	A	90	SER
1	A	98	THR
1	A	125	ARG
1	A	138	SER
1	A	150	ARG
1	A	185	SER
1	A	201	GLN
2	B	250	VAL
2	B	255	SER
2	B	289	SER
2	B	352	ASN
2	B	456	SER
2	B	469	GLU
2	B	492	ARG

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Mol	Chain	Res	Type
2	B	505	MET
2	B	507	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	85	GLN
1	A	99	HIS
1	A	161	GLN
1	A	202	GLN
1	A	216	ASN
1	A	226	ASN
2	B	352	ASN
2	B	417	GLN
2	B	437	GLN
2	B	491	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 ⓘ

7 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	$\# Z > 2$
3	NAG	C	1	3,2	14,14,15	0.74	0	17,19,21	3.18	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	2.05	5 (29%)
4	NAG	D	1	2,4	14,14,15	0.80	0	17,19,21	2.06	7 (41%)
4	NAG	D	2	4	14,14,15	0.65	0	17,19,21	1.68	3 (17%)
4	NAG	D	3	4	14,14,15	1.01	1 (7%)	17,19,21	2.24	6 (35%)
3	NAG	E	1	3,2	14,14,15	0.85	0	17,19,21	2.13	5 (29%)
3	NAG	E	2	3	14,14,15	1.04	0	17,19,21	1.86	6 (35%)

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
3	NAG	C	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	3	4	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3,2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	NAG	C1-C2	2.53	1.56	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	9.71	125.35	112.19
3	E	1	NAG	C1-C2-N2	-5.17	101.65	110.49
3	C	2	NAG	C1-O5-C5	4.89	118.82	112.19
3	E	2	NAG	C2-N2-C7	4.41	129.18	122.90
3	C	1	NAG	C1-C2-N2	4.39	117.98	110.49
4	D	2	NAG	C1-O5-C5	4.10	117.75	112.19
4	D	3	NAG	C1-O5-C5	3.98	117.59	112.19
4	D	3	NAG	C2-N2-C7	3.93	128.50	122.90
4	D	3	NAG	C1-C2-N2	3.63	116.68	110.49
3	C	1	NAG	C6-C5-C4	-3.61	104.55	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C3-C4-C5	-3.58	103.85	110.24
3	C	2	NAG	C8-C7-N2	3.46	121.96	116.10
4	D	1	NAG	C2-N2-C7	3.44	127.80	122.90
3	E	2	NAG	O4-C4-C5	3.43	117.81	109.30
4	D	1	NAG	C4-C3-C2	3.33	115.91	111.02
4	D	3	NAG	O7-C7-C8	-3.33	115.86	122.06
3	E	1	NAG	O5-C1-C2	3.32	116.54	111.29
4	D	1	NAG	C1-O5-C5	3.29	116.64	112.19
4	D	3	NAG	O5-C5-C6	3.19	112.20	107.20
3	C	1	NAG	C4-C3-C2	3.18	115.69	111.02
4	D	1	NAG	C3-C4-C5	-3.16	104.60	110.24
3	C	1	NAG	O4-C4-C5	2.95	116.62	109.30
3	C	2	NAG	C4-C3-C2	-2.94	106.70	111.02
3	C	2	NAG	O4-C4-C5	2.87	116.42	109.30
4	D	1	NAG	O4-C4-C5	2.65	115.88	109.30
4	D	2	NAG	O7-C7-C8	-2.65	117.14	122.06
4	D	2	NAG	O7-C7-N2	2.55	126.63	121.95
4	D	1	NAG	O5-C5-C6	-2.52	103.25	107.20
4	D	1	NAG	O7-C7-C8	-2.52	117.38	122.06
3	E	1	NAG	O3-C3-C2	2.47	114.58	109.47
3	E	2	NAG	C3-C4-C5	-2.32	106.10	110.24
3	C	1	NAG	O7-C7-N2	2.29	126.16	121.95
3	E	2	NAG	O4-C4-C3	2.25	115.56	110.35
3	E	2	NAG	C6-C5-C4	2.22	118.20	113.00
3	C	1	NAG	O7-C7-C8	-2.20	117.98	122.06
3	E	1	NAG	C1-O5-C5	2.17	115.14	112.19
4	D	3	NAG	C3-C4-C5	2.16	114.09	110.24
3	C	2	NAG	O7-C7-C8	-2.12	118.12	122.06
3	C	1	NAG	C2-N2-C7	2.11	125.90	122.90
3	E	2	NAG	O5-C1-C2	-2.07	108.03	111.29
3	C	1	NAG	O3-C3-C4	-2.06	105.60	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C3-C2-N2-C7
4	D	3	NAG	C3-C2-N2-C7

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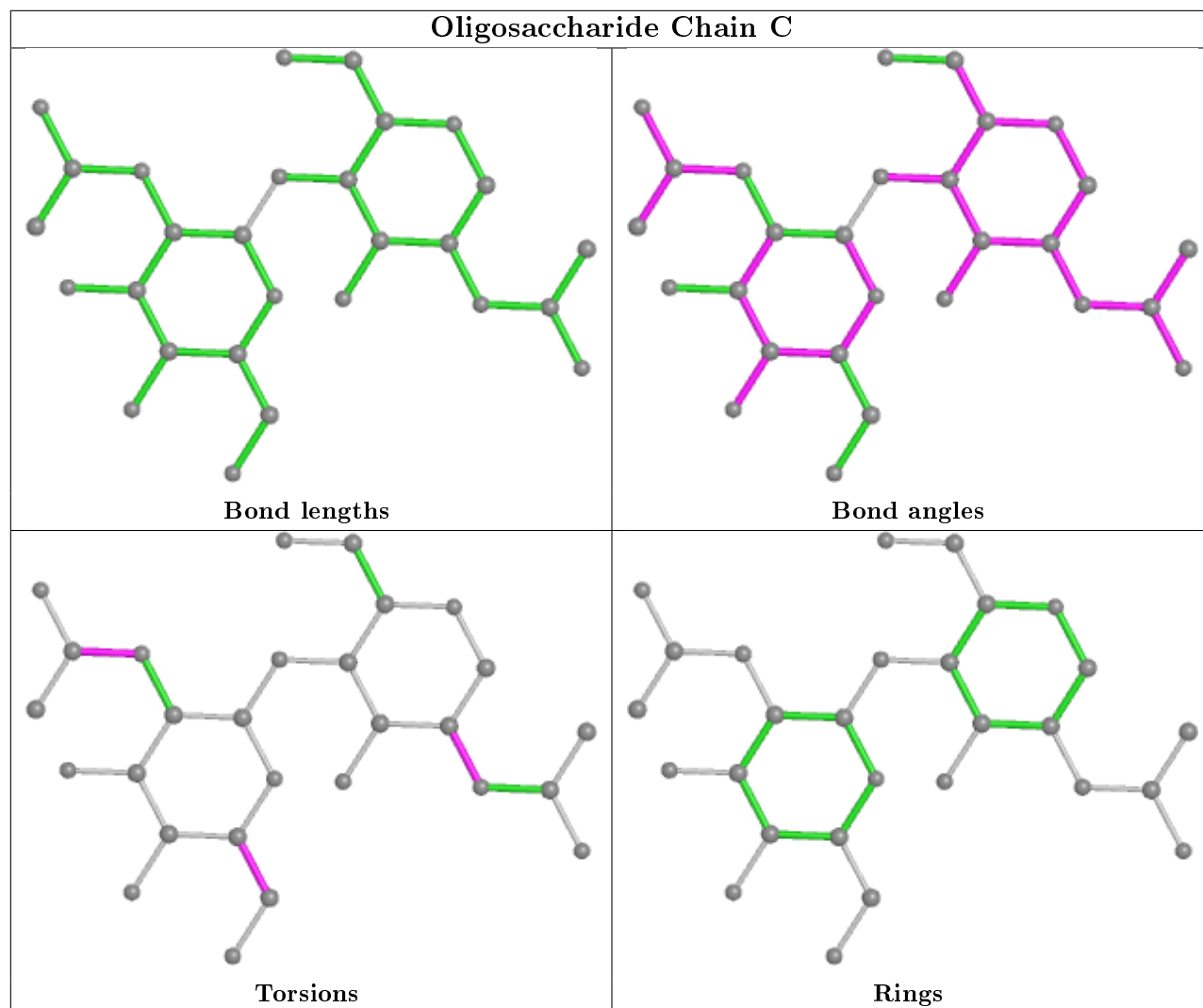
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	3	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	3	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	D	3	NAG	C1-C2-N2-C7
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7

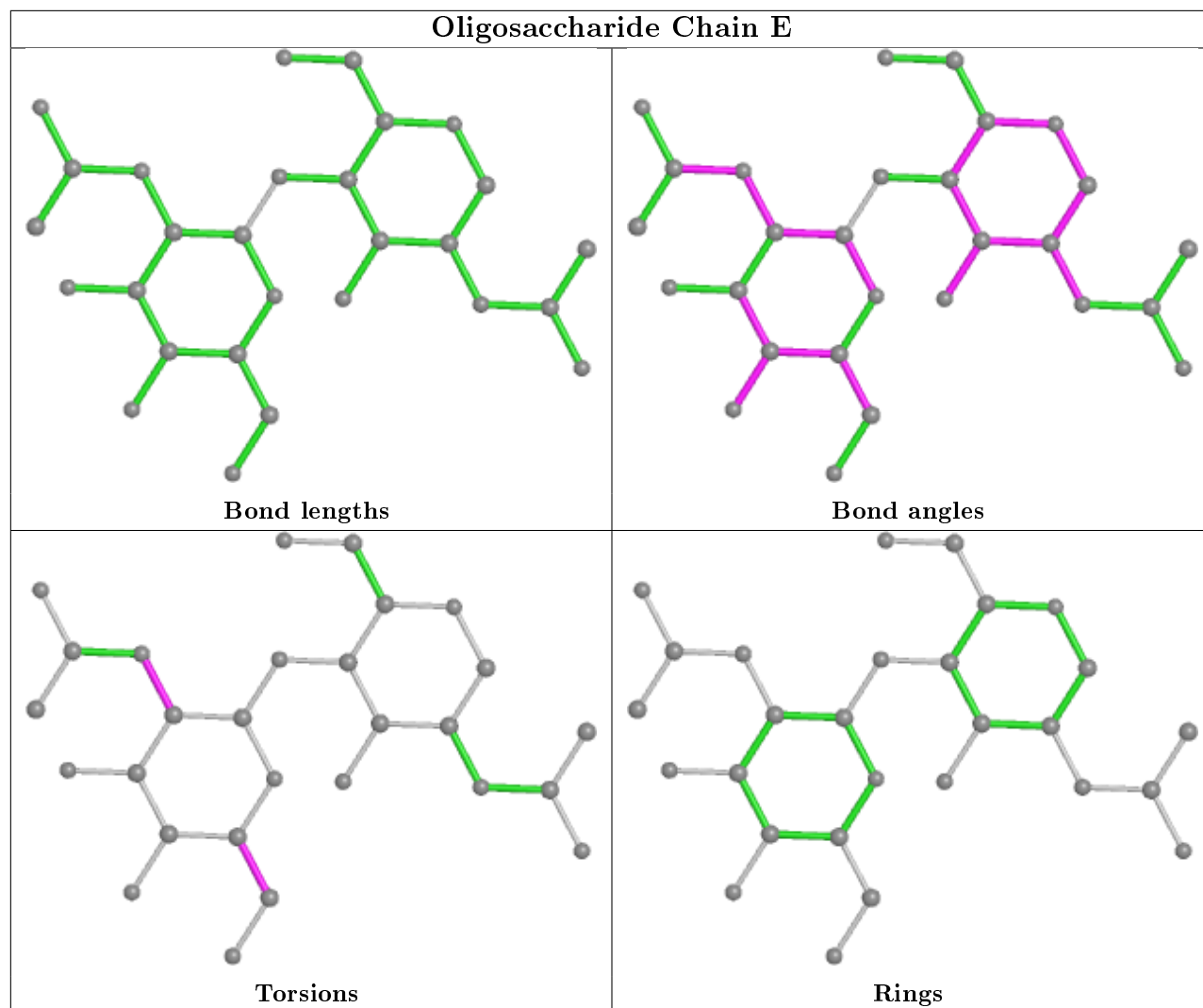
There are no ring outliers.

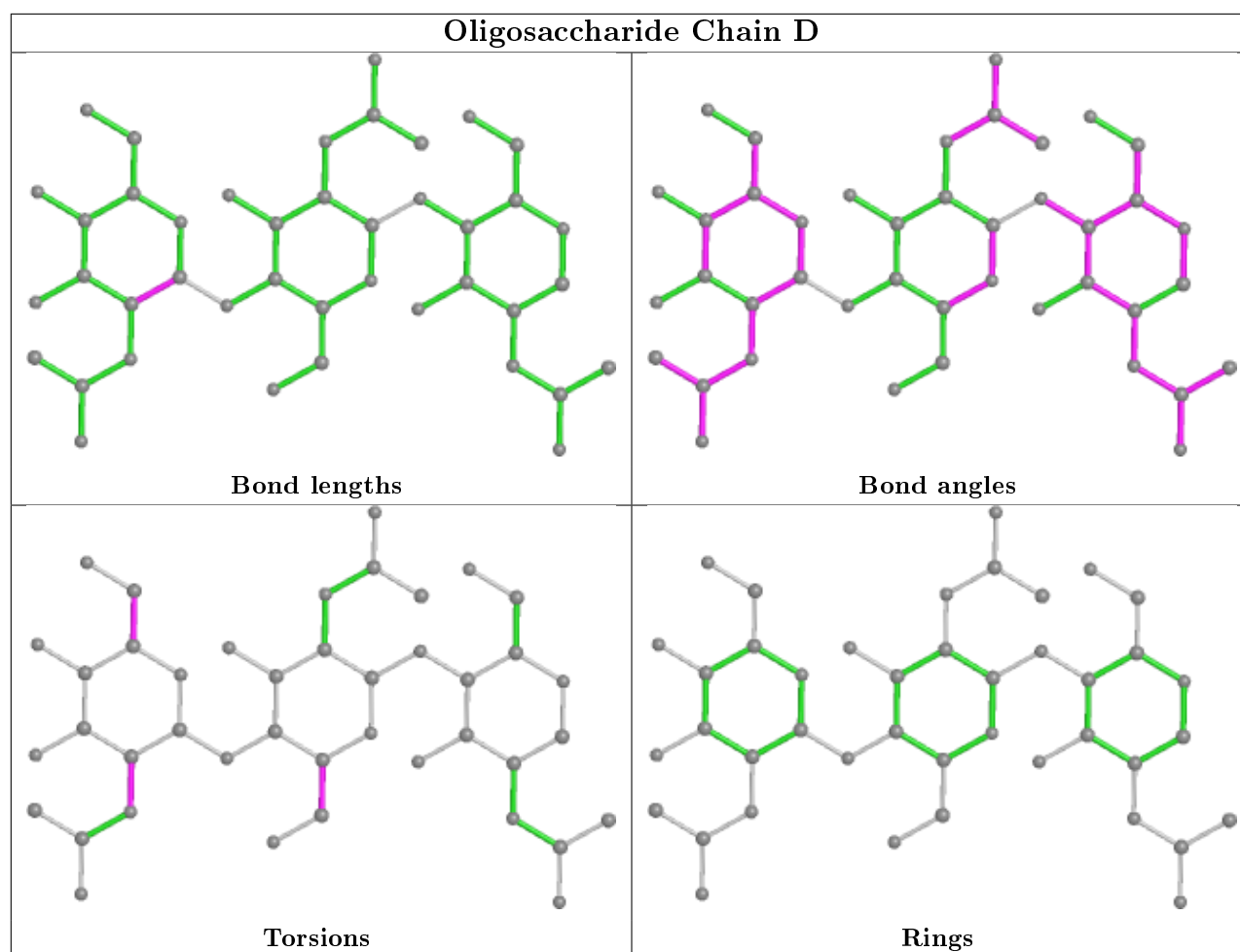
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	NAG	1	0
4	D	2	NAG	1	0
3	E	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
7	GOL	A	256	-	5,5,5	0.59	0	5,5,5	0.62	0
5	SO4	A	500	-	4,4,4	1.18	0	6,6,6	1.43	1 (16%)
6	NAG	A	601	1	14,14,15	0.79	0	17,19,21	2.87	7 (41%)
8	H35	A	255	-	12,18,18	1.91	2 (16%)	10,24,24	3.06	5 (50%)
7	GOL	B	511	-	5,5,5	1.20	1 (20%)	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	800	-	5,5,5	0.45	0	5,5,5	0.51	0
7	GOL	B	803	-	5,5,5	0.62	0	5,5,5	0.31	0
7	GOL	A	801	-	5,5,5	0.39	0	5,5,5	0.70	0
7	GOL	A	257	-	5,5,5	0.66	0	5,5,5	0.66	0
7	GOL	B	1	-	5,5,5	0.90	0	5,5,5	1.11	1 (20%)
7	GOL	A	802	-	5,5,5	0.95	0	5,5,5	1.39	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
7	GOL	A	256	-	-	2/4/4/4	-
6	NAG	A	601	1	-	5/6/23/26	0/1/1/1
8	H35	A	255	-	-	2/3/5/5	0/3/3/3
7	GOL	B	511	-	-	2/4/4/4	-
7	GOL	B	800	-	-	0/4/4/4	-
7	GOL	B	803	-	-	2/4/4/4	-
7	GOL	A	801	-	-	2/4/4/4	-
7	GOL	A	257	-	-	0/4/4/4	-
7	GOL	B	1	-	-	2/4/4/4	-
7	GOL	A	802	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	255	H35	CAM-CAK	-4.88	1.32	1.39
8	A	255	H35	C6-N6	-2.59	1.29	1.34
7	B	511	GOL	C1-C2	2.05	1.60	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	NAG	C2-N2-C7	7.28	133.26	122.90
8	A	255	H35	CAP-N6-C6	-6.28	114.73	123.11
6	A	601	NAG	C1-O5-C5	4.89	118.82	112.19
8	A	255	H35	N3-C2-N1	-4.82	121.14	128.68
6	A	601	NAG	C8-C7-N2	3.76	122.47	116.10
8	A	255	H35	C2-N3-C4	3.74	122.20	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	NAG	O5-C1-C2	-3.73	105.40	111.29
8	A	255	H35	CAK-CAP-N6	-3.20	105.78	112.71
6	A	601	NAG	O7-C7-N2	-2.84	116.74	121.95
5	A	500	SO4	O4-S-O3	-2.77	97.25	109.06
6	A	601	NAG	O5-C5-C4	2.65	117.26	110.83
6	A	601	NAG	C4-C3-C2	-2.43	107.46	111.02
7	B	1	GOL	C3-C2-C1	2.04	119.63	111.70
8	A	255	H35	N6-C6-N1	2.02	121.86	118.54

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	256	GOL	O1-C1-C2-C3
6	A	601	NAG	C3-C2-N2-C7
8	A	255	H35	N1-C6-N6-CAP
8	A	255	H35	C5-C6-N6-CAP
7	B	511	GOL	C1-C2-C3-O3
7	B	803	GOL	O1-C1-C2-C3
7	A	801	GOL	O1-C1-C2-C3
7	B	1	GOL	C1-C2-C3-O3
7	B	1	GOL	O2-C2-C3-O3
7	A	802	GOL	O1-C1-C2-C3
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	601	NAG	C8-C7-N2-C2
6	A	601	NAG	O7-C7-N2-C2
7	B	511	GOL	O2-C2-C3-O3
7	A	256	GOL	O1-C1-C2-O2
7	A	801	GOL	O1-C1-C2-O2
7	B	803	GOL	O1-C1-C2-O2
7	A	802	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	256	GOL	3	0
6	A	601	NAG	1	0
8	A	255	H35	5	0
7	B	511	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	800	GOL	2	0
7	B	1	GOL	5	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	248/254 (97%)	-0.52	4 (1%) 72 74	31, 46, 81, 103	0
2	B	262/263 (99%)	-0.48	6 (2%) 60 62	27, 38, 75, 133	0
All	All	510/517 (98%)	-0.50	10 (1%) 65 67	27, 42, 79, 133	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	485	GLN	3.2
2	B	489	SER	3.1
1	A	224	PRO	3.0
1	A	225	GLY	2.8
1	A	48	SER	2.8
2	B	291	ASN	2.7
2	B	254	ALA	2.4
2	B	490	LEU	2.3
1	A	44	THR	2.2
2	B	253	SER	2.2

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

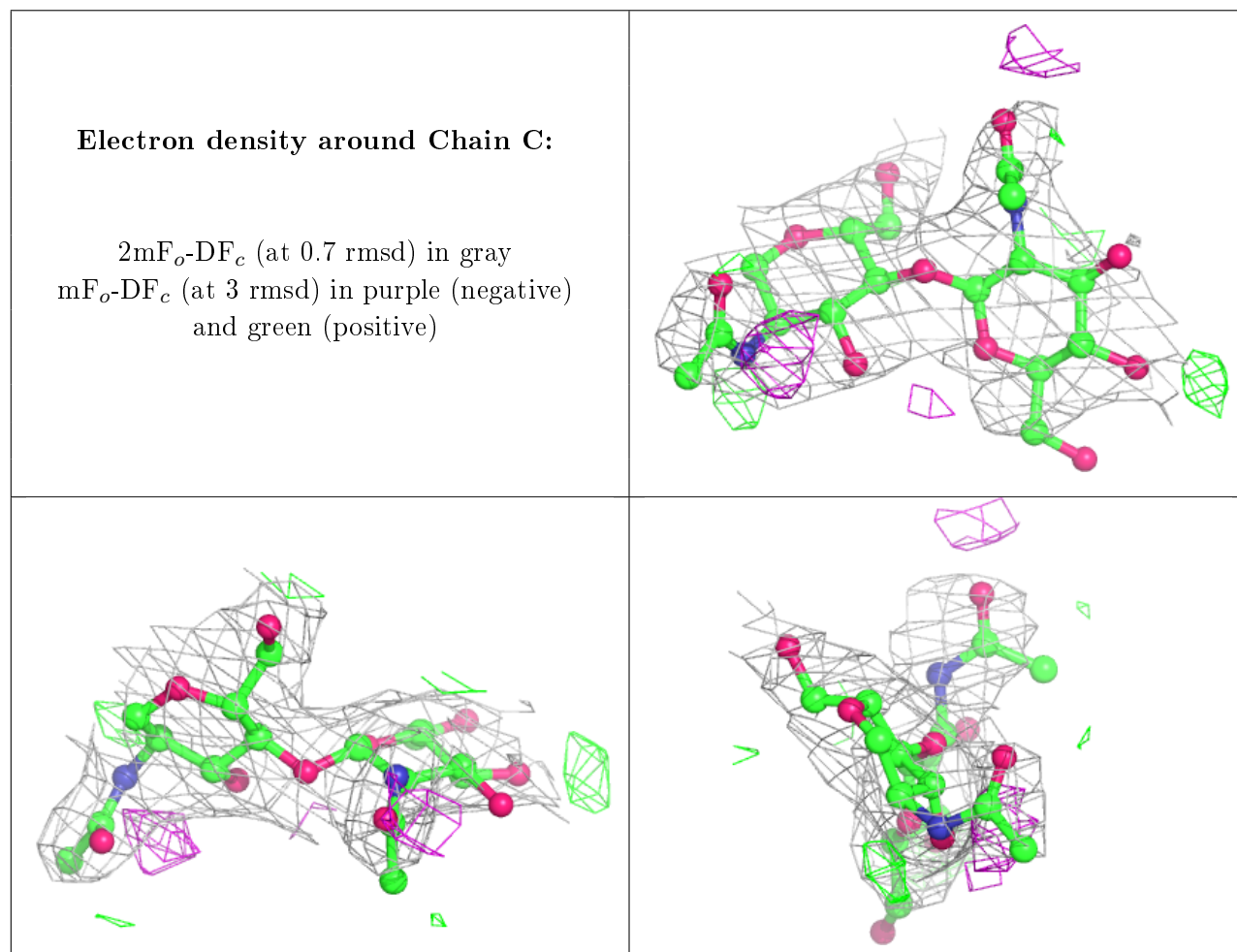
There are no non-standard protein/DNA/RNA residues in this entry.

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.

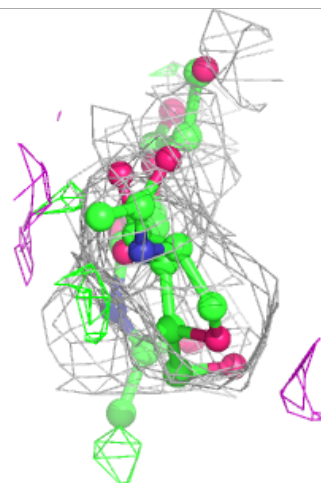
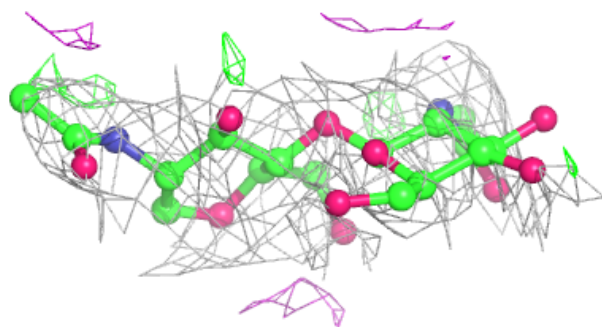
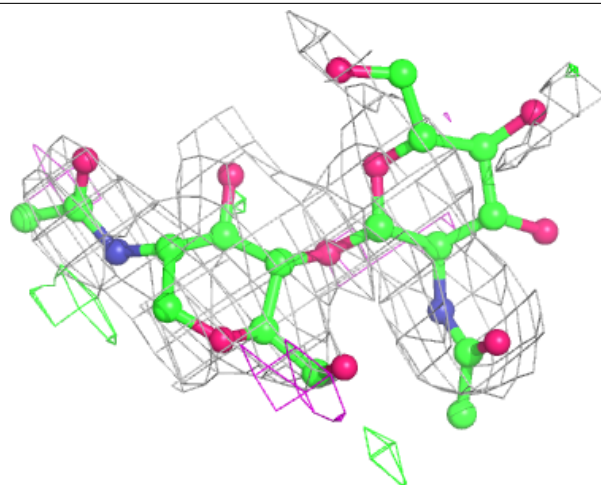
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	3	14/15	0.69	0.53	109,120,128,130	0
3	NAG	E	2	14/15	0.72	0.44	125,133,147,149	0
3	NAG	E	1	14/15	0.86	0.32	94,104,118,120	0
3	NAG	C	2	14/15	0.89	0.40	81,95,109,115	0
4	NAG	D	2	14/15	0.90	0.26	67,77,90,103	0
3	NAG	C	1	14/15	0.93	0.16	69,77,82,86	0
4	NAG	D	1	14/15	0.97	0.11	39,51,59,60	0

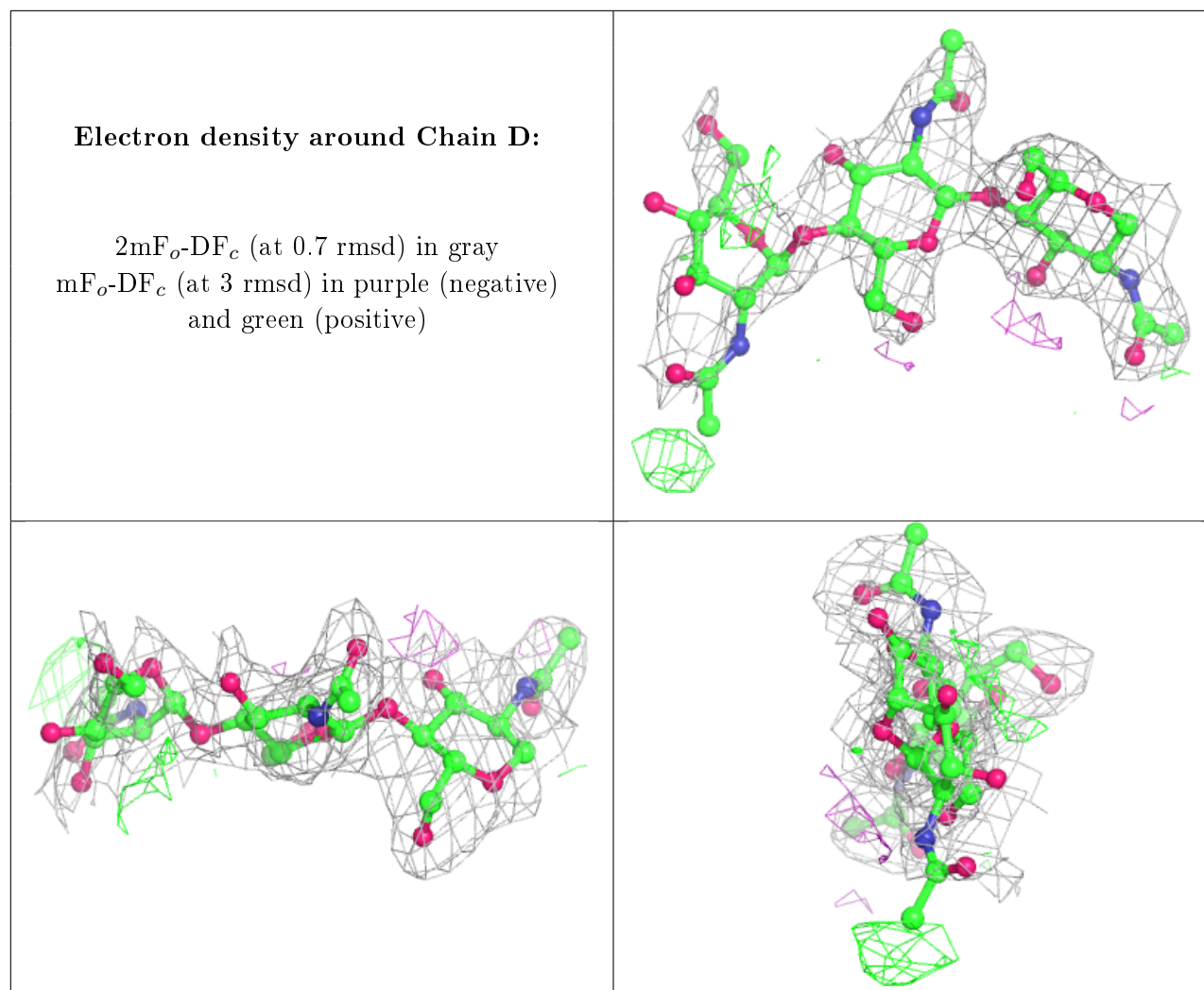
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o-DF_c$ (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
7	GOL	B	511	6/6	0.81	0.33	35,43,46,46	0
6	NAG	A	601	14/15	0.86	0.35	88,92,96,97	0
8	H35	A	255	16/16	0.88	0.20	52,54,57,57	16
7	GOL	A	256	6/6	0.93	0.19	46,48,50,50	0
7	GOL	A	257	6/6	0.94	0.26	46,49,51,52	0
7	GOL	A	801	6/6	0.95	0.15	70,75,77,81	0
7	GOL	B	800	6/6	0.95	0.14	53,56,58,59	0
7	GOL	B	1	6/6	0.95	0.22	38,42,43,43	0
7	GOL	A	802	6/6	0.95	0.19	34,37,39,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	500	5/5	0.98	0.15	32,37,40,42	0
7	GOL	B	803	6/6	0.98	0.14	57,60,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.