Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 06:04 pm GMT

PDB ID	:	5HYE
Title	:	Glycosylated Knob-Knob Fc fragment (P212121)
Authors	:	Kuglstatter, A.; Stihle, M.; Benz, J.
Deposited on	:	2016-02-01
Resolution	:	1.89 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 (i) 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 (i)) were used in the production of this report:

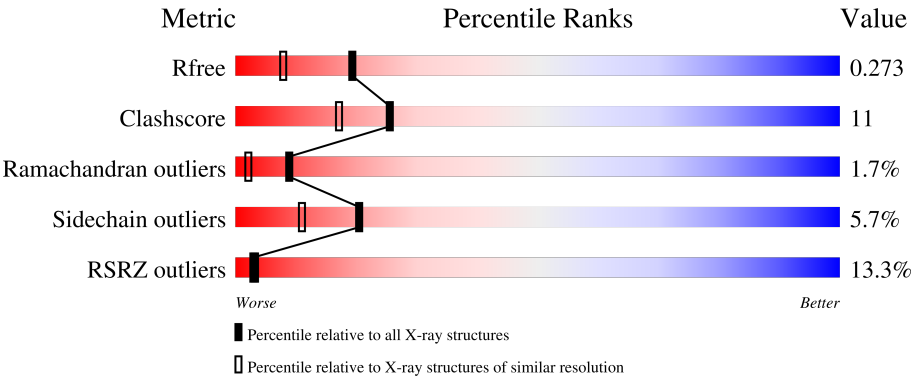
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	227	4% 74% 16% · 8%
1	C	227	20% 68% 18% 5% 9%
2	B	9	78% 22%
2	D	9	44% 56%

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
2	BMA	B	4	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3705 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.

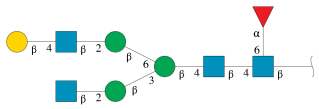
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1673	1068	281	317	7			
1	C	207	Total	C	N	O	S	0	0	0
			1665	1063	280	315	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	CYS	SER	engineered mutation	UNP P01857
A	366	TRP	THR	engineered mutation	UNP P01857
C	354	CYS	SER	engineered mutation	UNP P01857
C	366	TRP	THR	engineered mutation	UNP P01857

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			110	62	4	44			
2	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

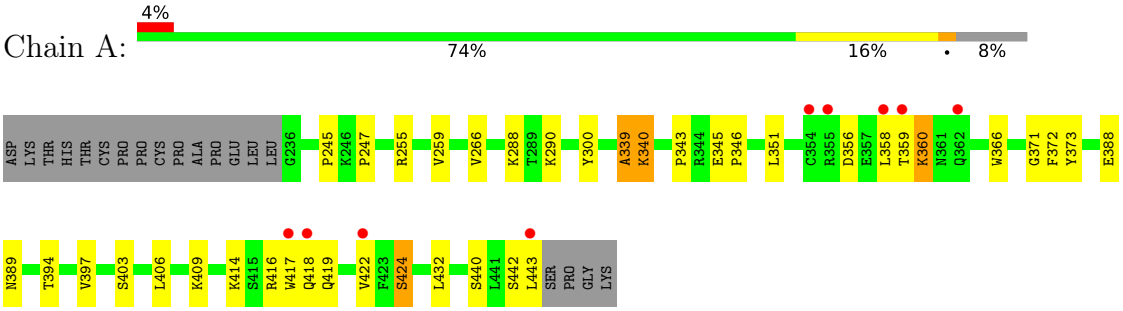
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	C	38	Total O 38 38	0	0

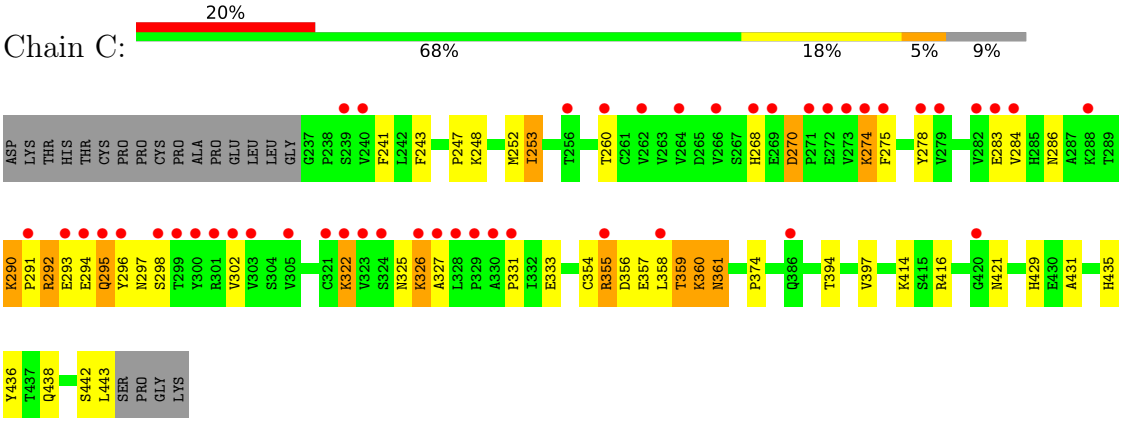
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

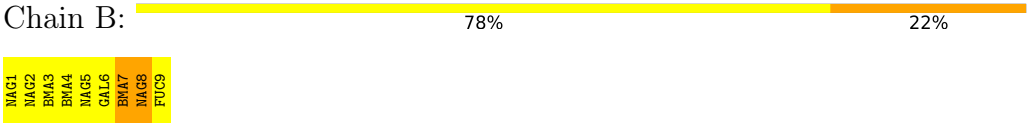
• Molecule 1: Ig gamma-1 chain C region



• Molecule 1: Ig gamma-1 chain C region



• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyran

ose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.03Å 81.62Å 136.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 1.89 46.13 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.17-1.89) 99.6 (46.13-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.275 0.220 , 0.273	Depositor DCC
R_{free} test set	2236 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3705	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GAL, FUC, NAG

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	0.95	0/1724	0.96	0/2350
1	C	0.82	1/1713 (0.1%)	0.86	0/2335
All	All	0.89	1/3437 (0.0%)	0.91	0/4685

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	LYS	CE-NZ	8.53	1.70	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	CYS	Peptide

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	1673	0	1638	26	0
1	C	1665	0	1628	47	0
2	B	110	0	94	1	0
2	D	110	0	94	6	0
3	A	109	0	0	3	0
3	C	38	0	0	3	0
All	All	3705	0	3454	74	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 11.

All (74) 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:C:274:LYS:CE	1:C:274:LYS:NZ	1.70	1.51
1:C:248:LYS:HG3	1:C:252:MET:HE1	1.38	0.99
1:A:255:ARG:HD2	3:A:601:HOH:O	1.81	0.79
1:C:292:ARG:HG2	1:C:292:ARG:HH11	1.47	0.78
1:C:248:LYS:HG3	1:C:252:MET:CE	2.14	0.74
1:C:243:PHE:CD2	2:D:5:NAG:H61	2.25	0.70
1:C:436:TYR:OH	1:C:438:GLN:NE2	2.21	0.70
1:C:435:HIS:HE1	3:C:629:HOH:O	1.77	0.68
2:B:7:BMA:O3	2:B:8:NAG:C1	2.43	0.67
2:D:2:NAG:H82	2:D:9:FUC:C1	2.31	0.60
1:C:325:ASN:OD1	1:C:327:ALA:HB3	2.01	0.60
1:C:359:THR:OG1	1:C:360:LYS:HE3	2.01	0.60
1:C:290:LYS:HE3	1:C:291:PRO:HD2	1.84	0.59
1:A:417:TRP:O	1:A:443:LEU:HB2	2.02	0.58
1:A:424:SER:OG	1:A:440:SER:OG	2.19	0.58
1:A:422:VAL:HA	1:A:442:SER:HB3	1.87	0.57
1:C:248:LYS:CG	1:C:252:MET:HE1	2.24	0.56
1:A:416:ARG:HA	1:A:419:GLN:HB2	1.86	0.55
1:A:366:TRP:CH2	1:A:409:LYS:HD2	2.40	0.55
1:C:429:HIS:CD2	1:C:431:ALA:H	2.24	0.55
1:C:270:ASP:OD2	1:C:327:ALA:HB2	2.07	0.55
1:C:248:LYS:CG	1:C:252:MET:CE	2.83	0.54
1:A:351:LEU:HB2	1:A:366:TRP:HB2	1.88	0.54
1:C:322:LYS:HE3	1:C:333:GLU:HG3	1.90	0.54
1:C:292:ARG:HG2	1:C:292:ARG:NH1	2.16	0.54
1:C:360:LYS:HA	1:C:360:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:C	1:A:406:LEU:HD12	2.29	0.53
1:C:274:LYS:NZ	1:C:274:LYS:CD	2.62	0.53
1:A:339:ALA:N	3:A:602:HOH:O	2.26	0.53
1:A:371:GLY:HA2	1:A:403:SER:OG	2.09	0.52
1:C:243:PHE:HD2	2:D:5:NAG:H61	1.74	0.52
1:A:290:LYS:HE3	3:A:675:HOH:O	2.09	0.51
1:C:361:ASN:H	1:C:361:ASN:ND2	2.09	0.51
1:C:360:LYS:HE2	1:C:360:LYS:CA	2.40	0.51
1:C:442:SER:O	1:C:443:LEU:C	2.49	0.50
1:A:417:TRP:CZ3	1:A:442:SER:HA	2.46	0.50
1:A:394:THR:HG22	1:C:397:VAL:HG21	1.93	0.49
1:A:359:THR:HA	1:A:414:LYS:HZ3	1.76	0.49
1:A:359:THR:HA	1:A:414:LYS:NZ	2.28	0.48
1:C:286:ASN:N	3:C:602:HOH:O	2.38	0.48
1:C:290:LYS:HE3	1:C:290:LYS:HB3	1.52	0.48
1:C:292:ARG:C	1:C:293:GLU:HG3	2.33	0.48
1:C:374:PRO:O	1:C:429:HIS:HE1	1.95	0.48
1:C:292:ARG:CB	1:C:302:VAL:HG22	2.44	0.47
1:A:360:LYS:NZ	1:A:360:LYS:HB2	2.29	0.47
1:C:241:PHE:CE1	2:D:3:BMA:H2	2.50	0.47
1:C:357:GLU:O	1:C:360:LYS:HB2	2.15	0.47
1:C:322:LYS:HE2	1:C:331:PRO:HB2	1.96	0.47
1:A:343:PRO:HA	1:A:373:TYR:O	2.15	0.46
1:A:418:GLN:HA	1:A:443:LEU:HD13	1.98	0.46
1:C:295:GLN:HB2	1:C:297:ASN:OD1	2.15	0.46
1:C:435:HIS:CE1	3:C:629:HOH:O	2.61	0.46
1:A:360:LYS:O	1:A:414:LYS:HD2	2.16	0.45
1:C:325:ASN:C	1:C:327:ALA:H	2.18	0.45
1:C:248:LYS:O	1:C:252:MET:HE2	2.16	0.45
1:C:360:LYS:O	1:C:414:LYS:HD3	2.17	0.45
1:A:442:SER:O	1:A:443:LEU:C	2.56	0.45
1:C:292:ARG:HB3	1:C:302:VAL:HG22	1.99	0.44
1:C:283:GLU:HG3	1:C:284:VAL:N	2.32	0.44
1:C:274:LYS:HG2	1:C:275:PHE:N	2.31	0.44
2:D:3:BMA:O2	2:D:7:BMA:C1	2.65	0.44
1:C:260:THR:HG21	2:D:5:NAG:O6	2.18	0.43
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.00	0.43
1:A:397:VAL:HG21	1:C:394:THR:HA	2.00	0.42
1:C:253:ILE:H	1:C:253:ILE:HG12	1.59	0.42
1:C:295:GLN:H	1:C:295:GLN:HG2	1.69	0.42
1:C:416:ARG:O	1:C:421:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LYS:CE	1:C:291:PRO:HD2	2.49	0.41
1:C:356:ASP:OD2	1:C:356:ASP:N	2.49	0.41
1:A:358:LEU:O	1:A:359:THR:CG2	2.68	0.41
1:A:266:VAL:HB	1:A:300:TYR:HB2	2.03	0.41
1:C:268:HIS:CD2	1:C:268:HIS:N	2.87	0.41
1:A:245:PRO:HD3	1:A:259:VAL:HG22	2.03	0.40
1:A:345:GLU:HG3	1:A:432:LEU:HD23	2.02	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	207/227 (91%)	196 (95%)	7 (3%)	4 (2%)	8 1
1	C	205/227 (90%)	193 (94%)	9 (4%)	3 (2%)	10 3
All	All	412/454 (91%)	389 (94%)	16 (4%)	7 (2%)	9 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	298	SER
1	C	355	ARG
1	A	388	GLU
1	A	389	ASN
1	A	339	ALA
1	C	326	LYS
1	A	340	LYS

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	194/210 (92%)	188 (97%)	6 (3%)	40 32
1	C	193/210 (92%)	177 (92%)	16 (8%)	11 4
All	All	387/420 (92%)	365 (94%)	22 (6%)	20 11

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	PRO
1	A	288	LYS
1	A	340	LYS
1	A	356	ASP
1	A	360	LYS
1	A	424	SER
1	C	247	PRO
1	C	253	ILE
1	C	270	ASP
1	C	278	TYR
1	C	290	LYS
1	C	292	ARG
1	C	294	GLU
1	C	295	GLN
1	C	296	TYR
1	C	322	LYS
1	C	326	LYS
1	C	355	ARG
1	C	358	LEU
1	C	359	THR
1	C	360	LYS
1	C	361	ASN

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

Mol	Chain	Res	Type
1	C	268	HIS
1	C	361	ASN
1	C	429	HIS
1	C	438	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GAL	D	6	2	11,11,12	0.91	1 (9%)	15,15,17	1.77	5 (33%)
2	GAL	B	6	2	11,11,12	1.38	3 (27%)	15,15,17	1.84	4 (26%)
2	NAG	D	8	2	14,14,15	0.61	0	17,19,21	1.86	4 (23%)
2	NAG	B	8	2	14,14,15	0.68	0	17,19,21	1.78	3 (17%)
2	NAG	B	2	2	14,14,15	1.33	3 (21%)	17,19,21	1.41	3 (17%)
2	NAG	B	1	1,2	14,14,15	0.87	0	17,19,21	1.40	3 (17%)
2	NAG	B	5	2	14,14,15	1.12	1 (7%)	17,19,21	1.33	2 (11%)
2	NAG	D	2	2	14,14,15	0.70	0	17,19,21	1.67	5 (29%)
2	NAG	D	5	2	14,14,15	1.00	2 (14%)	17,19,21	1.45	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.83	0	17,19,21	1.78	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
2	GAL	D	6	2	-	2/2/19/22	0/1/1/1
2	GAL	B	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	8	2	-	0/6/23/26	0/1/1/1
2	NAG	B	8	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	5	2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	5	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.79	1.39	1.43
2	B	2	NAG	C1-C2	2.54	1.56	1.52
2	B	5	NAG	O5-C5	-2.44	1.38	1.43
2	B	6	GAL	O3-C3	-2.42	1.37	1.43
2	D	6	GAL	O5-C1	-2.34	1.40	1.43
2	D	5	NAG	C1-C2	2.24	1.55	1.52
2	B	2	NAG	C8-C7	2.20	1.55	1.50
2	B	6	GAL	C4-C5	2.16	1.57	1.53
2	D	5	NAG	C3-C2	2.03	1.56	1.52
2	B	6	GAL	C2-C3	2.00	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	8	NAG	C1-O5-C5	6.12	120.48	112.19
2	B	6	GAL	O2-C2-C1	4.17	117.69	109.15
2	B	8	NAG	C1-O5-C5	3.84	117.39	112.19
2	B	8	NAG	O5-C1-C2	3.83	117.33	111.29
2	D	5	NAG	C4-C3-C2	3.79	116.57	111.02
2	D	6	GAL	C1-O5-C5	3.75	117.27	112.19
2	D	1	NAG	C2-N2-C7	3.74	128.22	122.90
2	B	6	GAL	C3-C4-C5	-3.47	104.06	110.24
2	B	2	NAG	C2-N2-C7	3.37	127.71	122.90
2	B	5	NAG	O5-C5-C6	-3.12	102.32	107.20
2	D	2	NAG	C1-C2-N2	3.07	115.73	110.49
2	D	2	NAG	C1-O5-C5	3.03	116.30	112.19
2	D	1	NAG	C4-C3-C2	3.00	115.41	111.02
2	D	2	NAG	C3-C4-C5	-2.96	104.96	110.24
2	D	2	NAG	O5-C1-C2	-2.86	106.78	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	GAL	O3-C3-C2	2.81	115.38	109.99
2	D	6	GAL	O5-C5-C6	-2.79	102.83	107.20
2	B	8	NAG	O5-C5-C6	2.77	111.54	107.20
2	B	6	GAL	C2-C3-C4	2.72	115.60	110.89
2	B	2	NAG	O5-C1-C2	-2.71	107.01	111.29
2	D	8	NAG	C2-N2-C7	2.64	126.66	122.90
2	D	1	NAG	O5-C5-C6	2.62	111.31	107.20
2	D	1	NAG	C1-O5-C5	2.52	115.61	112.19
2	B	1	NAG	C3-C4-C5	-2.42	105.91	110.24
2	B	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	D	1	NAG	O7-C7-C8	-2.28	117.83	122.06
2	D	1	NAG	C3-C4-C5	-2.26	106.21	110.24
2	D	8	NAG	C1-C2-N2	-2.13	106.85	110.49
2	D	6	GAL	C3-C4-C5	-2.12	106.46	110.24
2	D	6	GAL	O5-C1-C2	-2.10	107.53	110.77
2	D	6	GAL	O2-C2-C1	2.08	113.42	109.15
2	D	8	NAG	O5-C1-C2	2.07	114.55	111.29
2	D	5	NAG	O7-C7-C8	-2.05	118.25	122.06
2	B	5	NAG	O4-C4-C3	-2.03	105.66	110.35
2	D	2	NAG	O3-C3-C2	2.02	113.64	109.47
2	B	1	NAG	O7-C7-C8	-2.01	118.33	122.06
2	B	2	NAG	O5-C5-C6	2.00	110.35	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5	NAG	C4-C5-C6-O6
2	D	6	GAL	O5-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	D	6	GAL	C4-C5-C6-O6
2	B	5	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	NAG	1	0
2	D	2	NAG	1	0
2	D	5	NAG	3	0

5.5 Carbohydrates (i)

18 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	B	1	1,2	14,14,15	0.87	0	17,19,21	1.40	3 (17%)
2	NAG	B	2	2	14,14,15	1.33	3 (21%)	17,19,21	1.41	3 (17%)
2	BMA	B	3	2	11,11,12	1.15	2 (18%)	15,15,17	2.82	5 (33%)
2	BMA	B	4	2	11,11,12	1.02	0	15,15,17	2.00	5 (33%)
2	NAG	B	5	2	14,14,15	1.12	1 (7%)	17,19,21	1.33	2 (11%)
2	GAL	B	6	2	11,11,12	1.38	3 (27%)	15,15,17	1.84	4 (26%)
2	BMA	B	7	2	11,11,12	1.23	1 (9%)	15,15,17	3.82	6 (40%)
2	NAG	B	8	2	14,14,15	0.68	0	17,19,21	1.78	3 (17%)
2	FUC	B	9	2	10,10,11	1.11	1 (10%)	14,14,16	1.27	1 (7%)
2	NAG	D	1	1,2	14,14,15	0.83	0	17,19,21	1.78	6 (35%)
2	NAG	D	2	2	14,14,15	0.70	0	17,19,21	1.67	5 (29%)
2	BMA	D	3	2	11,11,12	0.68	0	15,15,17	2.21	5 (33%)
2	BMA	D	4	2	11,11,12	0.71	0	15,15,17	2.48	6 (40%)
2	NAG	D	5	2	14,14,15	1.00	2 (14%)	17,19,21	1.45	2 (11%)
2	GAL	D	6	2	11,11,12	0.91	1 (9%)	15,15,17	1.77	5 (33%)
2	BMA	D	7	2	11,11,12	0.83	0	15,15,17	1.46	3 (20%)
2	NAG	D	8	2	14,14,15	0.61	0	17,19,21	1.86	4 (23%)
2	FUC	D	9	2	10,10,11	0.78	0	14,14,16	1.64	4 (28%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	B	5	2	-	1/6/23/26	0/1/1/1
2	GAL	B	6	2	-	0/2/19/22	0/1/1/1
2	BMA	B	7	2	-	2/2/19/22	0/1/1/1
2	NAG	B	8	2	-	0/6/23/26	0/1/1/1
2	FUC	B	9	2	-	-	0/1/1/1
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	BMA	D	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	5	2	-	2/6/23/26	0/1/1/1
2	GAL	D	6	2	-	2/2/19/22	0/1/1/1
2	BMA	D	7	2	-	0/2/19/22	0/1/1/1
2	NAG	D	8	2	-	0/6/23/26	0/1/1/1
2	FUC	D	9	2	-	-	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	BMA	O5-C1	-3.10	1.38	1.43
2	B	2	NAG	O5-C1	-2.79	1.39	1.43
2	B	2	NAG	C1-C2	2.54	1.56	1.52
2	B	3	BMA	O5-C1	2.52	1.47	1.43
2	B	5	NAG	O5-C5	-2.44	1.38	1.43
2	B	6	GAL	O3-C3	-2.42	1.37	1.43
2	D	6	GAL	O5-C1	-2.34	1.40	1.43
2	D	5	NAG	C1-C2	2.24	1.55	1.52
2	B	2	NAG	C8-C7	2.20	1.55	1.50
2	B	6	GAL	C4-C5	2.16	1.57	1.53
2	B	9	FUC	C6-C5	2.07	1.56	1.51
2	D	5	NAG	C3-C2	2.03	1.56	1.52
2	B	3	BMA	O6-C6	2.03	1.51	1.42
2	B	6	GAL	C2-C3	2.00	1.55	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	7	BMA	C1-O5-C5	-13.02	94.55	112.19
2	B	3	BMA	O3-C3-C4	-7.24	93.61	110.35
2	D	8	NAG	C1-O5-C5	6.12	120.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BMA	C1-C2-C3	-5.46	102.95	109.67
2	D	3	BMA	C3-C4-C5	-5.26	100.86	110.24
2	D	4	BMA	O2-C2-C3	-4.25	101.63	110.14
2	D	4	BMA	C1-C2-C3	-4.22	104.47	109.67
2	D	7	BMA	O2-C2-C3	4.21	118.58	110.14
2	B	6	GAL	O2-C2-C1	4.17	117.69	109.15
2	D	4	BMA	C3-C4-C5	4.15	117.64	110.24
2	B	3	BMA	O3-C3-C2	4.06	117.76	109.99
2	D	3	BMA	O3-C3-C2	3.98	117.61	109.99
2	D	4	BMA	C1-O5-C5	-3.87	106.95	112.19
2	B	8	NAG	C1-O5-C5	3.84	117.39	112.19
2	B	8	NAG	O5-C1-C2	3.83	117.33	111.29
2	D	5	NAG	C4-C3-C2	3.79	116.57	111.02
2	D	6	GAL	C1-O5-C5	3.75	117.27	112.19
2	D	1	NAG	C2-N2-C7	3.74	128.22	122.90
2	B	6	GAL	C3-C4-C5	-3.47	104.06	110.24
2	B	4	BMA	O5-C1-C2	3.40	116.02	110.77
2	B	4	BMA	O5-C5-C6	3.39	112.52	107.20
2	B	2	NAG	C2-N2-C7	3.37	127.71	122.90
2	B	4	BMA	O2-C2-C3	-3.31	103.50	110.14
2	B	4	BMA	O6-C6-C5	-3.13	100.54	111.29
2	B	5	NAG	O5-C5-C6	-3.12	102.32	107.20
2	D	2	NAG	C1-C2-N2	3.07	115.73	110.49
2	D	9	FUC	C1-O5-C5	3.06	119.72	112.78
2	D	2	NAG	C1-O5-C5	3.03	116.30	112.19
2	B	7	BMA	O4-C4-C3	-3.03	103.35	110.35
2	D	1	NAG	C4-C3-C2	3.00	115.41	111.02
2	D	2	NAG	C3-C4-C5	-2.96	104.96	110.24
2	D	2	NAG	O5-C1-C2	-2.86	106.78	111.29
2	B	7	BMA	C3-C4-C5	2.83	115.28	110.24
2	B	6	GAL	O3-C3-C2	2.81	115.38	109.99
2	B	9	FUC	C1-C2-C3	-2.80	106.22	109.67
2	D	9	FUC	C3-C4-C5	2.80	114.13	109.77
2	D	6	GAL	O5-C5-C6	-2.79	102.83	107.20
2	B	8	NAG	O5-C5-C6	2.77	111.54	107.20
2	B	7	BMA	O5-C5-C6	2.73	111.48	107.20
2	D	3	BMA	O4-C4-C5	2.72	116.06	109.30
2	B	6	GAL	C2-C3-C4	2.72	115.60	110.89
2	B	2	NAG	O5-C1-C2	-2.71	107.01	111.29
2	D	8	NAG	C2-N2-C7	2.64	126.66	122.90
2	D	1	NAG	O5-C5-C6	2.62	111.31	107.20
2	B	7	BMA	O2-C2-C3	2.61	115.37	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	BMA	C2-C3-C4	2.61	115.41	110.89
2	D	1	NAG	C1-O5-C5	2.52	115.61	112.19
2	B	7	BMA	O6-C6-C5	-2.50	102.73	111.29
2	D	3	BMA	C2-C3-C4	-2.49	106.58	110.89
2	B	3	BMA	C6-C5-C4	-2.45	107.27	113.00
2	B	1	NAG	C3-C4-C5	-2.42	105.91	110.24
2	B	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	B	4	BMA	C3-C4-C5	2.35	114.44	110.24
2	D	4	BMA	O2-C2-C1	2.32	113.89	109.15
2	D	7	BMA	O2-C2-C1	2.28	113.82	109.15
2	D	1	NAG	O7-C7-C8	-2.28	117.83	122.06
2	D	1	NAG	C3-C4-C5	-2.26	106.21	110.24
2	D	9	FUC	O5-C1-C2	2.20	114.16	110.77
2	D	8	NAG	C1-C2-N2	-2.13	106.85	110.49
2	D	6	GAL	C3-C4-C5	-2.12	106.46	110.24
2	D	6	GAL	O5-C1-C2	-2.10	107.53	110.77
2	D	6	GAL	O2-C2-C1	2.08	113.42	109.15
2	D	3	BMA	O5-C5-C6	2.08	110.46	107.20
2	D	8	NAG	O5-C1-C2	2.07	114.55	111.29
2	D	7	BMA	C1-C2-C3	-2.06	107.13	109.67
2	D	5	NAG	O7-C7-C8	-2.05	118.25	122.06
2	B	3	BMA	O5-C5-C6	2.05	110.42	107.20
2	B	5	NAG	O4-C4-C3	-2.03	105.66	110.35
2	D	2	NAG	O3-C3-C2	2.02	113.64	109.47
2	B	1	NAG	O7-C7-C8	-2.01	118.33	122.06
2	B	2	NAG	O5-C5-C6	2.00	110.35	107.20
2	D	9	FUC	C1-C2-C3	2.00	112.13	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	4	BMA	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5	NAG	C4-C5-C6-O6
2	D	6	GAL	O5-C5-C6-O6
2	B	7	BMA	C4-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	D	6	GAL	C4-C5-C6-O6
2	B	7	BMA	O5-C5-C6-O6

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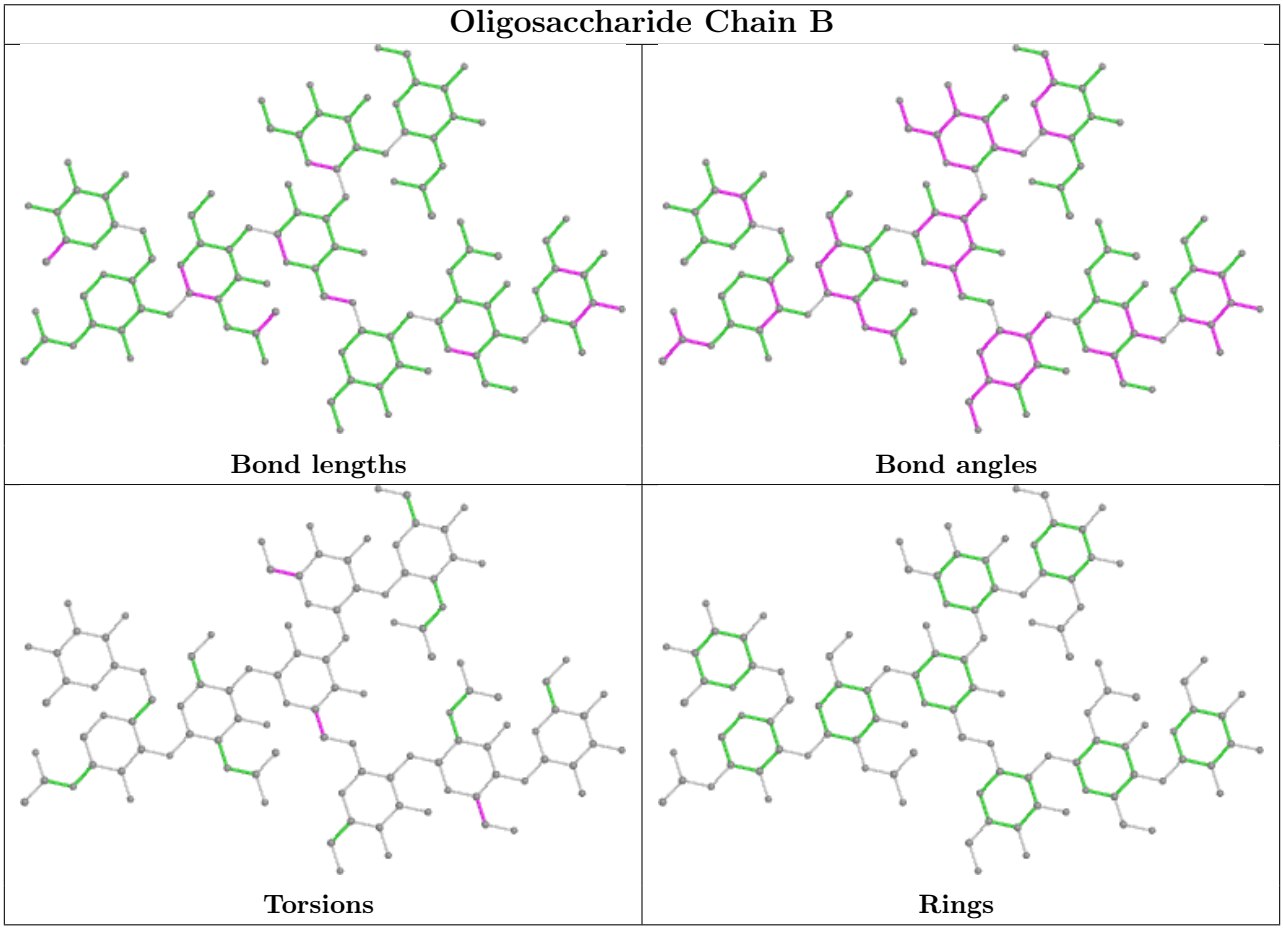
Mol	Chain	Res	Type	Atoms
2	B	5	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6

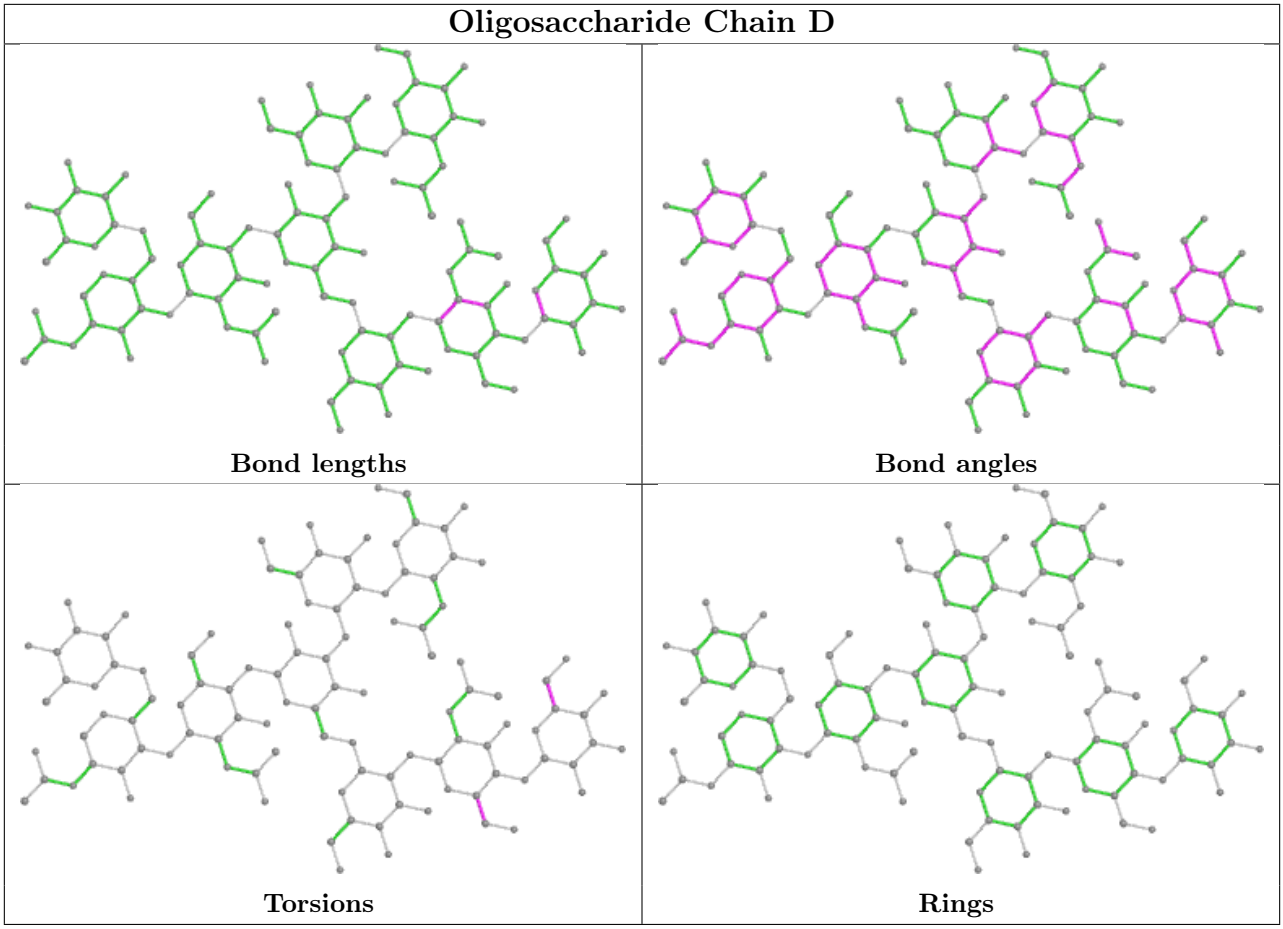
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7	BMA	1	0
2	D	3	BMA	2	0
2	B	8	NAG	1	0
2	D	2	NAG	1	0
2	D	9	FUC	1	0
2	D	5	NAG	3	0
2	D	7	BMA	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)

There are no ligands in this entry.

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, 95^{th} 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	208/227 (91%)	0.46	9 (4%) 35 38	29, 44, 94, 109	0
1	C	207/227 (91%)	1.19	46 (22%) 0 0	35, 67, 124, 152	0
All	All	415/454 (91%)	0.83	55 (13%) 3 3	29, 54, 109, 152	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	TYR	10.0
1	C	298	SER	7.4
1	C	330	ALA	6.2
1	C	323	VAL	5.6
1	C	273	VAL	5.5
1	C	358	LEU	5.3
1	C	326	LYS	5.2
1	C	328	LEU	5.1
1	A	355	ARG	5.0
1	C	278	TYR	5.0
1	C	302	VAL	4.8
1	C	324	SER	4.8
1	C	272	GLU	4.6
1	C	239	SER	4.5
1	A	358	LEU	4.4
1	C	268	HIS	4.3
1	C	331	PRO	4.1
1	C	300	TYR	4.1
1	C	299	THR	4.1
1	C	274	LYS	3.8
1	C	262	VAL	3.8
1	C	294	GLU	3.4
1	C	266	VAL	3.3
1	C	279	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	303	VAL	3.3
1	C	329	PRO	3.2
1	C	291	PRO	3.1
1	C	288	LYS	3.1
1	C	295	GLN	3.1
1	C	301	ARG	3.0
1	C	240	VAL	3.0
1	A	443	LEU	3.0
1	A	418	GLN	2.9
1	C	293	GLU	2.9
1	C	355	ARG	2.9
1	C	305	VAL	2.9
1	C	275	PHE	2.9
1	C	269	GLU	2.8
1	C	271	PRO	2.8
1	C	282	VAL	2.6
1	C	322	LYS	2.6
1	A	422	VAL	2.5
1	C	283	GLU	2.4
1	C	420	GLY	2.3
1	A	359	THR	2.3
1	C	284	VAL	2.3
1	A	362	GLN	2.2
1	C	264	VAL	2.2
1	A	417	TRP	2.1
1	C	260	THR	2.1
1	A	354	CYS	2.1
1	C	256	THR	2.0
1	C	327	ALA	2.0
1	C	321	CYS	2.0
1	C	386	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	NAG	D	8	14/15	0.70	0.26	109,116,121,128	0
2	NAG	D	1	14/15	0.72	0.19	107,123,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	8	14/15	0.77	0.20	85,91,99,103	0
2	NAG	D	2	14/15	0.83	0.13	87,121,126,128	0
2	NAG	D	5	14/15	0.86	0.20	76,87,91,99	0
2	GAL	D	6	11/12	0.91	0.15	63,67,84,85	0
2	GAL	B	6	11/12	0.94	0.11	33,38,43,53	0
2	NAG	B	1	14/15	0.95	0.10	36,40,49,50	0
2	NAG	B	5	14/15	0.97	0.11	35,39,48,50	0
2	NAG	B	2	14/15	0.97	0.10	31,36,45,47	0

6.3 Carbohydrates (i)

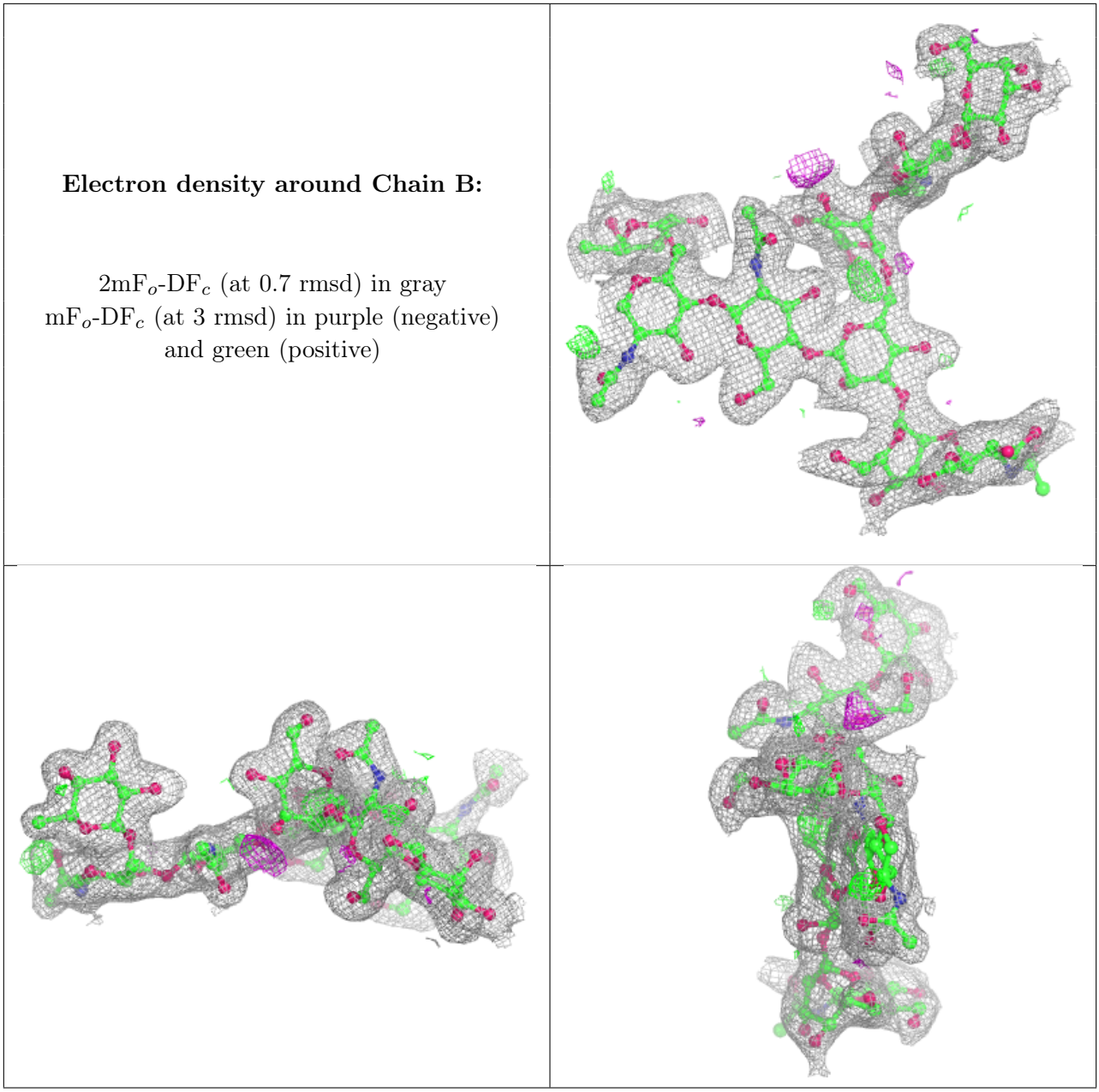
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	8	14/15	0.70	0.26	109,116,121,128	0
2	BMA	D	7	11/12	0.72	0.24	95,113,119,129	0
2	NAG	D	1	14/15	0.72	0.19	107,123,137,137	0
2	FUC	D	9	10/11	0.72	0.40	121,132,138,141	0
2	NAG	B	8	14/15	0.77	0.20	85,91,99,103	0
2	BMA	D	3	11/12	0.78	0.16	88,106,112,115	0
2	NAG	D	2	14/15	0.83	0.13	87,121,126,128	0
2	BMA	D	4	11/12	0.84	0.14	85,96,101,108	0
2	NAG	D	5	14/15	0.86	0.20	76,87,91,99	0
2	BMA	B	7	11/12	0.90	0.12	59,66,83,85	0
2	GAL	D	6	11/12	0.91	0.15	63,67,84,85	0
2	FUC	B	9	10/11	0.93	0.07	37,46,49,51	0
2	BMA	B	3	11/12	0.94	0.11	36,42,53,55	0
2	GAL	B	6	11/12	0.94	0.11	33,38,43,53	0
2	BMA	B	4	11/12	0.95	0.09	38,40,47,53	0
2	NAG	B	1	14/15	0.95	0.10	36,40,49,50	0
2	NAG	B	5	14/15	0.97	0.11	35,39,48,50	0
2	NAG	B	2	14/15	0.97	0.10	31,36,45,47	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.

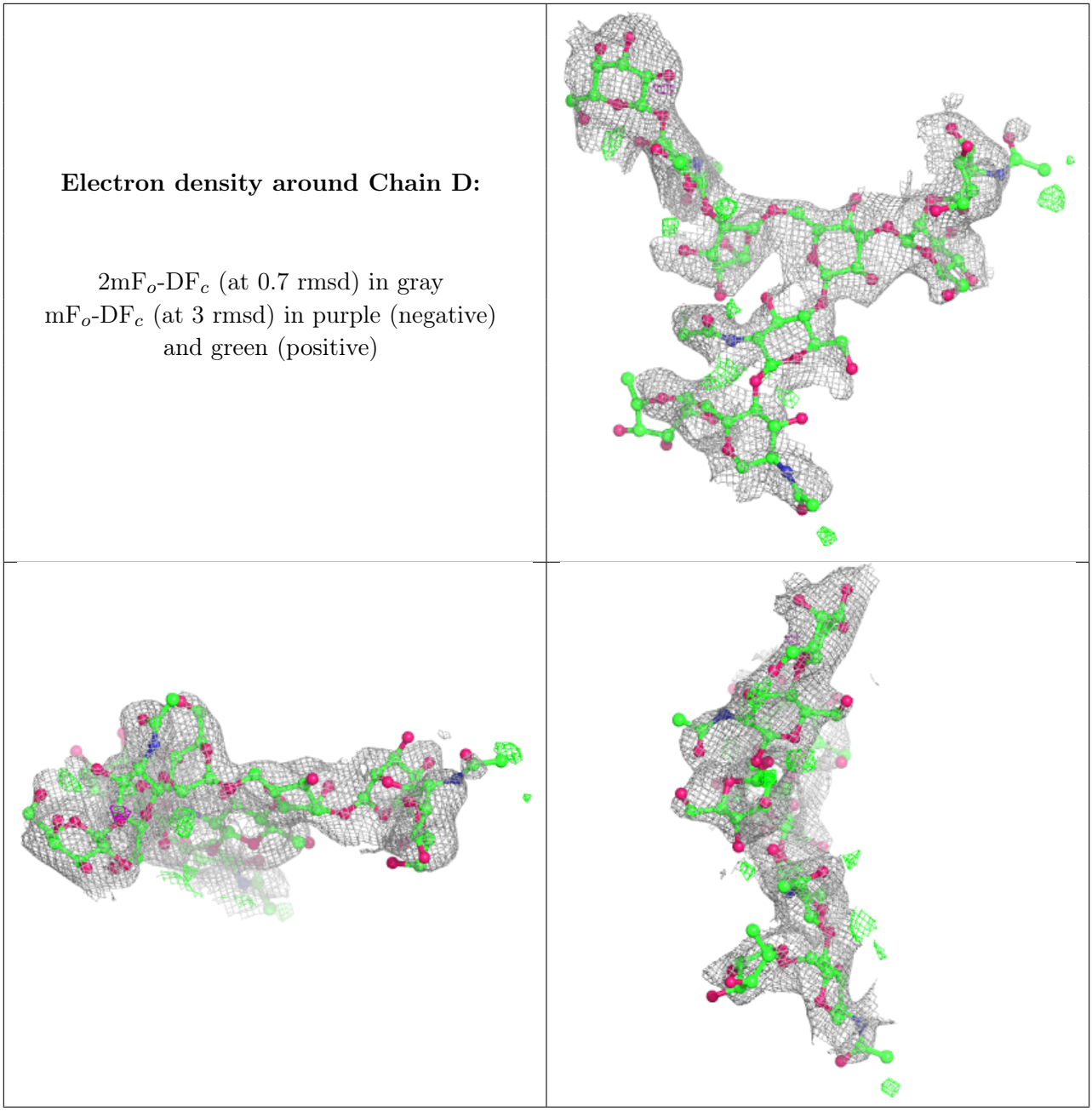
Electron density around Chain B:

$2mF_o$-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 D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.