



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:23 AM BST

PDB ID : 5YC5
Title : Crystal structure of human IgG-Fc in complex with aglycan and optimized Fc gamma receptor IIIa
Authors : Caaveiro, J.M.M.; Tamura, H.; Tsumoto, K.; Kiyoshi, M.
Deposited on : 2017-09-06
Resolution : 2.71 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

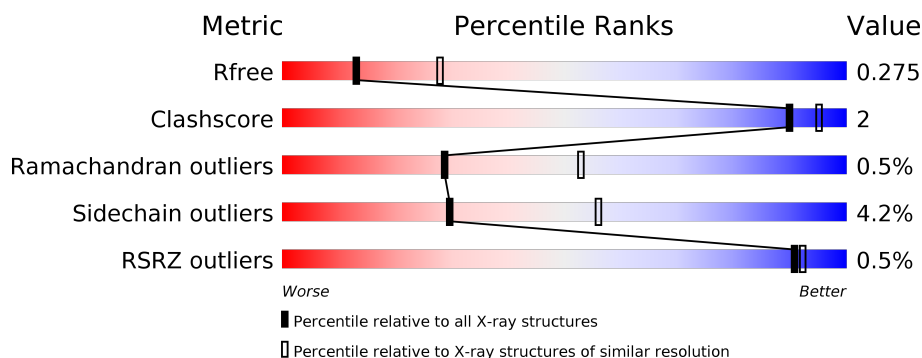
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	223	
1	B	223	
2	C	182	
3	D	9	
4	E	8	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4995 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1684	1073	283	322	6			
1	B	213	Total	C	N	O	S	0	0	0
			1700	1083	285	326	6			

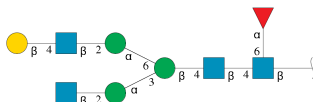
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1366	859	238	265	4			

There are 17 discrepancies between the modelled and reference sequences:

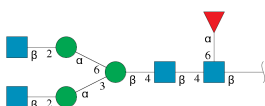
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	GLU	VAL	engineered mutation	UNP P08637
C	11	ILE	PHE	engineered mutation	UNP P08637
C	17	ASN	TYR	engineered mutation	UNP P08637
C	30	ARG	GLN	engineered mutation	UNP P08637
C	57	LEU	PHE	engineered mutation	UNP P08637
C	74	SER	ASN	engineered mutation	UNP P08637
C	99	GLU	VAL	engineered mutation	UNP P08637
C	103	GLY	GLU	engineered mutation	UNP P08637
C	153	SER	PHE	engineered mutation	UNP P08637
C	158	VAL	PHE	variant	UNP P08637
C	176	GLY	-	expression tag	UNP P08637
C	177	HIS	-	expression tag	UNP P08637
C	178	HIS	-	expression tag	UNP P08637
C	179	HIS	-	expression tag	UNP P08637
C	180	HIS	-	expression tag	UNP P08637
C	181	HIS	-	expression tag	UNP P08637
C	182	HIS	-	expression tag	UNP P08637

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-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
3	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
4	E	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	10	Total	O	0	0
			10	10		
6	C	7	Total	O	0	0
			7	7		

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: Immunoglobulin gamma-1 heavy chain

Chain A: 




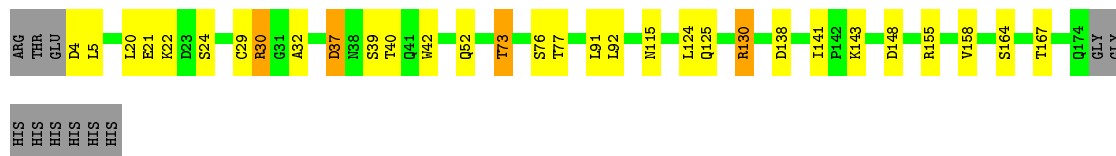
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain B: 




- Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C: 

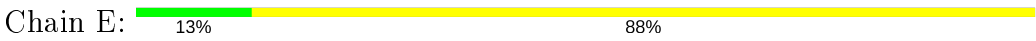


- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



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



MAG1
MAG2
ENC3
MAG4
MAG5
MAG6
MAG7
F008

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.79Å 101.42Å 122.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.71 46.89 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.90-2.71) 100.0 (46.89-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.209 , 0.273 0.214 , 0.275	Depositor DCC
R_{free} test set	1260 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, GAL, FUC, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/1730	0.96	3/2357 (0.1%)
1	B	0.79	0/1747	0.92	1/2380 (0.0%)
2	C	0.84	0/1400	0.95	4/1902 (0.2%)
All	All	0.82	0/4877	0.94	8/6639 (0.1%)

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
2	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	130	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	138	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	416	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	234	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	255	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	355	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	C	30	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	C	37	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	76	SER	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	1684	0	1655	3	0
1	B	1700	0	1669	4	0
2	C	1366	0	1317	11	0
3	D	110	0	94	2	0
4	E	99	0	85	0	0
5	A	1	0	0	0	0
6	A	18	0	0	0	0
6	B	10	0	0	0	0
6	C	7	0	0	0	0
All	All	4995	0	4820	18	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 2.

All (18) 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:C:20:LEU:HD21	2:C:92:LEU:HB2	1.78	0.64
1:B:272:GLU:O	1:B:325:ASN:ND2	2.33	0.59
2:C:155:ARG:HB3	2:C:164:SER:HB3	1.89	0.54
2:C:4:ASP:OD1	2:C:5:LEU:N	2.43	0.52
2:C:37:ASP:OD1	2:C:39:SER:OG	2.27	0.50
2:C:91:LEU:HD12	2:C:164:SER:HA	1.95	0.48
1:B:406:LEU:HD12	1:B:406:LEU:C	2.34	0.48
2:C:32:ALA:O	2:C:73:THR:CG2	2.62	0.47
2:C:141:ILE:HG21	2:C:148:ASP:OD1	2.15	0.47
1:A:246:LYS:HG2	3:D:6:GAL:O4	2.16	0.46
2:C:29:CYS:HB2	2:C:42:TRP:CZ2	2.52	0.45
1:A:433:HIS:CD2	1:A:434:ASN:ND2	2.86	0.44
2:C:158:VAL:O	2:C:158:VAL:HG12	2.17	0.44
1:B:308:VAL:HG12	1:B:319:TYR:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:GLU:O	2:C:22:LYS:HB2	2.18	0.42
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.54	0.42
2:C:125:GLN:OE1	2:C:130:ARG:NH1	2.44	0.41
1:A:334:LYS:HE3	3:D:8:NAG:H82	2.02	0.41

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	209/223 (94%)	203 (97%)	4 (2%)	2 (1%)	15	35
1	B	211/223 (95%)	200 (95%)	11 (5%)	0	100	100
2	C	169/182 (93%)	166 (98%)	2 (1%)	1 (1%)	25	48
All	All	589/628 (94%)	569 (97%)	17 (3%)	3 (0%)	29	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
2	C	77	THR
1	A	271	PRO

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	196/206 (95%)	190 (97%)	6 (3%)	40	68
1	B	198/206 (96%)	190 (96%)	8 (4%)	31	58
2	C	154/163 (94%)	145 (94%)	9 (6%)	20	42
All	All	548/575 (95%)	525 (96%)	23 (4%)	30	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LYS
1	A	298	SER
1	A	326	LYS
1	A	340	LYS
1	A	375	SER
1	A	418	GLN
1	B	254	SER
1	B	272	GLU
1	B	298	SER
1	B	376	ASP
1	B	389	ASN
1	B	424	SER
1	B	440	SER
1	B	444	SER
2	C	24	SER
2	C	30	ARG
2	C	40	THR
2	C	52	GLN
2	C	73	THR
2	C	115	ASN
2	C	124	LEU
2	C	143	LYS
2	C	167	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	386	GLN
1	A	390	ASN
1	A	434	ASN
1	B	386	GLN
1	B	434	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	15	GLN
2	C	52	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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
3	FUC	D	9	3	10,10,11	1.14	0	14,14,16	2.59	5 (35%)
3	NAG	D	8	3	14,14,15	1.30	1 (7%)	17,19,21	1.65	5 (29%)
3	MAN	D	7	3	11,11,12	0.61	0	15,15,17	2.29	3 (20%)
4	FUC	E	8	4	10,10,11	0.86	0	14,14,16	1.56	3 (21%)
4	MAN	E	6	4	11,11,12	0.68	0	15,15,17	1.62	3 (20%)
4	NAG	E	7	4	14,14,15	0.40	0	17,19,21	1.55	4 (23%)
3	GAL	D	6	3	11,11,12	1.54	4 (36%)	15,15,17	2.16	5 (33%)
3	NAG	D	2	3	14,14,15	0.61	0	17,19,21	0.90	0
4	NAG	E	1	1,4	14,14,15	0.67	0	17,19,21	1.13	0
4	NAG	E	5	4	14,14,15	0.67	0	17,19,21	1.55	4 (23%)
3	NAG	D	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	1.80	3 (17%)
3	MAN	D	4	3	11,11,12	0.59	0	15,15,17	2.03	5 (33%)
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	1.98	3 (20%)
3	NAG	D	5	3	14,14,15	0.94	0	17,19,21	2.68	8 (47%)
4	NAG	E	2	4	14,14,15	1.00	1 (7%)	17,19,21	1.40	3 (17%)

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	FUC	D	9	3	-	-	0/1/1/1
3	NAG	D	8	3	-	3/6/23/26	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
4	FUC	E	8	4	-	-	0/1/1/1
4	MAN	E	6	4	-	1/2/19/22	0/1/1/1
4	NAG	E	7	4	-	0/6/23/26	0/1/1/1
3	GAL	D	6	3	-	2/2/19/22	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	5	4	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GAL	C1-C2	2.80	1.58	1.52
3	D	6	GAL	C2-C3	2.14	1.55	1.52
3	D	1	NAG	O4-C4	2.12	1.48	1.43
3	D	6	GAL	O2-C2	2.12	1.47	1.43
3	D	6	GAL	O5-C1	2.11	1.47	1.43
4	E	2	NAG	O5-C1	-2.09	1.40	1.43
3	D	8	NAG	C3-C2	2.06	1.56	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	MAN	O5-C1-C2	-7.01	99.95	110.77
3	D	9	FUC	C3-C4-C5	6.51	119.91	109.77
3	D	5	NAG	C8-C7-N2	6.29	126.75	116.10
3	D	6	GAL	O5-C5-C6	5.35	115.59	107.20
4	E	4	MAN	C1-C2-C3	5.17	116.02	109.67
3	D	1	NAG	C1-C2-N2	5.07	119.15	110.49
3	D	4	MAN	C1-C2-C3	4.69	115.44	109.67
3	D	5	NAG	O7-C7-N2	-4.37	113.91	121.95
3	D	9	FUC	O4-C4-C3	-4.07	100.95	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	GAL	O5-C1-C2	3.68	116.46	110.77
4	E	4	MAN	O4-C4-C3	-3.54	102.18	110.35
3	D	5	NAG	O4-C4-C3	-3.49	102.27	110.35
3	D	9	FUC	O5-C1-C2	3.47	116.12	110.77
4	E	8	FUC	C3-C4-C5	3.31	114.93	109.77
3	D	9	FUC	O2-C2-C1	3.22	115.73	109.15
3	D	8	NAG	C2-N2-C7	3.17	127.41	122.90
3	D	4	MAN	O2-C2-C3	-3.14	103.85	110.14
3	D	4	MAN	C6-C5-C4	-3.11	105.71	113.00
3	D	7	MAN	O4-C4-C3	-3.09	103.20	110.35
4	E	7	NAG	C3-C4-C5	-3.07	104.76	110.24
4	E	6	MAN	O2-C2-C1	2.99	115.27	109.15
3	D	6	GAL	C1-O5-C5	2.96	116.20	112.19
3	D	6	GAL	O2-C2-C1	2.92	115.12	109.15
3	D	5	NAG	O5-C5-C6	-2.86	102.72	107.20
3	D	7	MAN	O3-C3-C4	-2.84	103.79	110.35
4	E	4	MAN	O2-C2-C3	-2.83	104.46	110.14
3	D	1	NAG	C1-O5-C5	2.79	115.97	112.19
4	E	6	MAN	O2-C2-C3	-2.71	104.70	110.14
3	D	5	NAG	C1-C2-N2	2.64	115.00	110.49
3	D	5	NAG	C4-C3-C2	-2.64	107.14	111.02
3	D	5	NAG	C1-O5-C5	-2.62	108.64	112.19
4	E	2	NAG	C2-N2-C7	2.60	126.61	122.90
4	E	5	NAG	O5-C1-C2	2.56	115.33	111.29
4	E	5	NAG	O3-C3-C4	2.55	116.23	110.35
3	D	5	NAG	C3-C4-C5	2.51	114.72	110.24
4	E	7	NAG	O4-C4-C3	2.44	115.99	110.35
4	E	7	NAG	O5-C1-C2	-2.35	107.57	111.29
4	E	8	FUC	O5-C1-C2	2.35	114.39	110.77
4	E	2	NAG	O7-C7-N2	2.34	126.26	121.95
3	D	8	NAG	O3-C3-C2	2.34	114.31	109.47
3	D	8	NAG	O7-C7-C8	-2.34	117.72	122.06
3	D	9	FUC	O5-C5-C4	2.29	113.63	109.52
4	E	2	NAG	O5-C1-C2	-2.25	107.73	111.29
3	D	6	GAL	O5-C5-C4	-2.25	105.36	110.83
3	D	1	NAG	O4-C4-C5	2.23	114.82	109.30
4	E	8	FUC	O5-C5-C6	2.22	112.10	107.33
4	E	5	NAG	O3-C3-C2	-2.13	105.06	109.47
4	E	5	NAG	C4-C3-C2	-2.10	107.93	111.02
3	D	8	NAG	C6-C5-C4	2.10	117.92	113.00
3	D	4	MAN	O5-C5-C6	2.07	110.46	107.20
3	D	8	NAG	O5-C5-C6	2.06	110.44	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	O3-C3-C4	-2.04	105.63	110.35
4	E	6	MAN	O6-C6-C5	-2.03	104.33	111.29
4	E	7	NAG	O5-C5-C4	-2.01	105.95	110.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	8	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
3	D	6	GAL	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	6	GAL	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	8	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	MAN	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	5	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	NAG	1	0
3	D	6	GAL	1	0

5.5 Carbohydrates

17 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	D	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	1.80	3 (17%)
3	NAG	D	2	3	14,14,15	0.61	0	17,19,21	0.90	0
3	BMA	D	3	3	11,11,12	0.85	0	15,15,17	1.72	3 (20%)
3	MAN	D	4	3	11,11,12	0.59	0	15,15,17	2.03	5 (33%)
3	NAG	D	5	3	14,14,15	0.94	0	17,19,21	2.68	8 (47%)
3	GAL	D	6	3	11,11,12	1.54	4 (36%)	15,15,17	2.16	5 (33%)
3	MAN	D	7	3	11,11,12	0.61	0	15,15,17	2.29	3 (20%)
3	NAG	D	8	3	14,14,15	1.30	1 (7%)	17,19,21	1.65	5 (29%)
3	FUC	D	9	3	10,10,11	1.14	0	14,14,16	2.59	5 (35%)
4	NAG	E	1	1,4	14,14,15	0.67	0	17,19,21	1.13	0
4	NAG	E	2	4	14,14,15	1.00	1 (7%)	17,19,21	1.40	3 (17%)
4	BMA	E	3	4	11,11,12	0.89	1 (9%)	15,15,17	1.04	1 (6%)
4	MAN	E	4	4	11,11,12	0.65	0	15,15,17	1.98	3 (20%)
4	NAG	E	5	4	14,14,15	0.67	0	17,19,21	1.55	4 (23%)
4	MAN	E	6	4	11,11,12	0.68	0	15,15,17	1.62	3 (20%)
4	NAG	E	7	4	14,14,15	0.40	0	17,19,21	1.55	4 (23%)
4	FUC	E	8	4	10,10,11	0.86	0	14,14,16	1.56	3 (21%)

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	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	3/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	NAG	E	5	4	-	2/6/23/26	0/1/1/1
4	MAN	E	6	4	-	1/2/19/22	0/1/1/1
4	NAG	E	7	4	-	0/6/23/26	0/1/1/1
4	FUC	E	8	4	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GAL	C1-C2	2.80	1.58	1.52
4	E	3	BMA	O5-C1	-2.22	1.40	1.43
3	D	6	GAL	C2-C3	2.14	1.55	1.52
3	D	1	NAG	O4-C4	2.12	1.48	1.43
3	D	6	GAL	O2-C2	2.12	1.47	1.43
3	D	6	GAL	O5-C1	2.11	1.47	1.43
4	E	2	NAG	O5-C1	-2.09	1.40	1.43
3	D	8	NAG	C3-C2	2.06	1.56	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	MAN	O5-C1-C2	-7.01	99.95	110.77
3	D	9	FUC	C3-C4-C5	6.51	119.91	109.77
3	D	5	NAG	C8-C7-N2	6.29	126.75	116.10
3	D	6	GAL	O5-C5-C6	5.35	115.59	107.20
4	E	4	MAN	C1-C2-C3	5.17	116.02	109.67
3	D	1	NAG	C1-C2-N2	5.07	119.15	110.49
3	D	4	MAN	C1-C2-C3	4.69	115.44	109.67
3	D	5	NAG	O7-C7-N2	-4.37	113.91	121.95
3	D	9	FUC	O4-C4-C3	-4.07	100.95	110.35
3	D	3	BMA	C1-C2-C3	3.91	114.47	109.67
3	D	6	GAL	O5-C1-C2	3.68	116.46	110.77
4	E	4	MAN	O4-C4-C3	-3.54	102.18	110.35
3	D	5	NAG	O4-C4-C3	-3.49	102.27	110.35
3	D	9	FUC	O5-C1-C2	3.47	116.12	110.77
4	E	8	FUC	C3-C4-C5	3.31	114.93	109.77
3	D	9	FUC	O2-C2-C1	3.22	115.73	109.15
3	D	8	NAG	C2-N2-C7	3.17	127.41	122.90
3	D	4	MAN	O2-C2-C3	-3.14	103.85	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C6-C5-C4	-3.11	105.71	113.00
3	D	7	MAN	O4-C4-C3	-3.09	103.20	110.35
4	E	7	NAG	C3-C4-C5	-3.07	104.76	110.24
4	E	6	MAN	O2-C2-C1	2.99	115.27	109.15
3	D	6	GAL	C1-O5-C5	2.96	116.20	112.19
3	D	6	GAL	O2-C2-C1	2.92	115.12	109.15
3	D	5	NAG	O5-C5-C6	-2.86	102.72	107.20
3	D	7	MAN	O3-C3-C4	-2.84	103.79	110.35
4	E	4	MAN	O2-C2-C3	-2.83	104.46	110.14
3	D	1	NAG	C1-O5-C5	2.79	115.97	112.19
4	E	6	MAN	O2-C2-C3	-2.71	104.70	110.14
3	D	5	NAG	C1-C2-N2	2.64	115.00	110.49
3	D	5	NAG	C4-C3-C2	-2.64	107.14	111.02
3	D	5	NAG	C1-O5-C5	-2.62	108.64	112.19
4	E	2	NAG	C2-N2-C7	2.60	126.61	122.90
4	E	3	BMA	O3-C3-C2	-2.56	105.09	109.99
4	E	5	NAG	O5-C1-C2	2.56	115.33	111.29
4	E	5	NAG	O3-C3-C4	2.55	116.23	110.35
3	D	5	NAG	C3-C4-C5	2.51	114.72	110.24
4	E	7	NAG	O4-C4-C3	2.44	115.99	110.35
4	E	7	NAG	O5-C1-C2	-2.35	107.57	111.29
4	E	8	FUC	O5-C1-C2	2.35	114.39	110.77
4	E	2	NAG	O7-C7-N2	2.34	126.26	121.95
3	D	8	NAG	O3-C3-C2	2.34	114.31	109.47
3	D	8	NAG	O7-C7-C8	-2.34	117.72	122.06
3	D	9	FUC	O5-C5-C4	2.29	113.63	109.52
4	E	2	NAG	O5-C1-C2	-2.25	107.73	111.29
3	D	6	GAL	O5-C5-C4	-2.25	105.36	110.83
3	D	1	NAG	O4-C4-C5	2.23	114.82	109.30
4	E	8	FUC	O5-C5-C6	2.22	112.10	107.33
4	E	5	NAG	O3-C3-C2	-2.13	105.06	109.47
4	E	5	NAG	C4-C3-C2	-2.10	107.93	111.02
3	D	8	NAG	C6-C5-C4	2.10	117.92	113.00
3	D	3	BMA	O6-C6-C5	-2.10	104.09	111.29
3	D	4	MAN	O5-C5-C6	2.07	110.46	107.20
3	D	8	NAG	O5-C5-C6	2.06	110.44	107.20
3	D	4	MAN	O3-C3-C4	-2.04	105.63	110.35
4	E	6	MAN	O6-C6-C5	-2.03	104.33	111.29
4	E	7	NAG	O5-C5-C4	-2.01	105.95	110.83
3	D	3	BMA	C3-C4-C5	2.00	113.81	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

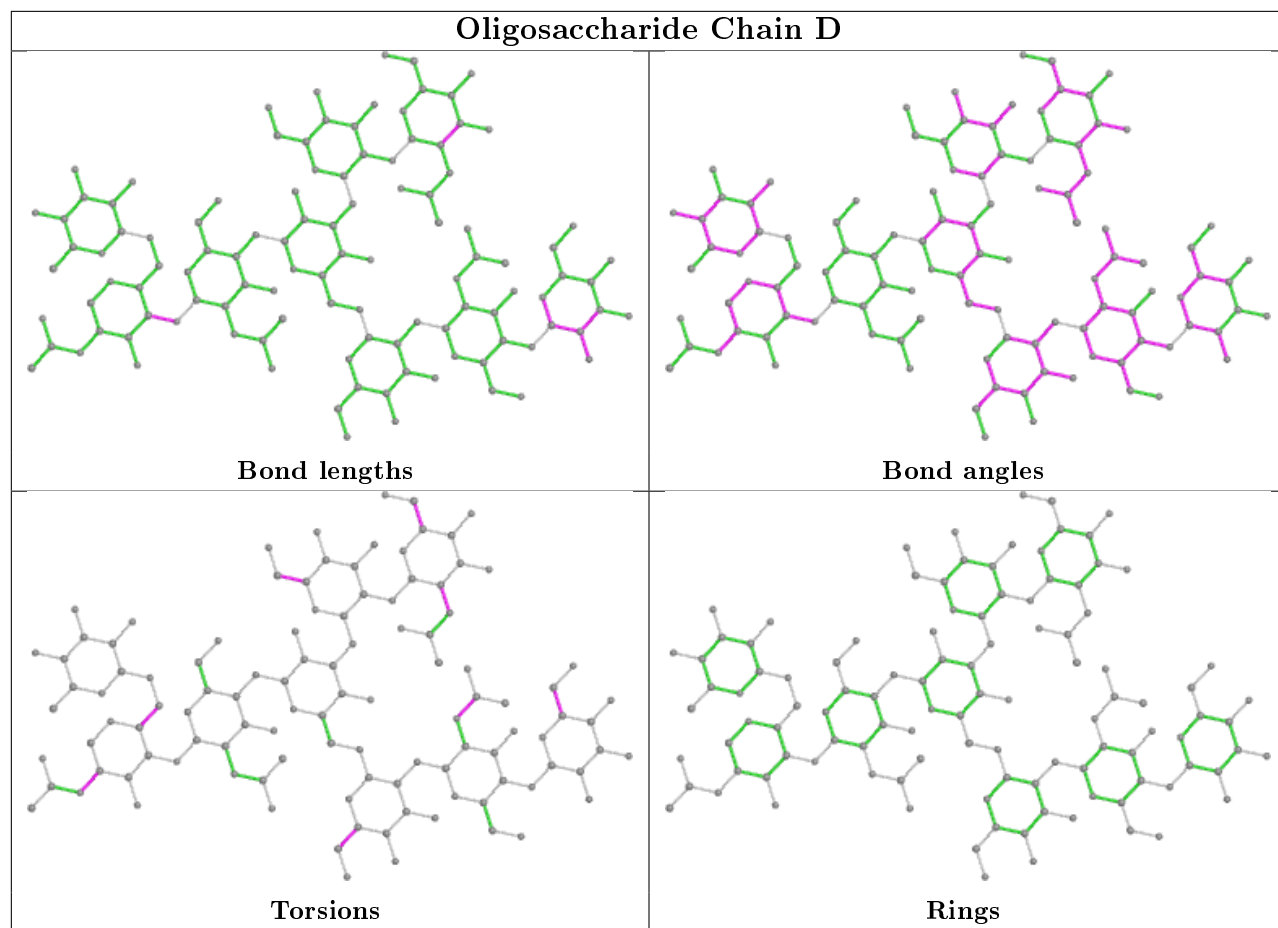
Mol	Chain	Res	Type	Atoms
3	D	8	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
3	D	6	GAL	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	6	GAL	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	8	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	MAN	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	5	NAG	C4-C5-C6-O6

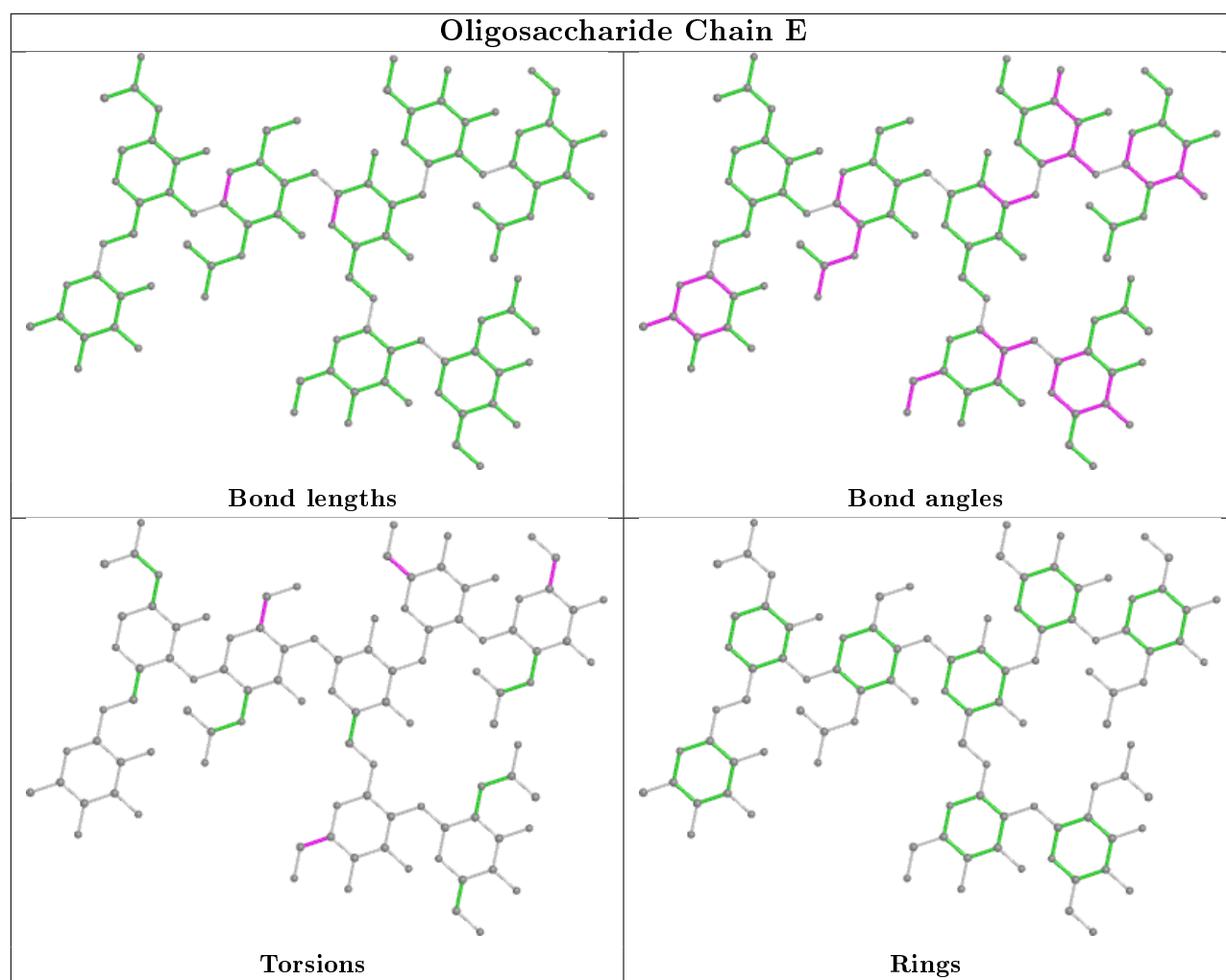
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	NAG	1	0
3	D	6	GAL	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	211/223 (94%)	-0.06	1 (0%) 91 92	36, 53, 76, 90	0
1	B	213/223 (95%)	-0.10	2 (0%) 84 85	38, 51, 78, 92	0
2	C	171/182 (93%)	-0.05	0 100 100	38, 54, 78, 107	0
All	All	595/628 (94%)	-0.07	3 (0%) 91 92	36, 53, 78, 107	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	3.1
1	B	389	ASN	2.6
1	A	234	LEU	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, 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
3	NAG	D	8	14/15	0.80	0.26	79,86,88,88	0
3	GAL	D	6	11/12	0.91	0.21	68,71,72,72	0
4	NAG	E	5	14/15	0.91	0.15	79,82,88,89	0
4	MAN	E	4	11/12	0.94	0.14	65,69,70,74	0
4	MAN	E	6	11/12	0.95	0.12	50,53,55,59	0
4	NAG	E	7	14/15	0.95	0.14	48,52,54,55	0
3	FUC	D	9	10/11	0.95	0.11	55,59,62,65	0
3	MAN	D	7	11/12	0.95	0.13	65,70,73,74	0
4	FUC	E	8	10/11	0.95	0.15	59,67,72,72	0
3	NAG	D	5	14/15	0.95	0.15	51,53,54,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	2	14/15	0.95	0.15	47,50,58,59	0
3	NAG	D	1	14/15	0.96	0.14	46,54,63,66	0
4	NAG	E	1	14/15	0.96	0.13	55,65,68,69	0
3	MAN	D	4	11/12	0.97	0.16	45,47,52,57	0
3	NAG	D	2	14/15	0.97	0.16	40,42,44,44	0

6.3 Carbohydrates

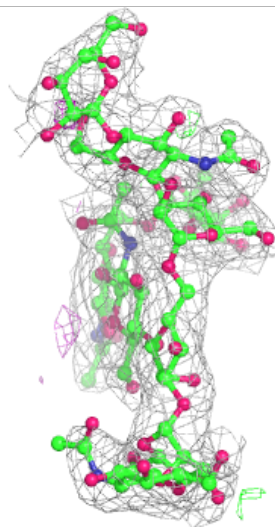
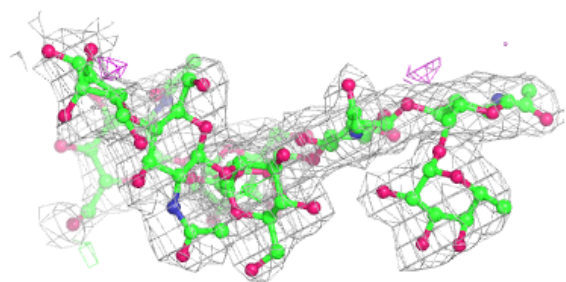
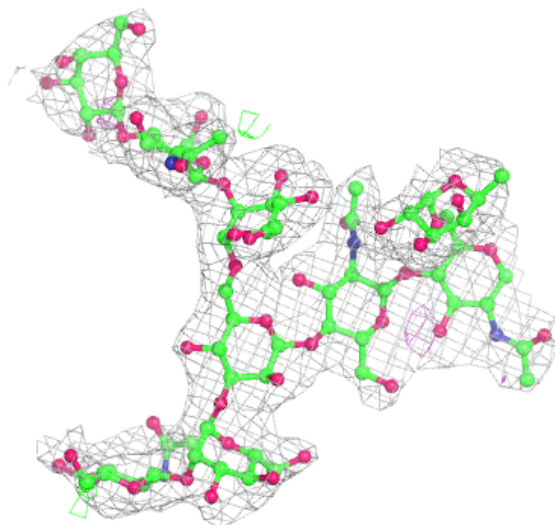
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

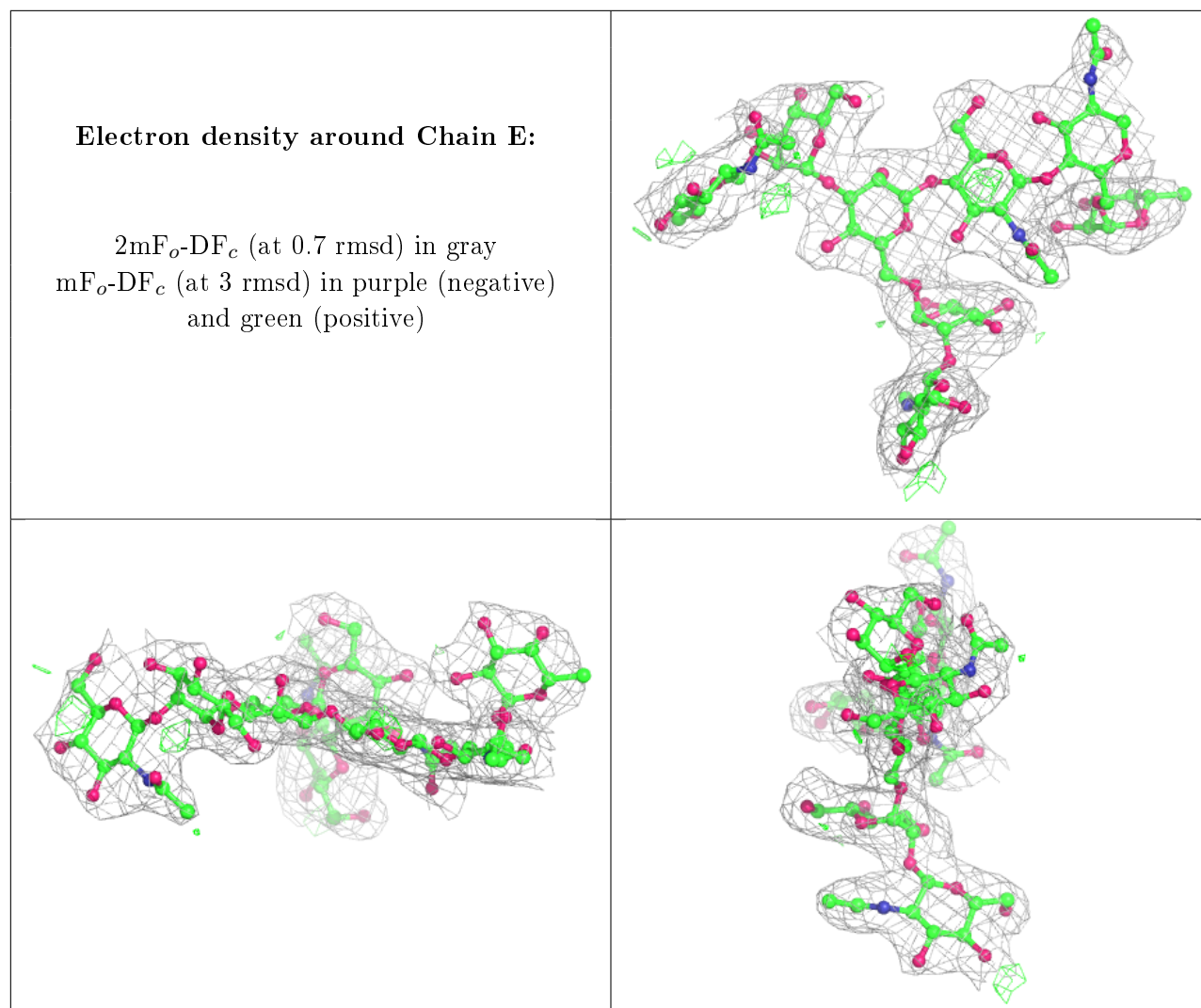
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	8	14/15	0.80	0.26	79,86,88,88	0
3	GAL	D	6	11/12	0.91	0.21	68,71,72,72	0
4	NAG	E	5	14/15	0.91	0.15	79,82,88,89	0
4	MAN	E	4	11/12	0.94	0.14	65,69,70,74	0
3	NAG	D	5	14/15	0.95	0.15	51,53,54,58	0
4	MAN	E	6	11/12	0.95	0.12	50,53,55,59	0
4	NAG	E	7	14/15	0.95	0.14	48,52,54,55	0
3	FUC	D	9	10/11	0.95	0.11	55,59,62,65	0
3	MAN	D	7	11/12	0.95	0.13	65,70,73,74	0
4	FUC	E	8	10/11	0.95	0.15	59,67,72,72	0
4	NAG	E	2	14/15	0.95	0.15	47,50,58,59	0
4	NAG	E	1	14/15	0.96	0.13	55,65,68,69	0
3	NAG	D	1	14/15	0.96	0.14	46,54,63,66	0
3	NAG	D	2	14/15	0.97	0.16	40,42,44,44	0
3	BMA	D	3	11/12	0.97	0.14	46,47,51,57	0
3	MAN	D	4	11/12	0.97	0.16	45,47,52,57	0
4	BMA	E	3	11/12	0.98	0.14	47,49,52,58	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)





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
5	CL	A	1012	1/1	0.92	0.09	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.