



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:01 AM UTC

PDB ID : 4X98 / pdb_00004x98
Title : Immunoglobulin Fc heterodimer variant
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Deposited on : 2014-12-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

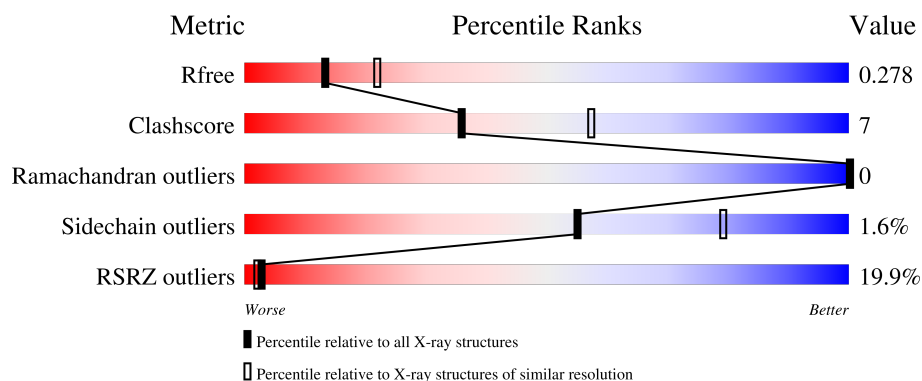
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	5% 86% 9% 5%
2	B	207	34% 82% 14% ..
3	C	8	50% 50%
3	D	8	88% 12%

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	FUC	C	8	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3542 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	0	0
			1669	1063	279	321	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLU	LYS	engineered mutation	UNP P01857
A	409	TRP	LYS	engineered mutation	UNP P01857

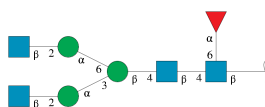
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1604	1019	274	305	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ARG	GLN	engineered mutation	UNP P01857
B	399	VAL	ASP	engineered mutation	UNP P01857
B	405	THR	PHE	engineered mutation	UNP P01857

- Molecule 3 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
3	C	8	Total 99	C 56	N 4	O 39	0	0	0
3	D	8	Total 99	C 56	N 4	O 39	0	0	0

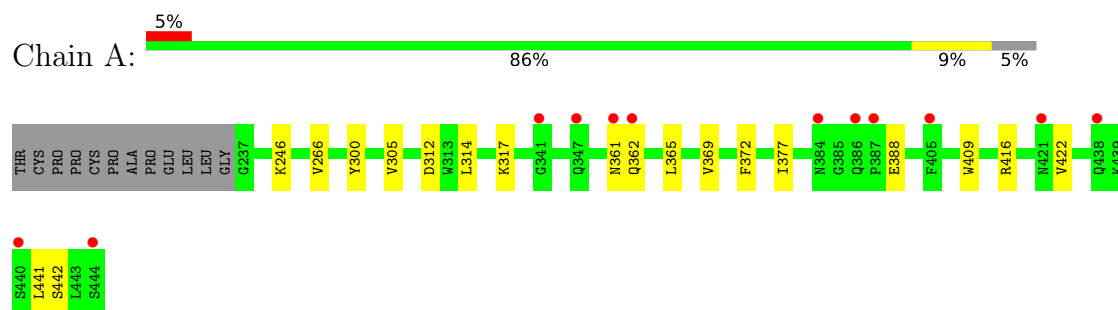
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total 47	O 47	0	0
4	B	24	Total 24	O 24	0	0

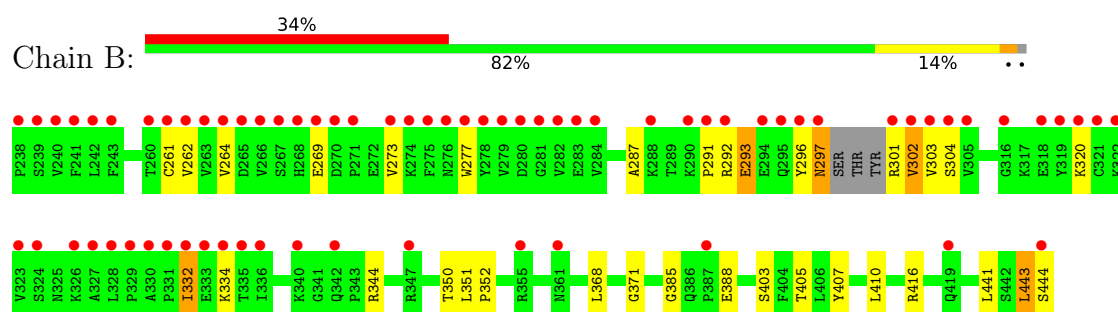
3 Residue-property plots

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

- Molecule 1: Ig gamma-1 chain C region



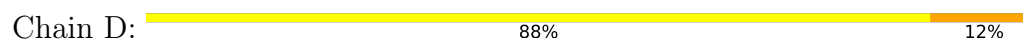
- Molecule 2: Ig gamma-1 chain C region



- Molecule 3: 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



- Molecule 3: 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
BMA3
MAN4
NAG5
MAN6
MAG7
FUC8

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.74Å 152.74Å 108.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.50 36.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.84-2.50) 95.5 (36.84-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.274 0.246 , 0.278	Depositor DCC
R_{free} test set	2000 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3542	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: NAG, BMA, MAN, FUC

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	0.65	0/1717	0.95	3/2343 (0.1%)
2	B	0.63	0/1645	0.97	2/2241 (0.1%)
All	All	0.64	0/3362	0.96	5/4584 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	264	VAL	N-CA-C	7.81	118.22	111.90
2	B	269	GLU	N-CA-C	-5.89	104.94	111.71
1	A	246	LYS	CA-C-N	5.40	124.86	119.24
1	A	246	LYS	C-N-CA	5.40	124.86	119.24
1	A	305	VAL	N-CA-C	5.17	115.29	107.80

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	1669	0	1619	11	0
2	B	1604	0	1578	23	0
3	C	99	0	82	12	0
3	D	99	0	85	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	47	0	0	1	0
4	B	24	0	0	1	0
All	All	3542	0	3364	50	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 7.

All (50) 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:296:TYR:O	2:B:297:ASN:HB3	1.53	1.09
3:C:1:NAG:H61	3:C:8:FUC:H5	1.36	1.07
3:C:4:MAN:C6	3:C:5:NAG:H83	1.98	0.93
3:C:4:MAN:O6	3:C:5:NAG:N2	2.00	0.93
3:C:4:MAN:H62	3:C:5:NAG:H83	1.53	0.89
3:D:1:NAG:H62	3:D:8:FUC:H5	1.54	0.87
2:B:292:ARG:C	2:B:293:GLU:HG2	2.02	0.84
3:C:1:NAG:H61	3:C:8:FUC:C5	2.07	0.84
2:B:291:PRO:O	2:B:293:GLU:HG2	1.87	0.74
2:B:371:GLY:H	2:B:405:THR:HG22	1.52	0.74
3:D:1:NAG:H62	3:D:8:FUC:C5	2.16	0.74
2:B:292:ARG:O	2:B:293:GLU:HG2	1.88	0.71
1:A:388:GLU:OE2	1:A:416:ARG:NH1	2.20	0.70
3:D:1:NAG:C6	3:D:8:FUC:H5	2.25	0.67
2:B:296:TYR:O	2:B:297:ASN:CB	2.38	0.65
3:C:1:NAG:C6	3:C:8:FUC:H5	2.22	0.63
2:B:350:THR:OG1	2:B:441:LEU:HB2	2.02	0.60
2:B:291:PRO:O	2:B:293:GLU:CG	2.49	0.59
3:C:5:NAG:O6	3:C:5:NAG:O4	2.17	0.56
3:D:1:NAG:C6	3:D:8:FUC:C5	2.85	0.54
1:A:369:VAL:HG12	1:A:372:PHE:CE1	2.43	0.54
2:B:262:VAL:HG22	2:B:303:VAL:HG22	1.91	0.52
2:B:344:ARG:NH1	2:B:403:SER:HB3	2.25	0.52
3:C:5:NAG:O7	3:C:5:NAG:H3	2.10	0.51
1:A:409:TRP:NE1	4:A:602:HOH:O	2.40	0.51
1:A:361:ASN:O	1:A:362:GLN:HG2	2.11	0.50
3:C:1:NAG:C6	3:C:8:FUC:C5	2.85	0.49
2:B:273:VAL:HG11	2:B:302:VAL:HG11	1.95	0.49
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.95	0.48
1:A:365:LEU:HB3	1:A:441:LEU:HD23	1.96	0.48
2:B:443:LEU:HD12	2:B:444:SER:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:372:PHE:CD1	2.51	0.46
2:B:261:CYS:HB2	2:B:277:TRP:CH2	2.51	0.44
2:B:334:LYS:HA	2:B:334:LYS:HD3	1.81	0.44
2:B:332:ILE:HD12	2:B:332:ILE:HA	1.82	0.44
1:A:422:VAL:HG22	1:A:442:SER:HB2	1.99	0.43
2:B:301:ARG:NH2	2:B:303:VAL:HG21	2.34	0.43
2:B:351:LEU:HA	2:B:352:PRO:HD3	1.84	0.43
2:B:388:GLU:HG2	2:B:410:LEU:HD11	2.00	0.43
3:C:4:MAN:C5	3:C:5:NAG:H83	2.48	0.43
2:B:368:LEU:HD13	2:B:407:TYR:CZ	2.54	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.78	0.42
2:B:388:GLU:CD	2:B:416:ARG:HH22	2.28	0.41
3:C:1:NAG:H61	3:C:8:FUC:H3	2.03	0.41
2:B:287:ALA:HB1	2:B:304:SER:OG	2.21	0.41
3:C:1:NAG:O5	3:C:8:FUC:H5	2.21	0.41
1:A:312:ASP:HB3	1:A:317:LYS:HD2	2.03	0.41
2:B:261:CYS:HB2	2:B:277:TRP:CZ2	2.56	0.41
2:B:385:GLY:N	4:B:602:HOH:O	2.53	0.41
1:A:369:VAL:HG11	1:A:377:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/220 (94%)	202 (98%)	4 (2%)	0	100	100
2	B	200/207 (97%)	194 (97%)	6 (3%)	0	100	100
All	All	406/427 (95%)	396 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/204 (95%)	194 (100%)	0	100	100
2	B	186/194 (96%)	180 (97%)	6 (3%)	34	62
All	All	380/398 (96%)	374 (98%)	6 (2%)	55	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	293	GLU
2	B	297	ASN
2	B	302	VAL
2	B	320	LYS
2	B	332	ILE
2	B	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
2	B	435	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 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	3,1	14,14,15	1.76	3 (21%)	17,19,21	2.83	4 (23%)
3	NAG	C	2	3	14,14,15	1.47	2 (14%)	17,19,21	1.39	3 (17%)
3	BMA	C	3	3	11,11,12	1.86	4 (36%)	15,15,17	1.77	5 (33%)
3	MAN	C	4	3	11,11,12	1.16	0	15,15,17	3.59	6 (40%)
3	NAG	C	5	3	14,14,15	0.51	0	17,19,21	1.70	4 (23%)
3	MAN	C	6	3	11,11,12	1.85	4 (36%)	15,15,17	1.64	2 (13%)
3	NAG	C	7	3	14,14,15	1.35	2 (14%)	17,19,21	1.62	5 (29%)
3	FUC	C	8	3	10,10,11	2.03	6 (60%)	14,14,16	1.54	3 (21%)
3	NAG	D	1	3,2	14,14,15	0.91	0	17,19,21	1.13	0
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
3	BMA	D	3	3	11,11,12	0.93	1 (9%)	15,15,17	1.28	2 (13%)
3	MAN	D	4	3	11,11,12	0.72	0	15,15,17	1.34	2 (13%)
3	NAG	D	5	3	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
3	MAN	D	6	3	11,11,12	0.82	0	15,15,17	1.50	2 (13%)
3	NAG	D	7	3	14,14,15	0.85	0	17,19,21	1.19	2 (11%)
3	FUC	D	8	3	10,10,11	1.17	1 (10%)	14,14,16	1.53	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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	NAG	C	7	3	-	2/6/23/26	0/1/1/1
3	FUC	C	8	3	-	-	0/1/1/1

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	-3.41	1.47	1.52
3	C	2	NAG	C1-C2	-3.12	1.48	1.52
3	C	1	NAG	C3-C2	-2.94	1.46	1.52
3	C	8	FUC	C4-C5	-2.91	1.46	1.52
3	C	3	BMA	O2-C2	-2.87	1.37	1.43
3	C	2	NAG	O5-C1	-2.84	1.38	1.43
3	C	6	MAN	O2-C2	-2.83	1.37	1.43
3	C	6	MAN	C4-C5	-2.80	1.47	1.53
3	C	8	FUC	O2-C2	-2.80	1.37	1.43
3	C	8	FUC	O5-C1	-2.77	1.39	1.43
3	C	3	BMA	O4-C4	-2.77	1.36	1.43
3	C	7	NAG	O4-C4	-2.66	1.36	1.43
3	C	6	MAN	O3-C3	-2.57	1.36	1.43
3	C	7	NAG	O3-C3	-2.46	1.36	1.43
3	C	3	BMA	C4-C5	-2.36	1.48	1.53
3	D	8	FUC	C4-C5	-2.33	1.47	1.52
3	C	3	BMA	C2-C3	-2.31	1.48	1.52
3	C	8	FUC	O5-C5	-2.27	1.39	1.43
3	C	8	FUC	O4-C4	-2.25	1.37	1.43
3	C	8	FUC	O3-C3	-2.22	1.37	1.43
3	C	1	NAG	O4-C4	-2.22	1.37	1.43
3	C	6	MAN	O5-C1	-2.17	1.40	1.43
3	D	3	BMA	C2-C3	-2.06	1.49	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	9.54	124.97	112.19
3	C	1	NAG	C1-O5-C5	8.09	123.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	O5-C5-C6	7.81	122.86	107.66
3	C	1	NAG	O5-C5-C6	-5.97	96.05	107.66
3	C	1	NAG	C6-C5-C4	-4.16	102.81	113.02
3	C	3	BMA	O3-C3-C2	-3.58	102.75	110.05
3	D	6	MAN	C3-C4-C5	-3.56	103.77	110.23
3	C	6	MAN	C1-O5-C5	3.34	116.67	112.19
3	C	5	NAG	C1-O5-C5	-3.17	107.94	112.19
3	C	2	NAG	C1-O5-C5	3.17	116.43	112.19
3	C	5	NAG	O5-C1-C2	-3.10	106.49	111.29
3	D	6	MAN	O5-C5-C6	3.03	113.57	107.66
3	D	4	MAN	O5-C5-C6	-2.99	101.84	107.66
3	D	8	FUC	C3-C4-C5	-2.96	105.32	109.81
3	C	7	NAG	C2-N2-C7	-2.95	118.95	122.90
3	D	2	NAG	O5-C1-C2	-2.92	106.77	111.29
3	C	4	MAN	C3-C4-C5	2.82	115.35	110.23
3	C	3	BMA	O2-C2-C3	-2.80	104.35	110.15
3	C	4	MAN	C2-C3-C4	2.80	115.78	110.86
3	C	5	NAG	O5-C5-C6	2.78	113.08	107.66
3	C	7	NAG	C1-C2-N2	-2.74	106.12	110.43
3	D	7	NAG	C2-N2-C7	-2.74	119.23	122.90
3	D	3	BMA	C1-C2-C3	-2.70	105.71	109.64
3	C	4	MAN	C6-C5-C4	-2.66	106.50	113.02
3	C	7	NAG	O5-C1-C2	-2.62	107.23	111.29
3	C	3	BMA	C1-O5-C5	2.61	115.68	112.19
3	C	4	MAN	O5-C1-C2	-2.61	104.57	110.79
3	C	7	NAG	C1-O5-C5	2.57	115.63	112.19
3	C	2	NAG	C6-C5-C4	-2.55	106.75	113.02
3	C	2	NAG	O5-C1-C2	-2.50	107.42	111.29
3	D	8	FUC	C6-C5-C4	-2.37	108.75	113.08
3	C	8	FUC	C6-C5-C4	-2.37	108.75	113.08
3	D	7	NAG	C1-O5-C5	2.35	115.33	112.19
3	C	5	NAG	C6-C5-C4	-2.28	107.43	113.02
3	C	8	FUC	C1-O5-C5	2.26	118.30	112.97
3	C	3	BMA	O5-C5-C4	-2.26	105.34	110.83
3	D	3	BMA	C1-O5-C5	2.25	115.20	112.19
3	C	8	FUC	O5-C5-C4	-2.22	105.55	109.55
3	C	6	MAN	O3-C3-C4	-2.22	105.14	110.38
3	C	1	NAG	O3-C3-C2	-2.21	104.80	109.40
3	D	8	FUC	O4-C4-C5	-2.15	105.00	109.74
3	C	3	BMA	C3-C4-C5	-2.14	106.35	110.23
3	C	7	NAG	C3-C4-C5	-2.13	106.36	110.23
3	D	5	NAG	O5-C1-C2	-2.11	108.03	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	O2-C2-C3	-2.02	105.96	110.15
3	D	8	FUC	O5-C5-C4	-2.01	105.93	109.55

There are no chirality outliers.

All (18) torsion outliers are listed below:

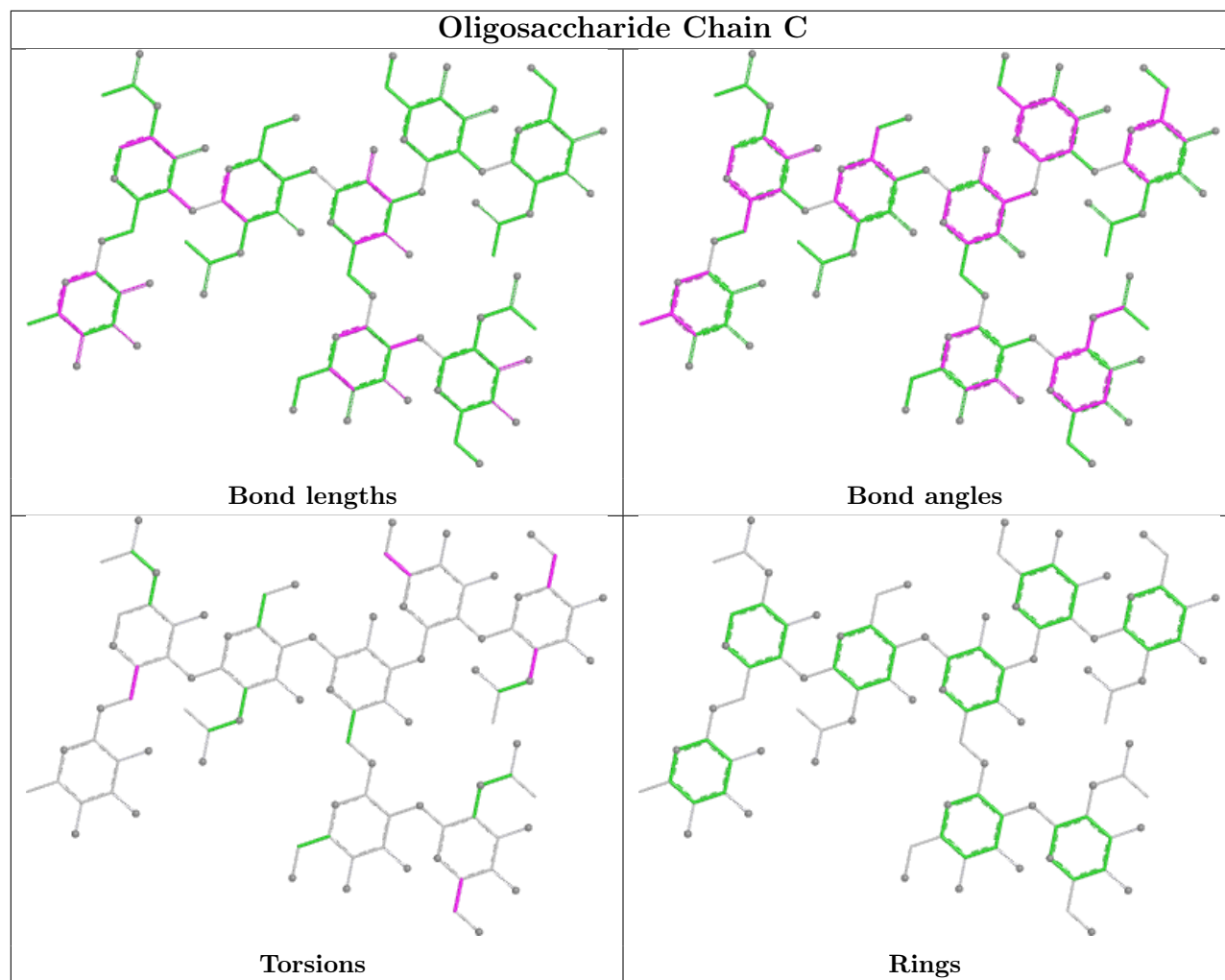
Mol	Chain	Res	Type	Atoms
3	C	5	NAG	C3-C2-N2-C7
3	D	5	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6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

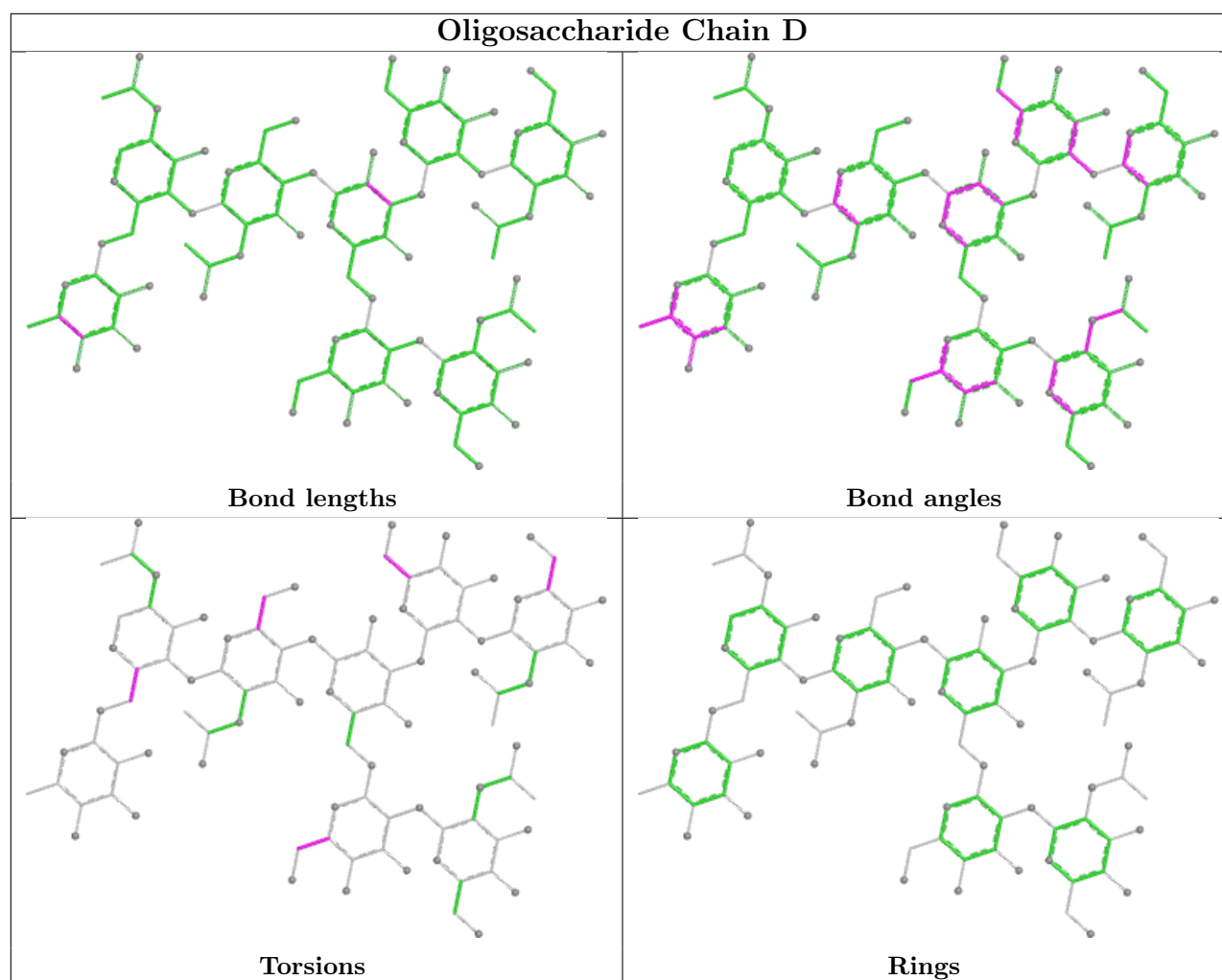
There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	8	FUC	6	0
3	C	1	NAG	6	0
3	D	1	NAG	4	0
3	D	8	FUC	4	0
3	C	5	NAG	6	0
3	C	4	MAN	4	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, 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	208/220 (94%)	0.37	12 (5%) 29 25	39, 52, 80, 95	0
2	B	204/207 (98%)	1.63	70 (34%) 1 1	25, 69, 118, 135	0
All	All	412/427 (96%)	0.99	82 (19%) 3 2	25, 58, 110, 135	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	10.8
2	B	297	ASN	9.4
2	B	332	ILE	8.3
2	B	296	TYR	7.7
2	B	240	VAL	6.9
2	B	241	PHE	6.3
2	B	263	VAL	5.9
2	B	271	PRO	5.8
2	B	330	ALA	5.7
2	B	295	GLN	5.4
2	B	273	VAL	5.3
2	B	331	PRO	5.0
2	B	329	PRO	4.8
2	B	268	HIS	4.8
2	B	262	VAL	4.7
2	B	323	VAL	4.7
2	B	303	VAL	4.6
2	B	266	VAL	4.6
2	B	238	PRO	4.3
2	B	336	ILE	4.2
2	B	243	PHE	4.2
2	B	324	SER	4.1
2	B	294	GLU	4.1
2	B	328	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	335	THR	4.0
2	B	282	VAL	3.8
2	B	239	SER	3.7
2	B	260	THR	3.6
2	B	281	GLY	3.6
2	B	291	PRO	3.6
2	B	242	LEU	3.6
2	B	264	VAL	3.5
2	B	275	PHE	3.5
2	B	304	SER	3.4
2	B	274	LYS	3.3
2	B	267	SER	3.2
2	B	270	ASP	3.2
2	B	320	LYS	3.2
2	B	277	TRP	3.2
2	B	278	TYR	3.2
2	B	319	TYR	3.1
2	B	292	ARG	3.0
2	B	301	ARG	3.0
1	A	444	SER	3.0
2	B	444	SER	3.0
2	B	283	GLU	2.9
2	B	269	GLU	2.9
2	B	333	GLU	2.8
1	A	341	GLY	2.8
2	B	321	CYS	2.8
2	B	347	ARG	2.7
2	B	280	ASP	2.7
2	B	290	LYS	2.7
2	B	318	GLU	2.7
2	B	322	LYS	2.6
1	A	362	GLN	2.6
2	B	279	VAL	2.6
2	B	261	CYS	2.6
2	B	334	LYS	2.6
2	B	265	ASP	2.5
1	A	361	ASN	2.5
2	B	327	ALA	2.5
2	B	419	GLN	2.5
2	B	326	LYS	2.4
2	B	387	PRO	2.4
1	A	421	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	342	GLN	2.3
1	A	387	PRO	2.3
1	A	405	PHE	2.3
1	A	440	SER	2.2
1	A	384	ASN	2.2
1	A	386	GLN	2.2
2	B	316	GLY	2.2
2	B	305	VAL	2.2
2	B	355	ARG	2.2
2	B	288	LYS	2.2
2	B	361	ASN	2.1
1	A	347	GLN	2.1
2	B	276	ASN	2.1
1	A	438	GLN	2.1
2	B	284	VAL	2.1
2	B	340	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

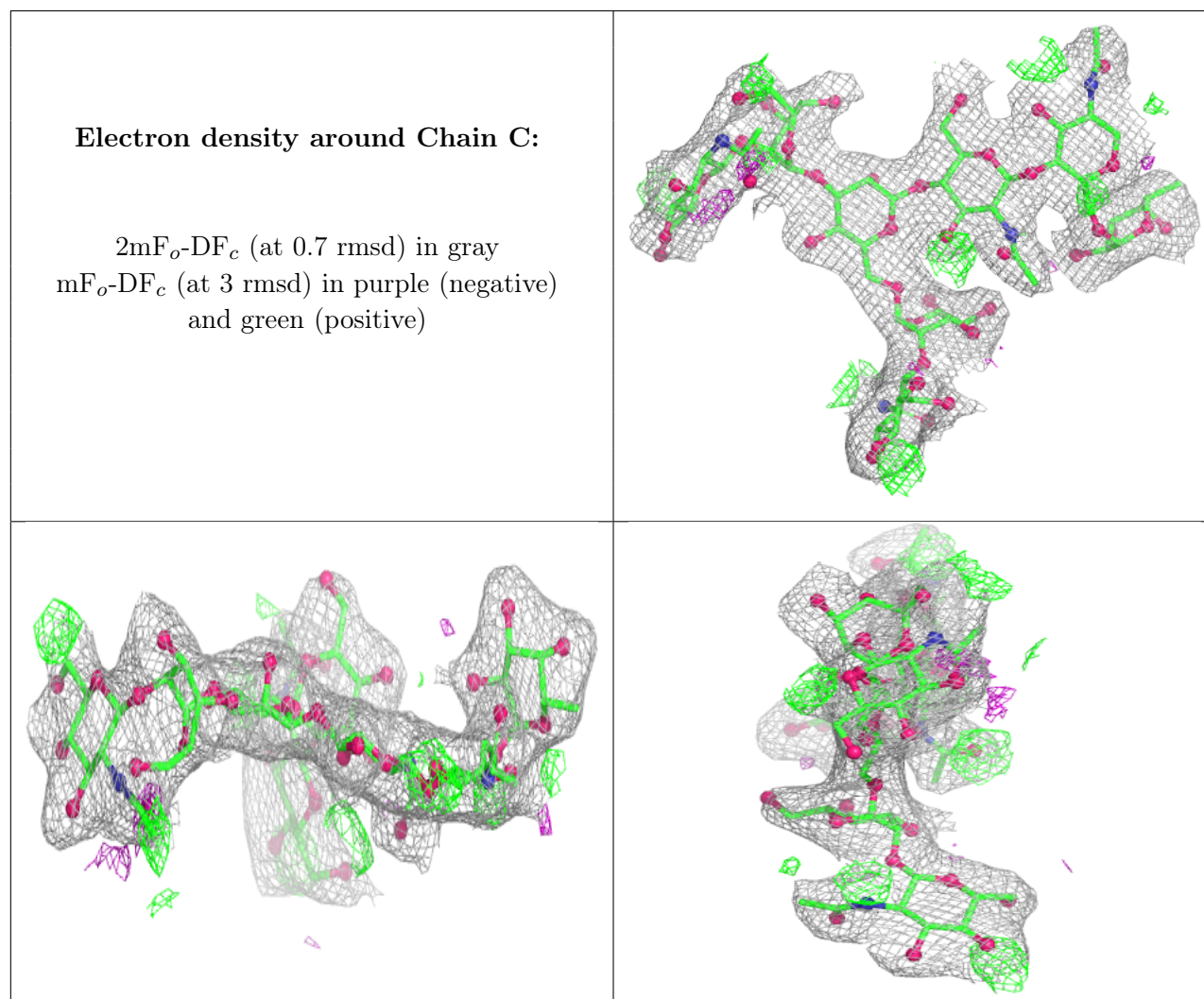
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	5	14/15	0.25	0.23	90,99,103,107	0
3	FUC	D	8	10/11	0.31	0.26	96,100,102,103	0
3	BMA	D	3	11/12	0.62	0.16	89,98,102,104	0
3	MAN	D	6	11/12	0.63	0.18	90,98,100,103	0
3	NAG	D	7	14/15	0.65	0.18	84,93,96,98	0
3	NAG	C	5	14/15	0.65	0.18	77,79,88,89	0
3	NAG	D	1	14/15	0.66	0.21	100,106,107,108	0
3	NAG	D	2	14/15	0.74	0.21	93,102,106,107	0
3	MAN	D	4	11/12	0.74	0.17	87,95,99,102	0
3	MAN	C	4	11/12	0.82	0.14	71,77,82,85	0
3	NAG	C	7	14/15	0.84	0.13	56,61,69,69	0
3	MAN	C	6	11/12	0.90	0.10	60,64,68,80	0

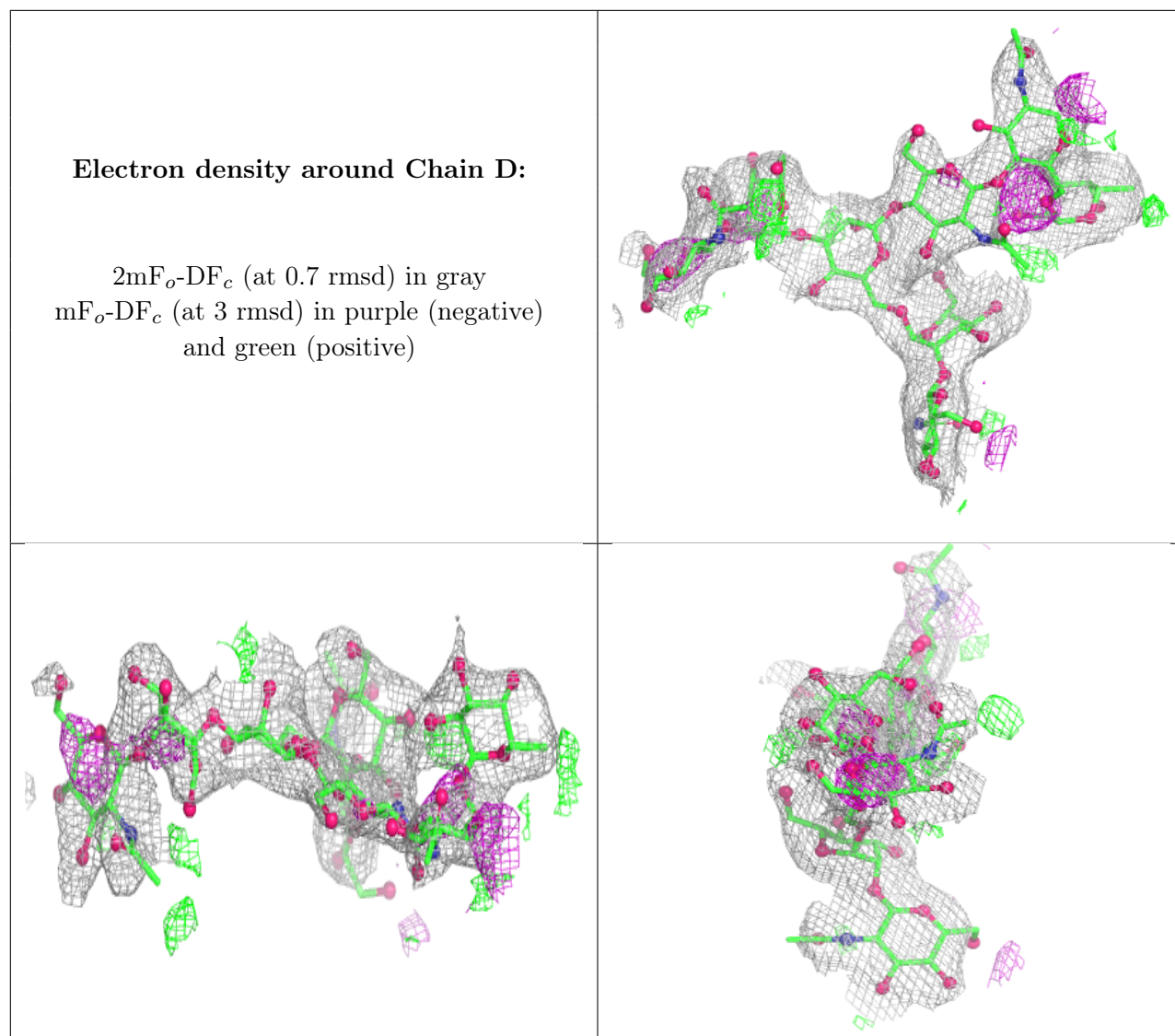
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	2	14/15	0.91	0.11	50,54,60,62	0
3	NAG	C	1	14/15	0.92	0.10	50,55,57,58	0
3	FUC	C	8	10/11	0.93	0.09	53,57,60,65	0
3	BMA	C	3	11/12	0.94	0.09	52,58,64,69	0

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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.