



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:11 AM UTC

PDB ID : 9CY6 / pdb_00009cy6
Title : Crystal structure of IgG1 FC M252H at pH 7.5
Authors : Reddem, E.R.; Shapiro, L.
Deposited on : 2024-08-01
Resolution : 2.06 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

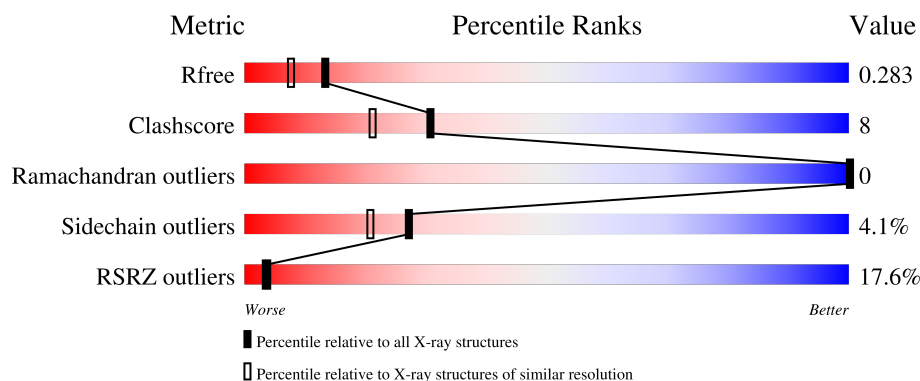
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	231	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	231	<div> <div>26%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>11%</div> </div> </div>
2	C	9	<div> <div>33%</div> <div>67%</div> </div>
3	D	9	<div> <div>22%</div> <div>33%</div> <div>44%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3735 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 Fc Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1666	1060	282	319	5			
1	B	206	Total	C	N	O	S	0	0	0
			1655	1053	280	317	5			

There are 40 discrepancies between the modelled and reference sequences:

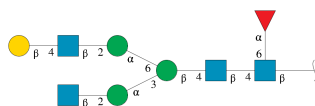
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP P0DOX5
A	218	GLY	-	expression tag	UNP P0DOX5
A	219	TRP	-	expression tag	UNP P0DOX5
A	220	SER	-	expression tag	UNP P0DOX5
A	221	CYS	-	expression tag	UNP P0DOX5
A	222	ILE	-	expression tag	UNP P0DOX5
A	223	ILE	-	expression tag	UNP P0DOX5
A	224	LEU	-	expression tag	UNP P0DOX5
A	225	PHE	-	expression tag	UNP P0DOX5
A	226	LEU	-	expression tag	UNP P0DOX5
A	227	VAL	-	expression tag	UNP P0DOX5
A	228	ALA	-	expression tag	UNP P0DOX5
A	229	THR	-	expression tag	UNP P0DOX5
A	230	ALA	-	expression tag	UNP P0DOX5
A	231	THR	-	expression tag	UNP P0DOX5
A	232	GLY	-	expression tag	UNP P0DOX5
A	233	VAL	-	expression tag	UNP P0DOX5
A	234	HIS	-	expression tag	UNP P0DOX5
A	235	SER	-	expression tag	UNP P0DOX5
A	252	HIS	MET	engineered mutation	UNP P0DOX5
B	217	MET	-	initiating methionine	UNP P0DOX5
B	218	GLY	-	expression tag	UNP P0DOX5
B	219	TRP	-	expression tag	UNP P0DOX5
B	220	SER	-	expression tag	UNP P0DOX5
B	221	CYS	-	expression tag	UNP P0DOX5

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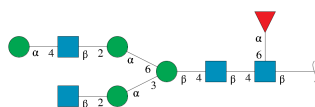
Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ILE	-	expression tag	UNP P0DOX5
B	223	ILE	-	expression tag	UNP P0DOX5
B	224	LEU	-	expression tag	UNP P0DOX5
B	225	PHE	-	expression tag	UNP P0DOX5
B	226	LEU	-	expression tag	UNP P0DOX5
B	227	VAL	-	expression tag	UNP P0DOX5
B	228	ALA	-	expression tag	UNP P0DOX5
B	229	THR	-	expression tag	UNP P0DOX5
B	230	ALA	-	expression tag	UNP P0DOX5
B	231	THR	-	expression tag	UNP P0DOX5
B	232	GLY	-	expression tag	UNP P0DOX5
B	233	VAL	-	expression tag	UNP P0DOX5
B	234	HIS	-	expression tag	UNP P0DOX5
B	235	SER	-	expression tag	UNP P0DOX5
B	252	HIS	MET	engineered mutation	UNP P0DOX5

- Molecule 2 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
2	C	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(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			

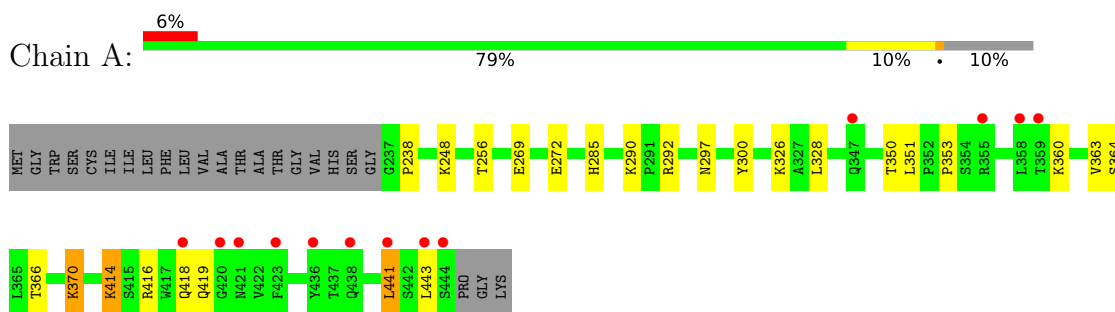
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	78	Total	O	0	0
			78	78		

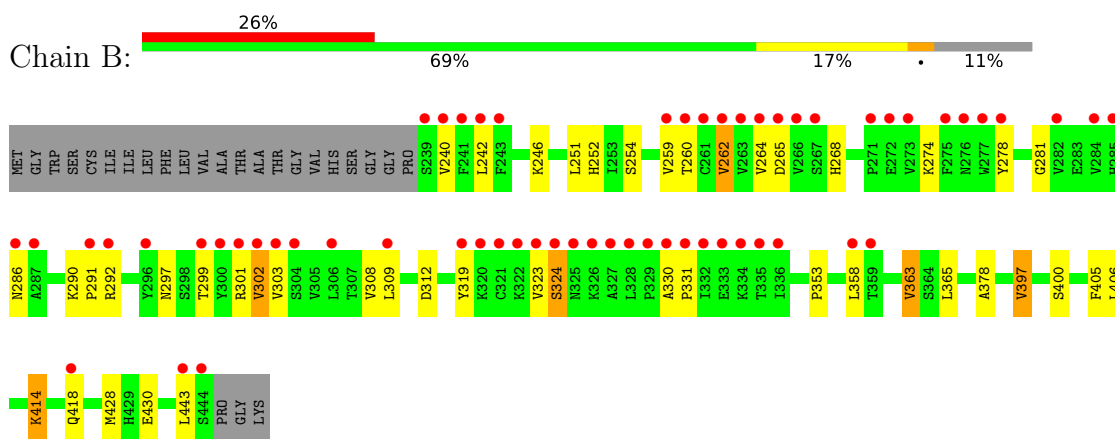
3 Residue-property plots

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: Immunoglobulin gamma-1 heavy chain Fc Fragment



- Molecule 1: Immunoglobulin gamma-1 heavy chain Fc Fragment




- Molecule 2: 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



- Molecule 3: alpha-D-mannopyranose-(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-mannopyr

anose-(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:  22% 33% 44%

NAG1	NAG2	BMA3	MAN4	NAG5	MAN6	MAN7	NAG8	FUC9
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.61Å 79.06Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.77 – 2.06 68.77 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.77-2.06) 99.8 (68.77-2.06)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.234 , 0.282 0.237 , 0.283	Depositor DCC
R_{free} test set	1713 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3735	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, GAL, 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	0.37	0/1713	0.56	0/2335
1	B	0.40	0/1701	0.63	0/2318
All	All	0.39	0/3414	0.59	0/4653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1666	0	1628	18	0
1	B	1655	0	1618	39	0
2	C	110	0	94	1	0
3	D	110	0	94	6	0
4	A	116	0	0	2	0
4	B	78	0	0	2	0
All	All	3735	0	3434	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG21	1:B:323:VAL:HG21	1.47	0.94
4:B:578:HOH:O	3:D:3:BMA:O2	2.10	0.69
1:A:272:GLU:OE1	1:A:326:LYS:NZ	2.27	0.68
1:B:418:GLN:HA	1:B:443:LEU:HD12	1.77	0.66
1:A:297:ASN:HD22	2:C:1:NAG:H83	1.62	0.65
1:A:416:ARG:HA	1:A:419:GLN:HE21	1.62	0.65
1:B:264:VAL:HG11	3:D:1:NAG:O4	1.98	0.64
1:A:292:ARG:HD2	1:A:300:TYR:CD1	2.34	0.63
1:B:264:VAL:HG12	1:B:265:ASP:H	1.64	0.62
1:A:269:GLU:N	1:A:269:GLU:OE1	2.34	0.59
1:B:414:LYS:O	1:B:418:GLN:HG3	2.04	0.57
1:A:416:ARG:HA	1:A:419:GLN:NE2	2.20	0.56
1:B:252:HIS:ND1	1:B:254:SER:OG	2.38	0.55
1:B:397:VAL:HG22	1:B:405:PHE:CE1	2.42	0.54
1:B:292:ARG:HD2	1:B:302:VAL:HB	1.89	0.54
1:B:301:ARG:HH11	3:D:2:NAG:H81	1.73	0.53
1:B:262:VAL:HB	1:B:303:VAL:HG12	1.91	0.52
1:B:290:LYS:HG2	1:B:291:PRO:N	2.26	0.51
1:A:350:THR:HB	1:A:441:LEU:HD13	1.93	0.51
1:B:414:LYS:HD3	1:B:418:GLN:NE2	2.26	0.51
1:B:290:LYS:HE3	1:B:291:PRO:O	2.11	0.50
1:A:360:LYS:O	1:A:414:LYS:HE2	2.12	0.50
1:B:264:VAL:HG12	1:B:265:ASP:N	2.27	0.50
1:B:309:LEU:HB2	1:B:312:ASP:HB2	1.94	0.48
1:A:256:THR:HG23	4:A:564:HOH:O	2.12	0.48
1:A:370:LYS:HE2	4:B:535:HOH:O	2.12	0.47
1:B:240:VAL:CG2	1:B:323:VAL:HG21	2.33	0.47
1:B:353:PRO:HG3	1:B:363:VAL:CG1	2.45	0.47
1:B:414:LYS:HD3	1:B:418:GLN:CD	2.41	0.46
1:B:246:LYS:HG2	3:D:6:MAN:H4	1.98	0.46
1:A:353:PRO:HB3	1:A:363:VAL:HG22	1.98	0.46
1:B:290:LYS:HD3	1:B:303:VAL:HG22	1.98	0.45
1:B:292:ARG:H	1:B:292:ARG:HG2	1.37	0.45
1:B:259:VAL:HG23	1:B:308:VAL:HG11	1.99	0.45
1:B:278:TYR:HB3	1:B:281:GLY:O	2.16	0.45
1:B:406:LEU:HD12	1:B:406:LEU:C	2.42	0.45
1:B:301:ARG:NH1	3:D:2:NAG:H81	2.31	0.45
1:B:290:LYS:HB3	1:B:303:VAL:HG22	2.00	0.44
1:B:353:PRO:HG3	1:B:363:VAL:HG13	2.00	0.44
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.17	0.44
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:OG	4:A:501:HOH:O	2.20	0.43
1:B:260:THR:OG1	3:D:5:NAG:H61	2.19	0.43
1:B:297:ASN:OD1	1:B:299:THR:HG22	2.18	0.43
1:A:269:GLU:CD	1:A:269:GLU:H	2.14	0.43
1:B:330:ALA:HB1	1:B:331:PRO:HD2	2.00	0.43
1:B:274:LYS:HB3	1:B:324:SER:O	2.18	0.43
1:B:353:PRO:HD3	1:B:365:LEU:HD12	2.00	0.43
1:A:238:PRO:HD2	1:A:328:LEU:HD21	2.02	0.41
1:A:351:LEU:HB2	1:A:366:THR:HB	2.01	0.41
1:A:238:PRO:HD2	1:A:328:LEU:CD2	2.51	0.41
1:B:251:LEU:HD23	1:B:251:LEU:HA	1.86	0.41
1:B:246:LYS:HE3	1:B:246:LYS:HB3	1.60	0.40
1:A:418:GLN:HA	1:A:443:LEU:HD11	2.04	0.40
1:B:378:ALA:HB3	1:B:428:MET:HB2	2.03	0.40
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.90	0.40
1:A:292:ARG:HD2	1:A:300:TYR:CG	2.56	0.40
1:B:268:HIS:CD2	1:B:268:HIS:H	2.40	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	206/231 (89%)	204 (99%)	2 (1%)	0	100	100
1	B	204/231 (88%)	195 (96%)	9 (4%)	0	100	100
All	All	410/462 (89%)	399 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/211 (92%)	188 (97%)	6 (3%)	35	30
1	B	193/211 (92%)	183 (95%)	10 (5%)	21	14
All	All	387/422 (92%)	371 (96%)	16 (4%)	27	21

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	A	285	HIS
1	A	290	LYS
1	A	370	LYS
1	A	414	LYS
1	A	441	LEU
1	B	262	VAL
1	B	286	ASN
1	B	302	VAL
1	B	324	SER
1	B	358	LEU
1	B	363	VAL
1	B	397	VAL
1	B	400	SER
1	B	414	LYS
1	B	430	GLU

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

Mol	Chain	Res	Type
1	A	347	GLN
1	A	389	ASN
1	A	418	GLN
1	A	419	GLN
1	B	286	ASN
1	B	311	GLN

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Mol	Chain	Res	Type
1	B	362	GLN
1	B	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	C	1	1,2	14,14,15	0.41	0	17,19,21	0.48	0
2	NAG	C	2	2	14,14,15	0.61	1 (7%)	17,19,21	0.69	0
2	BMA	C	3	2	11,11,12	1.04	1 (9%)	15,15,17	1.11	1 (6%)
2	MAN	C	4	2	11,11,12	1.05	1 (9%)	15,15,17	1.37	2 (13%)
2	NAG	C	5	2	14,14,15	0.23	0	17,19,21	0.57	0
2	GAL	C	6	2	11,11,12	1.70	4 (36%)	15,15,17	1.21	1 (6%)
2	MAN	C	7	2	11,11,12	1.11	1 (9%)	15,15,17	1.44	2 (13%)
2	NAG	C	8	2	14,14,15	0.50	0	17,19,21	0.58	0
2	FUC	C	9	2	10,10,11	0.97	0	14,14,16	0.94	0
3	NAG	D	1	1,3	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.56	0
3	BMA	D	3	3	11,11,12	1.25	1 (9%)	15,15,17	0.75	0
3	MAN	D	4	3	11,11,12	0.93	0	15,15,17	1.72	2 (13%)
3	NAG	D	5	3	14,14,15	0.79	1 (7%)	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	6	3	11,11,12	1.42	2 (18%)	15,15,17	1.32	1 (6%)
3	MAN	D	7	3	11,11,12	1.22	1 (9%)	15,15,17	1.43	2 (13%)
3	NAG	D	8	3	14,14,15	0.29	0	17,19,21	0.70	0
3	FUC	D	9	3	10,10,11	0.89	0	14,14,16	0.88	0

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	C2-C3	3.16	1.57	1.52
2	C	6	GAL	C1-C2	3.05	1.59	1.52
3	D	5	NAG	O5-C1	-2.81	1.39	1.43
2	C	4	MAN	O5-C5	2.55	1.48	1.43
2	C	7	MAN	C2-C3	-2.46	1.48	1.52
3	D	7	MAN	C4-C5	2.35	1.58	1.53
2	C	6	GAL	C2-C3	2.32	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	GAL	O2-C2	2.32	1.48	1.43
2	C	6	GAL	C4-C3	2.22	1.58	1.52
3	D	6	MAN	O2-C2	2.19	1.47	1.43
2	C	3	BMA	O5-C1	-2.13	1.40	1.43
3	D	6	MAN	O5-C5	2.09	1.47	1.43
2	C	2	NAG	O5-C1	-2.09	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	5.24	119.21	112.19
2	C	7	MAN	O2-C2-C3	-4.38	101.08	110.15
2	C	4	MAN	C1-O5-C5	4.10	117.68	112.19
3	D	6	MAN	C1-O5-C5	3.73	117.19	112.19
3	D	7	MAN	O2-C2-C3	-3.24	103.45	110.15
3	D	4	MAN	O2-C2-C3	-3.16	103.61	110.15
3	D	7	MAN	C1-O5-C5	2.97	116.16	112.19
2	C	6	GAL	C1-O5-C5	2.88	116.05	112.19
2	C	7	MAN	C1-O5-C5	2.58	115.65	112.19
2	C	4	MAN	O2-C2-C3	-2.42	105.13	110.15
2	C	3	BMA	O2-C2-C3	-2.36	105.27	110.15
3	D	1	NAG	C1-O5-C5	2.23	115.18	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	8	NAG	C1-C2-N2-C7
3	D	8	NAG	C1-C2-N2-C7
2	C	8	NAG	C3-C2-N2-C7
3	D	8	NAG	C3-C2-N2-C7
3	D	7	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6

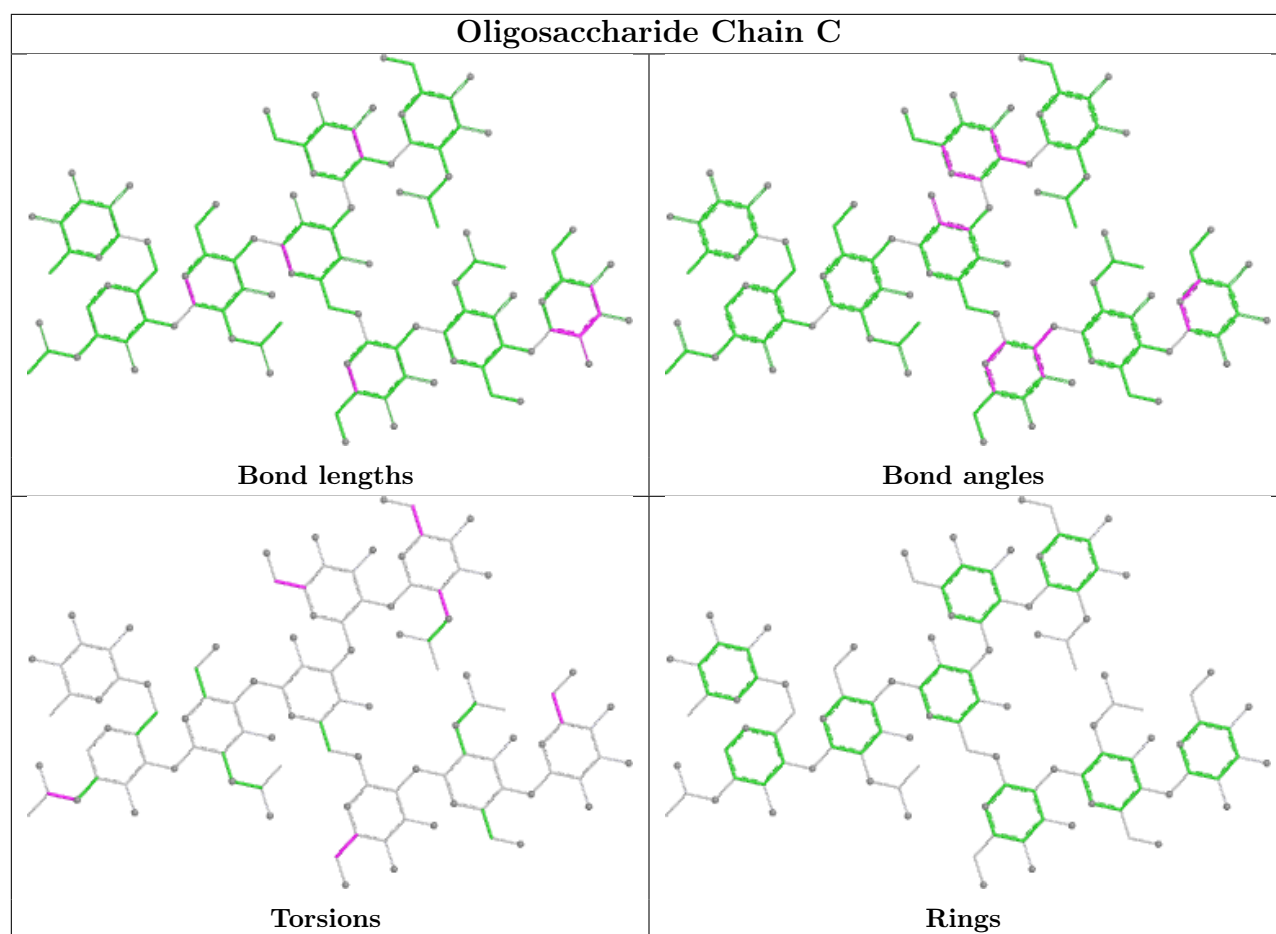
All (1) ring outliers are listed below:

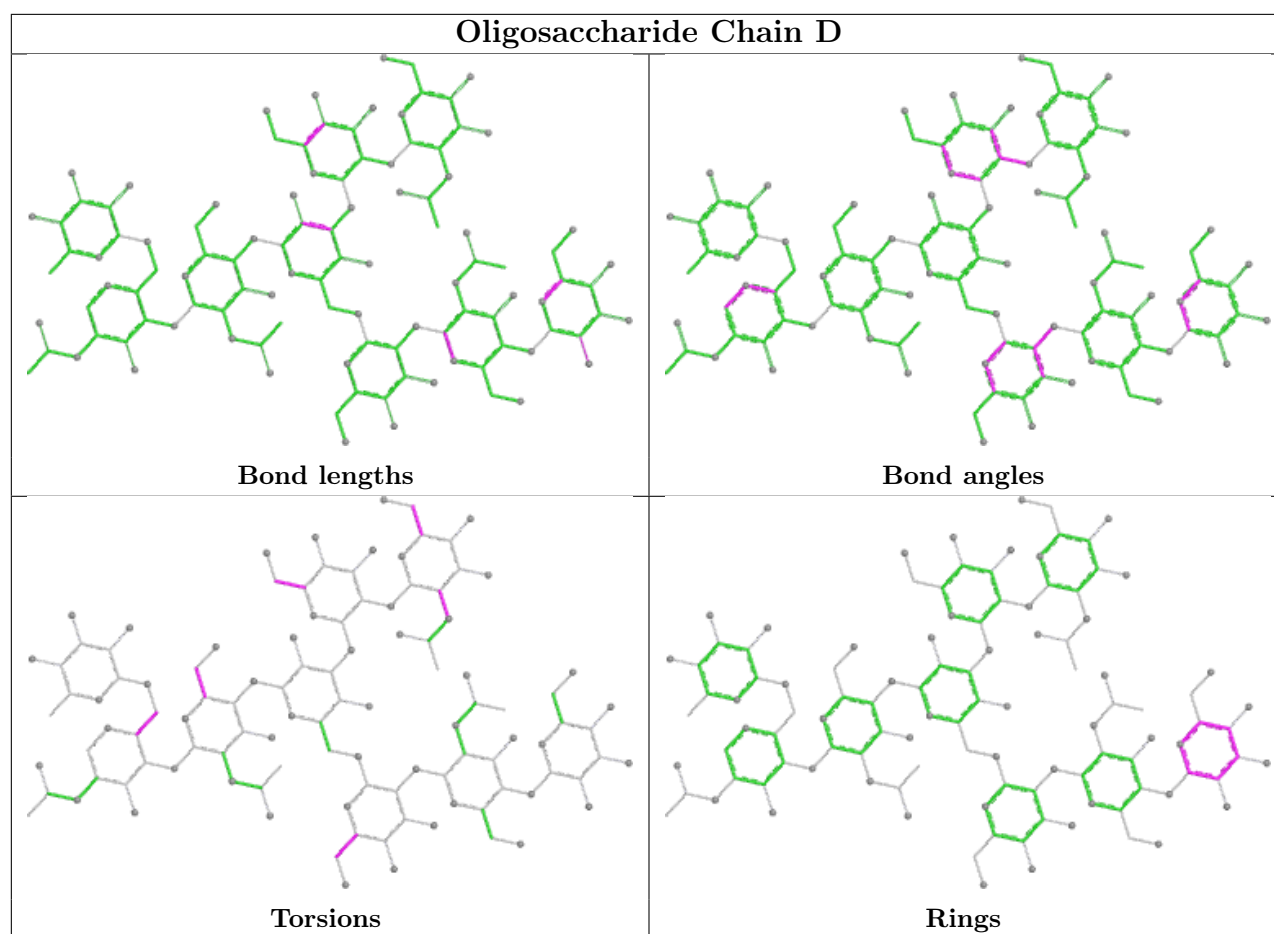
Mol	Chain	Res	Type	Atoms
3	D	6	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	2	0
3	D	6	MAN	1	0
2	C	1	NAG	1	0
3	D	5	NAG	1	0
3	D	1	NAG	1	0
3	D	3	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, 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	208/231 (90%)	0.50	13 (6%) 26 25	32, 44, 68, 90	0
1	B	206/231 (89%)	1.48	60 (29%) 1 1	30, 53, 99, 124	0
All	All	414/462 (89%)	0.99	73 (17%) 4 3	30, 47, 92, 124	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	SER	6.7
1	B	328	LEU	6.6
1	B	323	VAL	6.2
1	B	240	VAL	5.9
1	B	262	VAL	5.8
1	B	273	VAL	5.6
1	B	241	PHE	5.0
1	B	324	SER	4.9
1	B	330	ALA	4.6
1	B	266	VAL	4.5
1	B	302	VAL	4.4
1	B	300	TYR	4.3
1	B	329	PRO	4.3
1	B	271	PRO	4.3
1	B	321	CYS	4.2
1	B	332	ILE	4.1
1	B	303	VAL	4.1
1	B	264	VAL	4.1
1	B	296	TYR	4.0
1	B	263	VAL	3.8
1	B	275	PHE	3.8
1	B	325	ASN	3.7
1	B	278	TYR	3.7
1	B	287	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	242	LEU	3.6
1	B	277	TRP	3.5
1	B	327	ALA	3.5
1	B	301	ARG	3.4
1	B	358	LEU	3.3
1	B	335	THR	3.2
1	B	359	THR	3.1
1	B	299	THR	3.1
1	B	322	LYS	3.1
1	B	284	VAL	3.1
1	B	444	SER	3.1
1	A	347	GLN	3.1
1	B	243	PHE	3.0
1	B	282	VAL	3.0
1	B	331	PRO	3.0
1	B	260	THR	2.9
1	B	285	HIS	2.9
1	B	291	PRO	2.9
1	B	306	LEU	2.9
1	A	355	ARG	2.8
1	B	320	LYS	2.8
1	B	261	CYS	2.7
1	B	304	SER	2.7
1	B	292	ARG	2.7
1	A	444	SER	2.6
1	B	319	TYR	2.6
1	B	272	GLU	2.6
1	B	326	LYS	2.6
1	B	267	SER	2.6
1	B	443	LEU	2.5
1	B	265	ASP	2.5
1	B	418	GLN	2.5
1	A	358	LEU	2.5
1	B	333	GLU	2.5
1	B	259	VAL	2.4
1	A	438	GLN	2.4
1	A	359	THR	2.3
1	B	334	LYS	2.3
1	A	423	PHE	2.3
1	A	420	GLY	2.2
1	A	436	TYR	2.2
1	A	421	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	443	LEU	2.2
1	B	309	LEU	2.2
1	B	276	ASN	2.2
1	B	286	ASN	2.1
1	A	441	LEU	2.1
1	A	418	GLN	2.0
1	B	336	ILE	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](#)

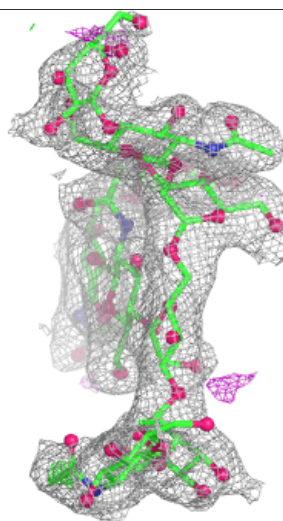
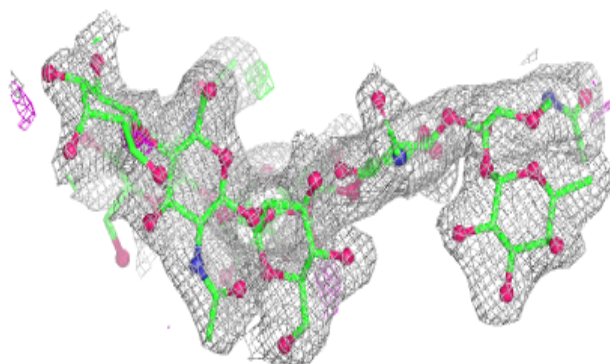
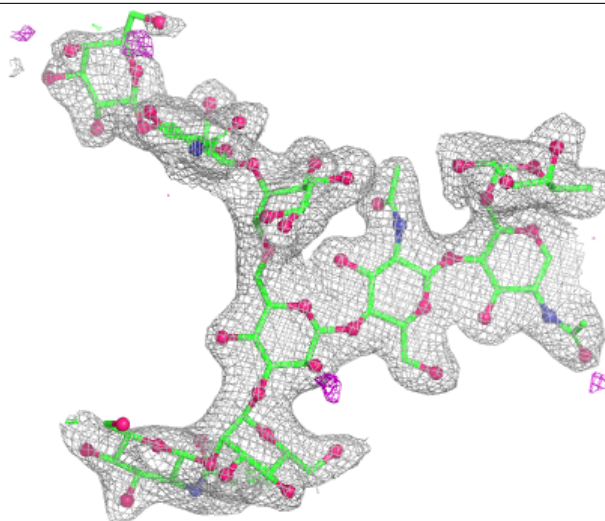
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

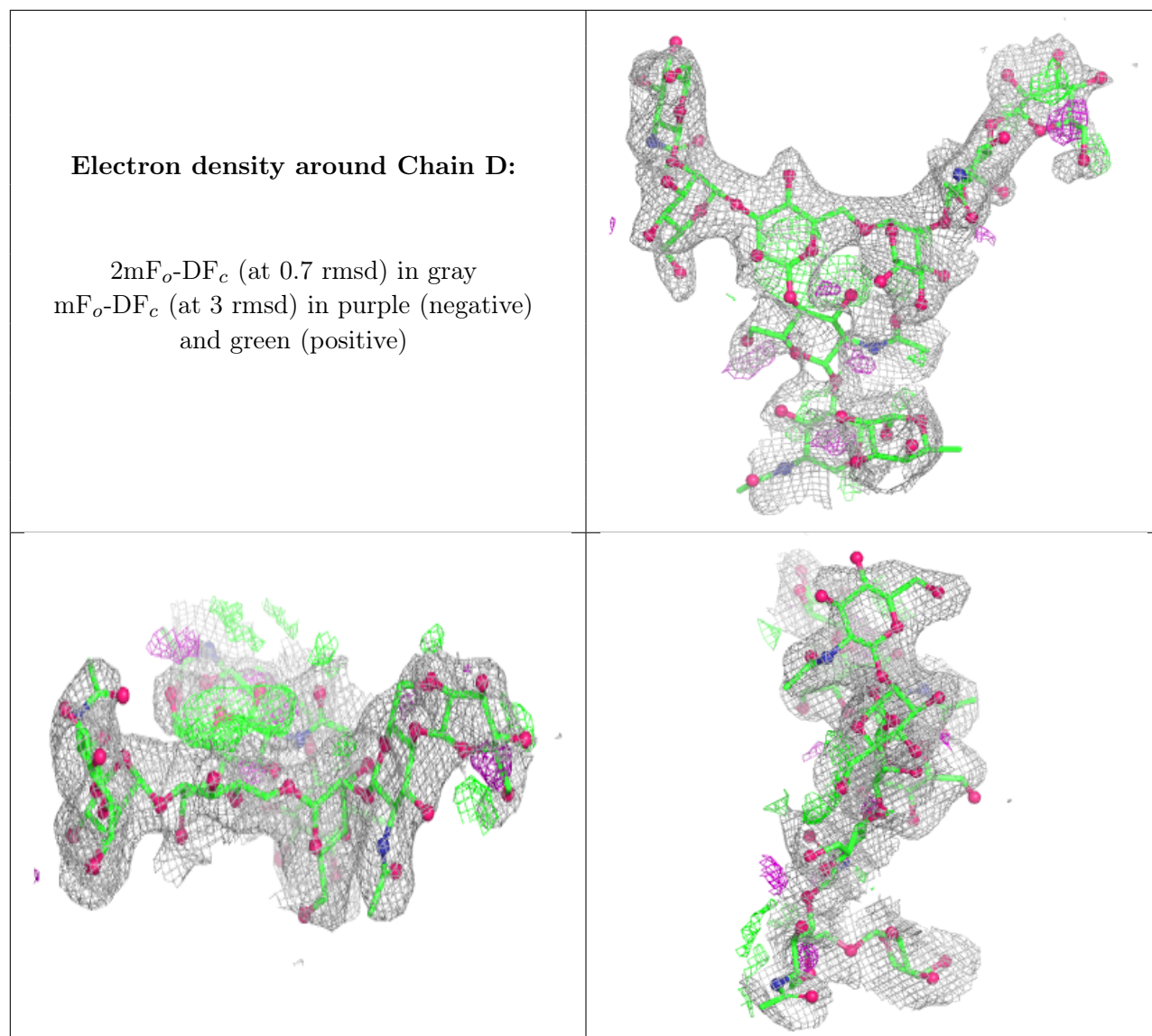
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.36	0.22	88,96,103,104	0
3	NAG	D	1	14/15	0.49	0.17	104,108,112,113	0
2	NAG	C	8	14/15	0.50	0.15	72,82,89,90	0
3	MAN	D	6	11/12	0.66	0.19	55,67,76,76	0
3	BMA	D	3	11/12	0.67	0.14	73,80,88,89	0
3	FUC	D	9	10/11	0.70	0.11	108,110,111,111	0
3	NAG	D	8	14/15	0.71	0.12	80,86,92,97	0
3	MAN	D	4	11/12	0.73	0.13	73,75,79,87	0
3	NAG	D	5	14/15	0.81	0.13	65,70,76,77	0
2	FUC	C	9	10/11	0.81	0.11	48,53,59,60	0
2	GAL	C	6	11/12	0.84	0.17	45,55,61,63	0
3	MAN	D	7	11/12	0.86	0.11	66,73,77,78	0
2	NAG	C	5	14/15	0.87	0.11	45,53,57,59	0
2	BMA	C	3	11/12	0.89	0.09	46,48,53,55	0
2	MAN	C	7	11/12	0.90	0.09	58,63,67,75	0
2	NAG	C	1	14/15	0.91	0.08	45,49,51,58	0
2	MAN	C	4	11/12	0.91	0.08	45,51,54,59	0
2	NAG	C	2	14/15	0.94	0.08	42,46,49,53	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 C:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.