



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 09:27 PM JST

PDB ID : 5Y56  
Title : Fc mutant (K392D/K409D/D399K)  
Authors : Ye, S.; Xu, T.; Yu, J.; Wang, X.; Xu, T.; Jin, Q.; Duan, J.; Wu, J.; Wu, H.  
Deposited on : 2017-08-07  
Resolution : 2.65 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](mailto: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>.

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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 : 2.36  
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

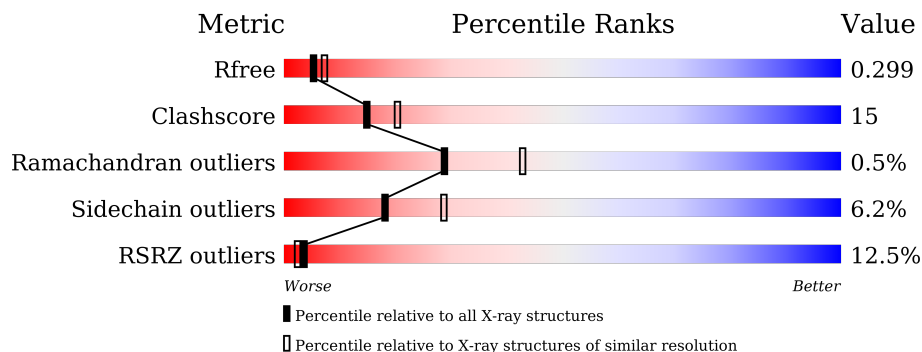
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	208	
1	B	208	
2	C	9	
3	D	7	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3613 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.

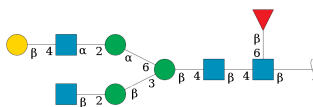
- Molecule 1 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total 1661	C 1056	N 279	O 320	S 6	0	0	0
1	B	208	Total 1661	C 1056	N 279	O 320	S 6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASP	LYS	engineered mutation	UNP P0DOX5
A	399	LYS	ASP	engineered mutation	UNP P0DOX5
A	409	ASP	LYS	engineered mutation	UNP P0DOX5
B	392	ASP	LYS	engineered mutation	UNP P0DOX5
B	399	LYS	ASP	engineered mutation	UNP P0DOX5
B	409	ASP	LYS	engineered mutation	UNP P0DOX5

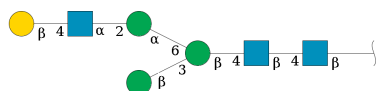
- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	7	86	48	3	35	0	0	0

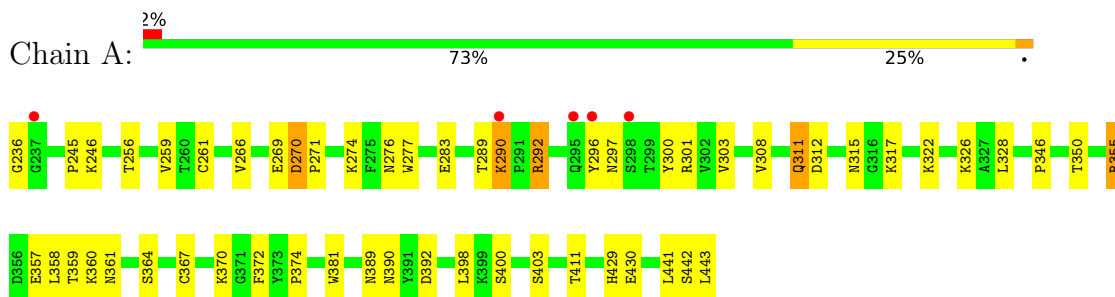
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	36	Total	O	0	0
			36	36		

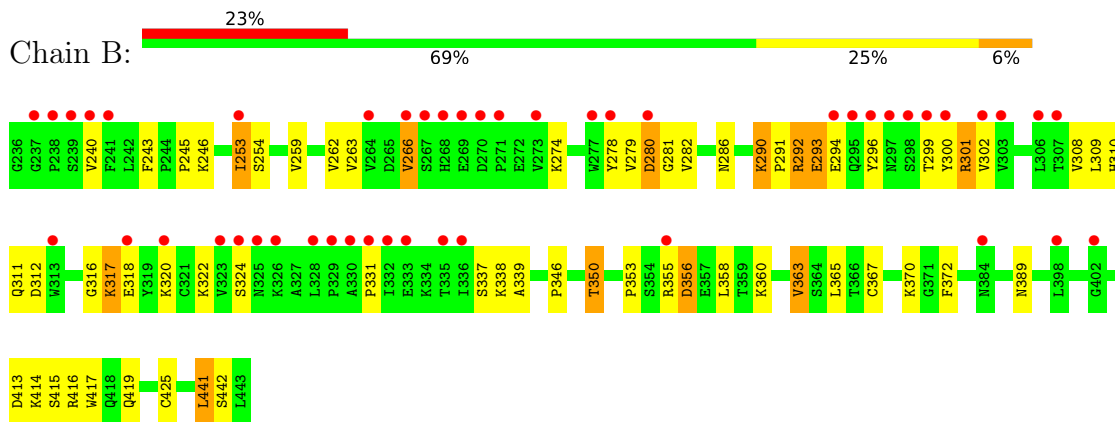
### 3 Residue-property plots [i](#)

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.

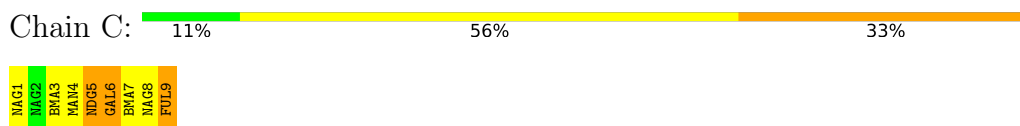
- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



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



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

Chain D:

43%

57%

MG1
MG2
MG3
MG4
MG5
MG6
MG7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.13Å 65.13Å 477.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.45 – 2.65 36.45 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.1 (36.45-2.65) 96.1 (36.45-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.65Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.260 , 0.298 0.260 , 0.299	Depositor DCC
$R_{free}$ test set	1804 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.2	Xtrriage
Anisotropy	0.199	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GAL, MAN, BMA, FUL, NDG

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	0.45	0/1707	0.62	1/2327 (0.0%)
1	B	0.39	0/1707	0.57	0/2327
All	All	0.42	0/3414	0.59	1/4654 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	CA-CB-CG	5.12	127.07	115.30

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	1661	0	1619	47	1
1	B	1661	0	1619	54	2
2	C	110	0	93	7	0
3	D	86	0	72	7	1
4	A	59	0	0	18	1
4	B	36	0	0	16	0
All	All	3613	0	3403	105	3



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 15.

All (105) 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:A:370:LYS:NZ	4:A:601:HOH:O	1.91	1.02
1:B:367:CYS:SG	4:B:634:HOH:O	2.20	0.99
1:A:271:PRO:O	4:A:602:HOH:O	1.91	0.88
1:B:274:LYS:NZ	4:B:602:HOH:O	1.97	0.84
1:A:276:ASN:OD1	4:A:603:HOH:O	1.99	0.80
1:B:360:LYS:O	1:B:414:LYS:NZ	2.16	0.77
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.67	0.75
1:A:283:GLU:OE1	4:A:604:HOH:O	2.05	0.74
4:B:603:HOH:O	3:D:7:BMA:O2	2.06	0.72
1:B:322:LYS:HZ3	1:B:331:PRO:HB3	1.55	0.71
1:B:311:GLN:OE1	4:B:604:HOH:O	2.07	0.71
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.72	0.71
1:B:292:ARG:HG3	1:B:302:VAL:HG22	1.73	0.71
1:A:236:GLY:O	4:A:605:HOH:O	2.09	0.70
1:B:350:THR:HB	1:B:441:LEU:CD2	2.22	0.70
1:B:290:LYS:HG3	1:B:291:PRO:HD2	1.74	0.69
1:A:256:THR:OG1	4:A:606:HOH:O	2.10	0.69
1:B:310:HIS:NE2	4:B:607:HOH:O	2.26	0.69
1:B:416:ARG:NH1	1:B:419:GLN:OE1	2.24	0.69
1:A:297:ASN:O	4:A:607:HOH:O	2.11	0.69
1:A:361:ASN:ND2	4:A:614:HOH:O	2.26	0.69
1:A:290:LYS:HD2	1:A:303:VAL:H	1.60	0.67
1:B:243:PHE:HE1	3:D:4:MAN:H2	1.60	0.66
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.77	0.66
1:A:266:VAL:HG23	1:A:300:TYR:HB2	1.76	0.66
1:A:245:PRO:HA	2:C:6:GAL:H61	1.77	0.66
3:D:5:NDG:H4	3:D:6:GAL:O2	1.95	0.66
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.78	0.66
1:B:286:ASN:HA	4:B:616:HOH:O	1.97	0.65
1:A:296:TYR:HA	4:A:621:HOH:O	1.98	0.64
1:B:312:ASP:O	4:B:605:HOH:O	2.14	0.64
1:B:322:LYS:NZ	4:B:610:HOH:O	2.32	0.63
1:B:350:THR:HB	1:B:441:LEU:HG	1.82	0.61
1:A:276:ASN:ND2	4:A:604:HOH:O	2.25	0.61
4:A:608:HOH:O	2:C:9:FUL:O2	2.16	0.61
1:A:355:ARG:NH1	4:A:619:HOH:O	2.33	0.60
2:C:5:NDG:H4	2:C:6:GAL:O2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:THR:HB	4:B:612:HOH:O	2.02	0.59
1:A:292:ARG:HG3	1:A:300:TYR:CE2	2.38	0.59
1:B:316:GLY:N	4:B:605:HOH:O	2.36	0.58
1:B:293:GLU:HG3	1:B:301:ARG:HB3	1.85	0.58
1:A:290:LYS:NZ	1:A:301:ARG:O	2.37	0.57
1:B:338:LYS:NZ	1:B:339:ALA:O	2.35	0.57
1:A:350:THR:HB	1:A:441:LEU:HD22	1.86	0.56
1:A:359:THR:OG1	4:A:610:HOH:O	2.18	0.56
1:B:246:LYS:HE3	3:D:6:GAL:H3	1.87	0.56
1:B:356:ASP:O	1:B:360:LYS:NZ	2.38	0.55
1:A:357:GLU:OE1	4:A:609:HOH:O	2.17	0.54
1:A:364:SER:O	4:A:611:HOH:O	2.18	0.54
1:A:246:LYS:HG2	2:C:6:GAL:H5	1.90	0.54
1:B:254:SER:N	4:B:601:HOH:O	1.90	0.54
1:B:350:THR:HB	1:B:441:LEU:CG	2.38	0.53
1:B:350:THR:HB	1:B:441:LEU:HD23	1.90	0.53
1:B:353:PRO:HB3	1:B:363:VAL:HG22	1.91	0.53
1:A:357:GLU:C	1:A:359:THR:H	2.12	0.53
1:A:311:GLN:O	1:A:315:ASN:ND2	2.43	0.50
1:A:270:ASP:N	1:A:270:ASP:OD1	2.45	0.50
1:A:322:LYS:NZ	4:A:623:HOH:O	2.37	0.49
1:A:296:TYR:HB2	2:C:9:FUL:H61	1.95	0.49
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.41	0.49
1:B:389:ASN:OD1	1:B:389:ASN:N	2.45	0.49
1:B:417:TRP:CH2	1:B:442:SER:HA	2.48	0.49
1:A:389:ASN:HA	4:A:635:HOH:O	2.13	0.49
1:B:280:ASP:CB	1:B:317:LYS:HE3	2.43	0.49
1:B:280:ASP:HB3	1:B:317:LYS:HE3	1.95	0.48
1:A:312:ASP:HB3	1:A:317:LYS:HD2	1.95	0.48
1:B:294:GLU:HA	1:B:300:TYR:HA	1.96	0.48
1:A:374:PRO:O	1:A:429:HIS:HE1	1.97	0.47
1:B:425:CYS:SG	4:B:634:HOH:O	2.61	0.47
1:B:253:ILE:H	1:B:253:ILE:HG13	1.49	0.47
1:B:246:LYS:HG2	3:D:6:GAL:H5	1.96	0.47
1:B:279:VAL:O	1:B:281:GLY:N	2.47	0.47
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.50	0.47
1:B:360:LYS:H	1:B:360:LYS:HD2	1.81	0.46
1:B:425:CYS:HB2	4:B:634:HOH:O	2.16	0.45
1:A:346:PRO:HD3	1:A:429:HIS:CD2	2.52	0.45
1:B:266:VAL:HG22	1:B:300:TYR:HB2	1.99	0.45
1:A:290:LYS:HD3	1:A:290:LYS:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.99	0.45
1:B:245:PRO:HA	3:D:6:GAL:H61	2.00	0.44
1:A:259:VAL:HG23	1:A:308:VAL:HG11	2.00	0.44
1:B:259:VAL:HG23	1:B:308:VAL:HG11	2.00	0.44
1:A:360:LYS:HD2	1:A:361:ASN:H	1.83	0.44
1:B:253:ILE:HD12	4:B:601:HOH:O	2.18	0.44
1:B:318:GLU:HG2	1:B:337:SER:HB2	2.00	0.43
1:A:398:LEU:HD12	1:A:403:SER:O	2.19	0.43
1:B:417:TRP:CZ3	1:B:442:SER:HA	2.54	0.43
1:A:296:TYR:HB2	2:C:9:FUL:C6	2.49	0.43
1:B:266:VAL:N	4:B:612:HOH:O	2.33	0.42
1:B:353:PRO:HB3	1:B:363:VAL:CG2	2.49	0.42
1:B:266:VAL:CG2	1:B:300:TYR:HB2	2.48	0.42
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.55	0.42
1:B:365:LEU:HD21	1:B:417:TRP:CZ3	2.55	0.42
1:A:274:LYS:HB3	1:A:274:LYS:HE2	1.73	0.42
1:A:442:SER:O	1:A:443:LEU:HB2	2.19	0.42
1:A:269:GLU:O	1:A:271:PRO:HD3	2.20	0.42
1:B:370:LYS:HB2	1:B:370:LYS:HE3	1.75	0.41
1:B:262:VAL:HG11	3:D:2:NAG:H81	2.01	0.41
1:A:290:LYS:HE3	1:A:303:VAL:HB	2.02	0.41
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.90	0.41
1:B:322:LYS:NZ	1:B:324:SER:OG	2.53	0.41
1:A:245:PRO:HA	2:C:6:GAL:C6	2.47	0.40
1:A:297:ASN:HB2	4:A:612:HOH:O	2.20	0.40
1:A:390:ASN:OD1	1:A:411:THR:OG1	2.39	0.40
1:B:254:SER:CB	4:B:601:HOH:O	2.69	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:O	1:B:292:ARG:NH1[8_555]	2.06	0.14
1:B:296:TYR:OH	3:D:1:NAG:O6[8_555]	2.13	0.07
4:A:614:HOH:O	4:A:655:HOH:O[12_444]	2.17	0.03

## 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	206/208 (99%)	197 (96%)	8 (4%)	1 (0%)	29	43
1	B	206/208 (99%)	196 (95%)	9 (4%)	1 (0%)	29	43
All	All	412/416 (99%)	393 (95%)	17 (4%)	2 (0%)	29	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	A	358	LEU

### 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	193/193 (100%)	184 (95%)	9 (5%)	26	40
1	B	193/193 (100%)	178 (92%)	15 (8%)	12	20
All	All	386/386 (100%)	362 (94%)	24 (6%)	18	29

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

Mol	Chain	Res	Type
1	A	270	ASP
1	A	289	THR
1	A	290	LYS
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	326	LYS
1	A	355	ARG
1	A	392	ASP
1	A	430	GLU
1	B	253	ILE
1	B	266	VAL
1	B	282	VAL
1	B	290	LYS
1	B	292	ARG
1	B	293	GLU
1	B	301	ARG
1	B	309	LEU
1	B	317	LYS
1	B	350	THR
1	B	356	ASP
1	B	363	VAL
1	B	413	ASP
1	B	415	SER
1	B	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	B	347	GLN
1	B	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](#)

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
2	NAG	C	1	2,1	14,14,15	1.08	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	0.41	0
2	BMA	C	3	2	11,11,12	1.11	1 (9%)	15,15,17	1.82	3 (20%)
2	MAN	C	4	2	11,11,12	1.07	1 (9%)	15,15,17	2.11	4 (26%)
2	NDG	C	5	2	14,14,15	1.00	1 (7%)	17,19,21	1.26	1 (5%)
2	GAL	C	6	2	11,11,12	1.56	3 (27%)	15,15,17	2.04	3 (20%)
2	BMA	C	7	2	11,11,12	1.19	1 (9%)	15,15,17	1.70	3 (20%)
2	NAG	C	8	2	14,14,15	1.25	1 (7%)	17,19,21	1.22	1 (5%)
2	FUL	C	9	2	10,10,11	2.10	3 (30%)	14,14,16	1.87	3 (21%)
3	NAG	D	1	3,1	14,14,15	0.36	0	17,19,21	0.37	0
3	NAG	D	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	BMA	D	3	3	11,11,12	1.27	2 (18%)	15,15,17	1.78	3 (20%)
3	MAN	D	4	3	11,11,12	1.02	0	15,15,17	1.42	1 (6%)
3	NDG	D	5	3	14,14,15	0.99	1 (7%)	17,19,21	1.36	2 (11%)
3	GAL	D	6	3	11,11,12	1.32	1 (9%)	15,15,17	1.80	3 (20%)
3	BMA	D	7	3	11,11,12	1.14	2 (18%)	15,15,17	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	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NDG	C	5	2	-	2/6/23/26	0/1/1/1
2	GAL	C	6	2	-	1/2/19/22	0/1/1/1
2	BMA	C	7	2	-	0/2/19/22	0/1/1/1
2	NAG	C	8	2	-	0/6/23/26	0/1/1/1

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9	FUL	O5-C1	5.62	1.52	1.43
2	C	8	NAG	O5-C1	4.29	1.50	1.43
2	C	1	NAG	O5-C1	3.89	1.49	1.43
3	D	6	GAL	C1-C2	3.31	1.59	1.52
2	C	6	GAL	C2-C3	-3.27	1.47	1.52
3	D	5	NDG	C1-C2	3.21	1.57	1.52
2	C	5	NDG	C1-C2	3.19	1.57	1.52
2	C	4	MAN	O5-C5	2.88	1.49	1.43
3	D	3	BMA	C2-C3	2.86	1.56	1.52
2	C	7	BMA	C4-C5	2.77	1.58	1.53
3	D	7	BMA	C4-C5	2.53	1.58	1.53
2	C	6	GAL	O5-C5	2.48	1.48	1.43
2	C	6	GAL	C1-C2	2.44	1.57	1.52
2	C	9	FUL	C2-C3	-2.28	1.49	1.52
2	C	9	FUL	O5-C5	2.20	1.48	1.43
3	D	3	BMA	C1-C2	2.13	1.57	1.52
2	C	3	BMA	O3-C3	2.13	1.48	1.43
3	D	7	BMA	O5-C1	-2.01	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	5.95	120.25	112.19
2	C	3	BMA	O3-C3-C2	5.33	120.20	109.99
2	C	9	FUL	C1-C2-C3	-5.26	103.20	109.67
3	D	3	BMA	O3-C3-C2	5.07	119.70	109.99
2	C	7	BMA	C1-C2-C3	-4.82	103.75	109.67
2	C	8	NAG	C1-O5-C5	4.80	118.70	112.19
2	C	6	GAL	O2-C2-C1	4.77	118.92	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	GAL	O2-C2-C1	4.57	118.51	109.15
3	D	4	MAN	C1-O5-C5	4.22	117.91	112.19
2	C	6	GAL	O5-C1-C2	-3.97	104.65	110.77
2	C	6	GAL	O2-C2-C3	-3.70	102.74	110.14
3	D	6	GAL	O2-C2-C3	-3.22	103.69	110.14
3	D	3	BMA	C1-C2-C3	-3.18	105.76	109.67
3	D	6	GAL	O5-C1-C2	-3.17	105.88	110.77
2	C	1	NAG	C1-O5-C5	3.08	116.36	112.19
2	C	5	NDG	C1-O5-C5	3.02	116.29	112.19
2	C	4	MAN	C1-C2-C3	-2.76	106.27	109.67
2	C	4	MAN	O2-C2-C3	-2.71	104.70	110.14
3	D	5	NDG	C1-O5-C5	2.71	115.86	112.19
2	C	9	FUL	O5-C1-C2	-2.65	106.67	110.77
2	C	7	BMA	O3-C3-C2	2.50	114.79	109.99
2	C	7	BMA	O5-C1-C2	-2.38	107.10	110.77
2	C	9	FUL	C1-O5-C5	-2.36	107.44	112.78
2	C	4	MAN	C2-C3-C4	-2.33	106.87	110.89
2	C	3	BMA	C1-C2-C3	-2.33	106.81	109.67
3	D	5	NDG	C1-C2-N2	2.28	114.39	110.49
2	C	3	BMA	C1-O5-C5	2.26	115.26	112.19
3	D	3	BMA	C3-C4-C5	-2.01	106.66	110.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	5	NDG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	6	GAL	O5-C5-C6-O6
3	D	5	NDG	O5-C5-C6-O6
2	C	5	NDG	C4-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	5	NDG	C4-C5-C6-O6

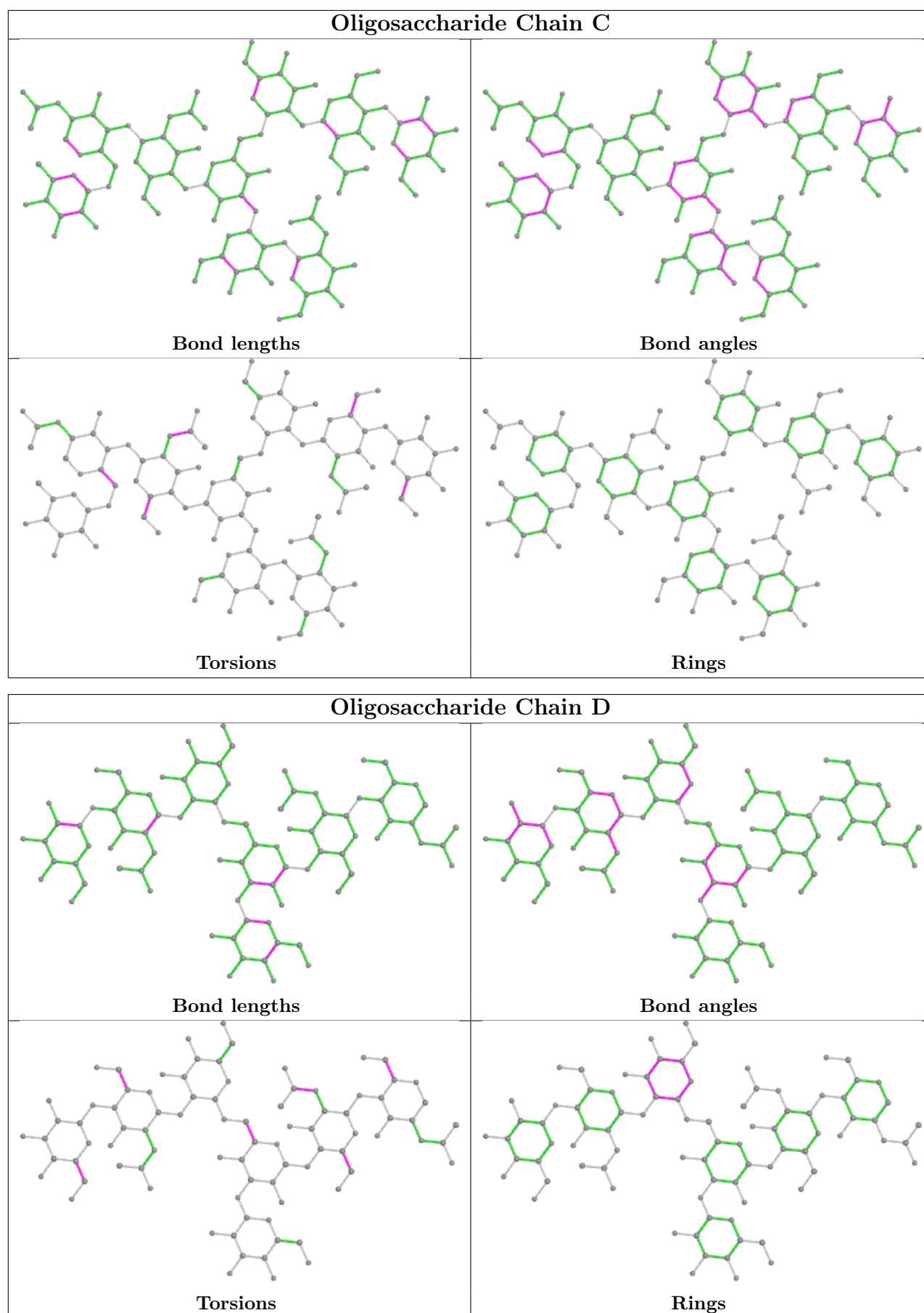
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	MAN	1	0
3	D	5	NDG	1	0
2	C	6	GAL	4	0
3	D	7	BMA	1	0
2	C	5	NDG	1	0
3	D	6	GAL	4	0
3	D	2	NAG	1	0
3	D	1	NAG	0	1
2	C	9	FUL	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/208 (100%)	0.36	5 (2%) 59 54	54, 88, 133, 159	4 (1%)
1	B	208/208 (100%)	1.35	47 (22%) 0 0	65, 119, 199, 257	3 (1%)
All	All	416/416 (100%)	0.86	52 (12%) 3 2	54, 101, 183, 257	7 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	PRO	9.0
1	B	237	GLY	7.9
1	B	299	THR	7.7
1	B	271	PRO	7.3
1	B	300	TYR	7.2
1	B	295	GLN	7.2
1	B	269	GLU	6.8
1	B	267	SER	5.3
1	B	297	ASN	5.2
1	B	323	VAL	5.1
1	B	266	VAL	5.1
1	B	294	GLU	4.9
1	B	298	SER	4.8
1	B	240	VAL	4.7
1	B	273	VAL	4.7
1	A	296	TYR	4.6
1	B	302	VAL	4.6
1	A	237	GLY	4.6
1	B	296	TYR	4.1
1	B	333	GLU	4.0
1	B	268	HIS	4.0
1	B	320	LYS	3.8
1	B	270	ASP	3.7
1	B	239	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	3.6
1	B	335	THR	3.6
1	B	402	GLY	3.4
1	B	331	PRO	3.4
1	B	384	ASN	3.3
1	B	326	LYS	3.2
1	B	241	PHE	3.2
1	B	313	TRP	3.1
1	A	298	SER	3.0
1	B	264	VAL	3.0
1	B	330	ALA	3.0
1	B	253	ILE	2.9
1	B	332	ILE	2.9
1	B	277	TRP	2.6
1	B	278	TYR	2.6
1	B	336	ILE	2.4
1	B	355	ARG	2.4
1	A	290	LYS	2.4
1	A	295	GLN	2.2
1	B	324	SER	2.2
1	B	306	LEU	2.1
1	B	307	THR	2.1
1	B	398	LEU	2.1
1	B	303	VAL	2.1
1	B	318	GLU	2.1
1	B	325	ASN	2.1
1	B	329	PRO	2.1
1	B	280	ASP	2.1

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

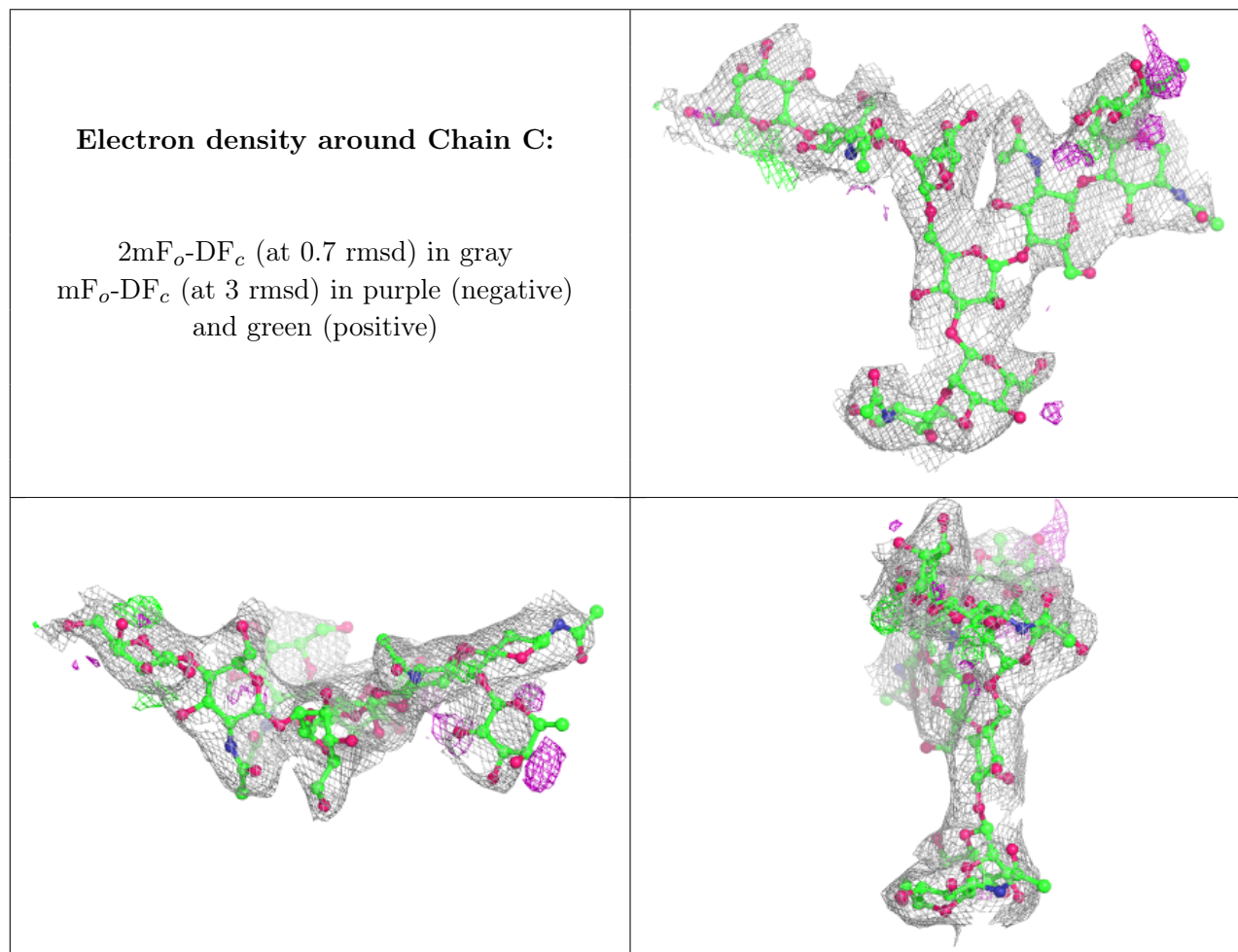
There are no non-standard protein/DNA/RNA residues in this entry.

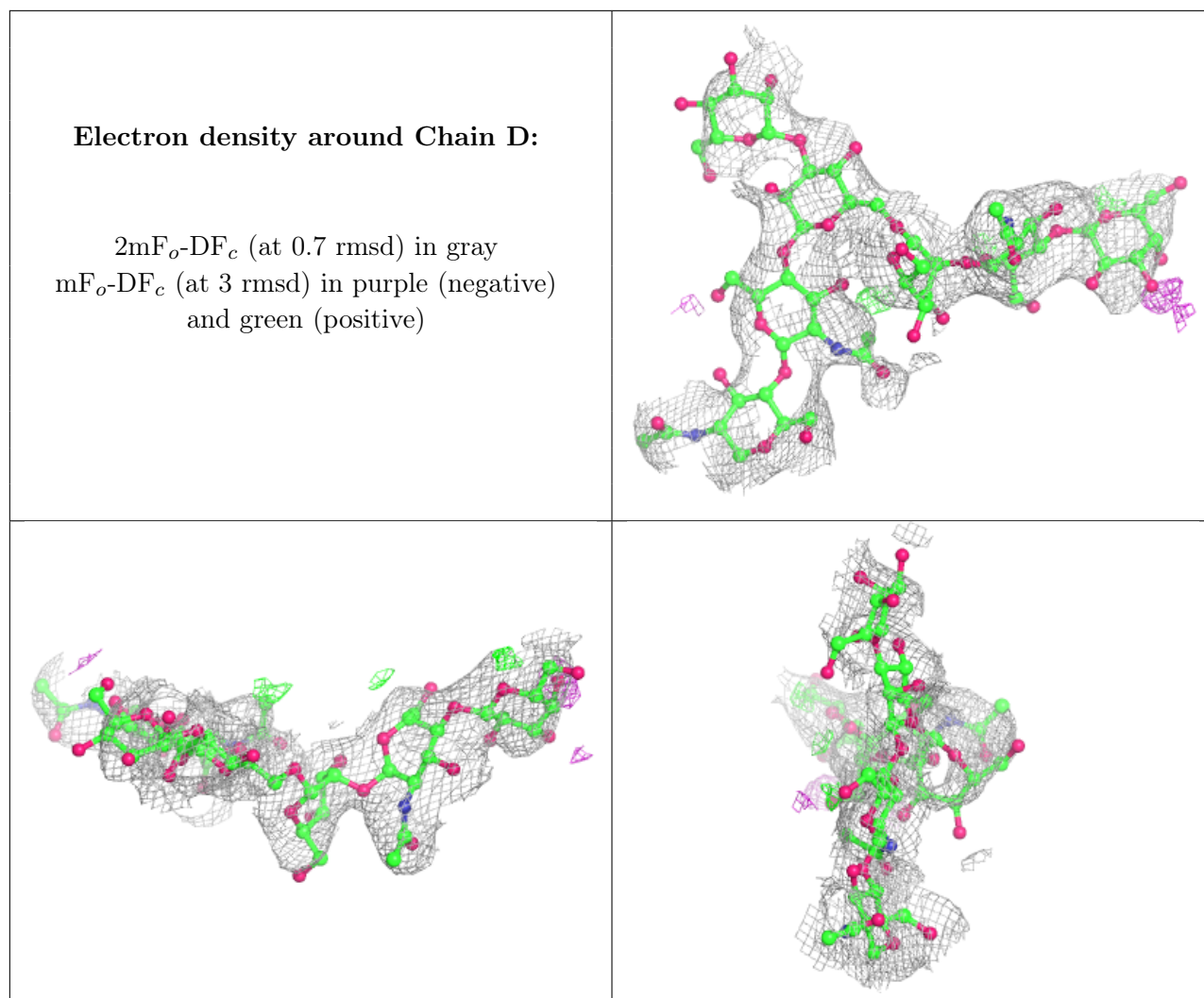
## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MAN	D	4	11/12	0.79	0.24	155,161,180,184	0
3	BMA	D	3	11/12	0.80	0.14	155,163,175,177	0
2	FUL	C	9	10/11	0.80	0.50	101,136,154,159	0
3	NAG	D	2	14/15	0.82	0.22	133,180,188,195	0
2	NAG	C	8	14/15	0.83	0.21	124,154,162,162	0
3	GAL	D	6	11/12	0.85	0.35	141,158,168,181	0
2	GAL	C	6	11/12	0.88	0.22	81,107,124,142	0
3	NAG	D	1	14/15	0.88	0.20	112,149,162,173	0
2	NAG	C	1	14/15	0.88	0.18	96,107,146,150	0
3	BMA	D	7	11/12	0.88	0.26	135,158,168,175	0
3	NDG	D	5	14/15	0.89	0.26	112,130,143,144	0
2	BMA	C	7	11/12	0.90	0.14	116,137,144,145	0
2	MAN	C	4	11/12	0.91	0.13	95,103,117,126	0
2	NDG	C	5	14/15	0.92	0.12	88,111,126,127	0
2	NAG	C	2	14/15	0.94	0.17	95,110,130,133	0
2	BMA	C	3	11/12	0.95	0.16	91,100,113,117	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.