



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 04:14 PM EDT

PDB ID : 8SM2  
Title : Crystal Structure of the macaque Fc $\alpha$ RI bound to macaque IgA Fc.  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2023-04-25  
Resolution : 3.15 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

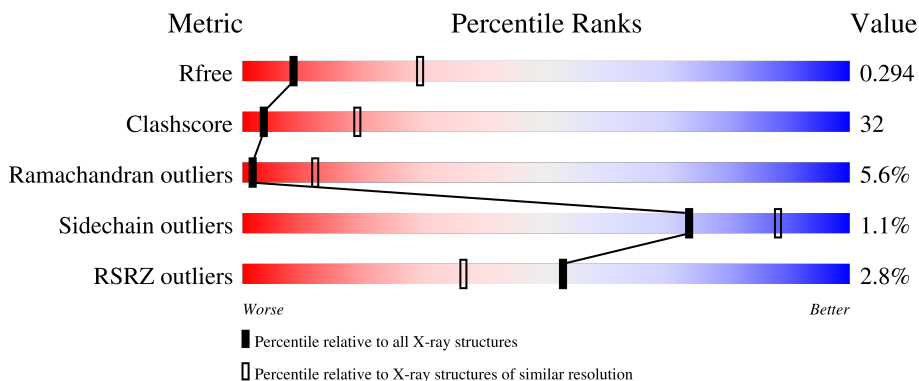
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	216	
2	C	207	
3	G	5	

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	MAN	G	4	-	-	-	X
4	NAG	C	701	-	-	-	X
4	NAG	C	703	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3241 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-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1599	1005	276	310	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	expression tag	UNP H9H2V9
A	326	ASN	ASP	conflict	UNP H9H2V9
A	454	LYS	-	expression tag	UNP H9H2V9

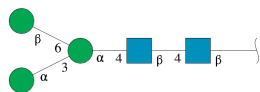
- Molecule 2 is a protein called Immunoglobulin subtype domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	190	1520	972	261	279	8	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	78	ARG	GLN	conflict	UNP G7NN72
C	202	HIS	TYR	conflict	UNP G7NN72
C	203	HIS	-	expression tag	UNP G7NN72
C	204	HIS	-	expression tag	UNP G7NN72
C	205	HIS	-	expression tag	UNP G7NN72
C	206	HIS	-	expression tag	UNP G7NN72
C	207	HIS	-	expression tag	UNP G7NN72

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-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	G	5	61	34	2	25	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).

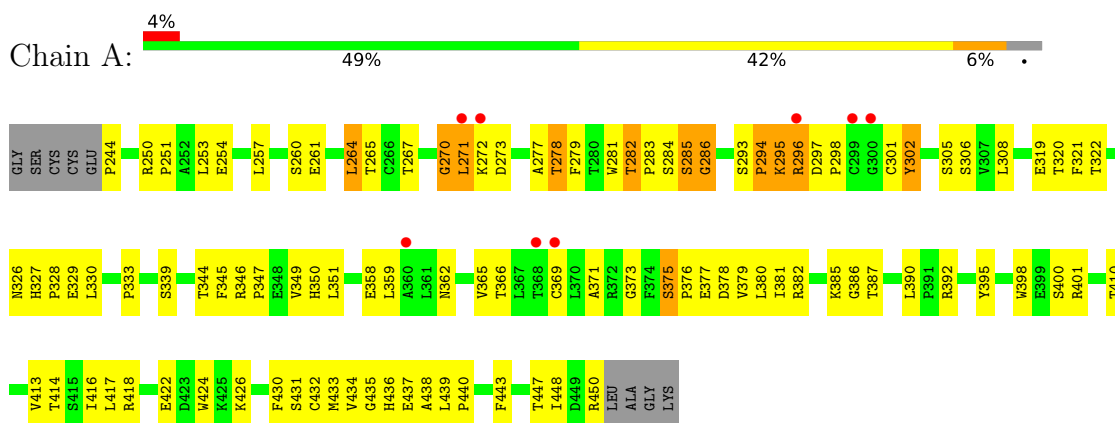


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

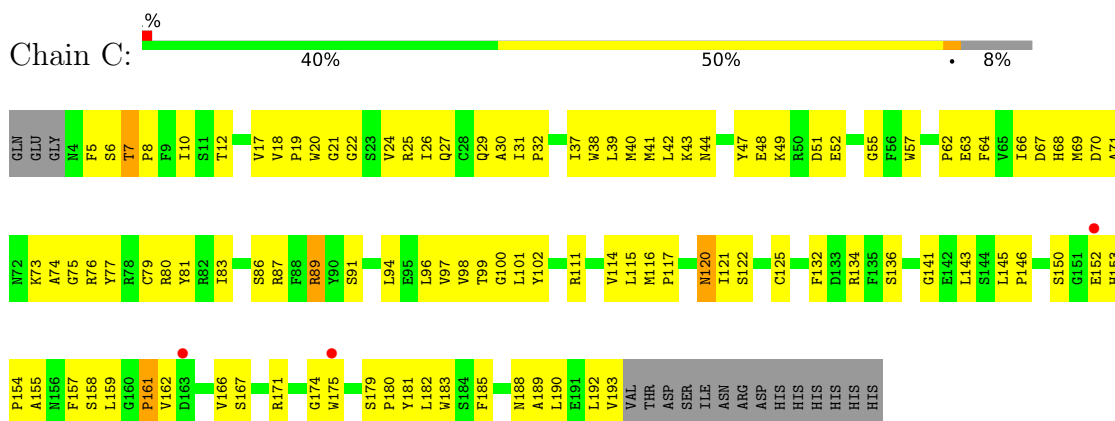
### 3 Residue-property plots [i](#)

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

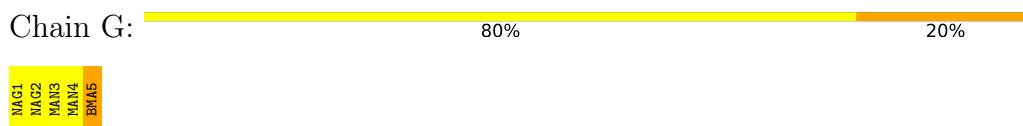
- Molecule 1: Ig-like domain-containing protein



- Molecule 2: Immunoglobulin subtype domain-containing protein



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.05Å 160.05Å 52.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.29 – 3.15 28.29 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.29-3.15) 98.0 (28.29-3.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.17Å)	Xtrriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, $R_{free}$	0.273 , 0.296 0.272 , 0.294	Depositor DCC
$R_{free}$ test set	612 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.4	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 80.2	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	0.93	EDS
Total number of atoms	3241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/1638	0.73	0/2235
2	C	0.35	0/1567	0.70	0/2131
All	All	0.34	0/3205	0.72	0/4366

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

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	1599	0	1582	101	0
2	C	1520	0	1457	105	0
3	G	61	0	52	1	0
4	C	56	0	52	4	0
5	C	5	0	0	0	0
All	All	3241	0	3143	205	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 32.

All (205) 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:282:THR:HG23	1:A:283:PRO:CD	1.65	1.24
1:A:282:THR:HG23	1:A:283:PRO:HD2	1.24	1.14
1:A:282:THR:HG21	1:A:321:PHE:HA	1.36	1.06
1:A:270:GLY:HA2	1:A:301:CYS:HA	1.37	1.06
2:C:37:ILE:HD13	2:C:57:TRP:HZ3	1.24	1.02
1:A:346:ARG:HE	1:A:440:PRO:HD3	1.24	1.00
1:A:282:THR:HG23	1:A:283:PRO:HD3	1.43	1.00
1:A:271:LEU:HD21	1:A:329:GLU:HG3	1.46	0.97
2:C:115:LEU:HD13	2:C:121:ILE:HB	1.45	0.96
1:A:270:GLY:HA2	1:A:301:CYS:CA	1.96	0.95
2:C:117:PRO:HB3	2:C:162:VAL:HB	1.49	0.95
1:A:282:THR:CG2	1:A:283:PRO:CD	2.51	0.89
2:C:136:SER:HB3	2:C:146:PRO:HG3	1.57	0.86
1:A:282:THR:CG2	1:A:283:PRO:HD3	2.06	0.85
2:C:97:VAL:HG12	2:C:181:TYR:HA	1.58	0.84
2:C:26:ILE:HD11	2:C:96:LEU:HD11	1.57	0.84
1:A:271:LEU:HD21	1:A:329:GLU:CG	2.08	0.83
2:C:66:ILE:HD11	2:C:77:TYR:CE2	2.17	0.80
1:A:282:THR:HB	1:A:322:THR:HG22	1.62	0.79
2:C:12:THR:HG22	2:C:26:ILE:HG12	1.65	0.79
1:A:279:PHE:CD2	1:A:306:SER:HB2	2.18	0.78
2:C:179:SER:HB2	2:C:182:LEU:HB2	1.67	0.77
1:A:271:LEU:HD21	1:A:329:GLU:CB	2.14	0.77
2:C:37:ILE:HD13	2:C:57:TRP:CZ3	2.16	0.76
1:A:327:HIS:CD2	1:A:329:GLU:HB3	2.21	0.76
2:C:66:ILE:HD11	2:C:77:TYR:HE2	1.50	0.74
2:C:38:TRP:HE3	2:C:80:ARG:HD3	1.51	0.74
1:A:346:ARG:NE	1:A:440:PRO:HD3	2.01	0.73
1:A:270:GLY:O	1:A:271:LEU:HB2	1.88	0.72
1:A:270:GLY:CA	1:A:301:CYS:HA	2.19	0.72
1:A:385:LYS:HG3	1:A:430:PHE:HE1	1.55	0.71
1:A:244:PRO:HG3	1:A:271:LEU:HB2	1.73	0.71
2:C:175:TRP:HD1	2:C:183:TRP:NE1	1.88	0.71
1:A:375:SER:OG	1:A:376:PRO:HD3	1.91	0.70
2:C:17:VAL:HG23	2:C:97:VAL:HG23	1.73	0.70
2:C:122:SER:HA	2:C:158:SER:HA	1.73	0.70
2:C:40:MET:HE2	2:C:49:LYS:HA	1.76	0.68
1:A:283:PRO:HG2	1:A:321:PHE:CE1	2.29	0.67
1:A:283:PRO:HG2	1:A:321:PHE:HE1	1.59	0.67
1:A:271:LEU:HD21	1:A:329:GLU:HB2	1.75	0.66
1:A:344:THR:HA	1:A:375:SER:OG	1.96	0.66
2:C:66:ILE:HG23	2:C:73:LYS:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:HIS:CD2	2:C:154:PRO:HD3	2.31	0.66
1:A:373:GLY:HA2	1:A:410:THR:HB	1.80	0.64
2:C:51:ASP:OD1	2:C:52:GLU:N	2.28	0.64
1:A:385:LYS:HB2	1:A:390:LEU:HD11	1.81	0.63
1:A:271:LEU:CD2	1:A:329:GLU:HB2	2.29	0.62
1:A:277:ALA:H	1:A:328:PRO:HD3	1.64	0.62
1:A:385:LYS:HG3	1:A:430:PHE:CE1	2.33	0.62
2:C:31:ILE:HG21	2:C:83:ILE:HD11	1.81	0.62
2:C:39:LEU:HD21	2:C:77:TYR:CD2	2.34	0.62
1:A:351:LEU:HD22	1:A:448:ILE:HB	1.81	0.62
2:C:38:TRP:HB3	2:C:40:MET:HE3	1.81	0.62
2:C:101:LEU:HD21	2:C:182:LEU:HD22	1.83	0.61
1:A:279:PHE:HD2	1:A:306:SER:HB2	1.64	0.60
2:C:74:ALA:HB1	2:C:181:TYR:HB3	1.82	0.60
2:C:8:PRO:HG3	2:C:81:TYR:CE2	2.36	0.60
1:A:284:SER:O	1:A:286:GLY:N	2.35	0.60
1:A:349:VAL:O	1:A:350:HIS:ND1	2.34	0.59
1:A:284:SER:OG	1:A:285:SER:N	2.34	0.59
1:A:379:VAL:HG21	1:A:413:VAL:HG21	1.83	0.59
1:A:253:LEU:HD21	1:A:437:GLU:HG3	1.85	0.59
1:A:347:PRO:HD2	1:A:439:LEU:HG	1.84	0.59
1:A:381:ILE:HG12	1:A:434:VAL:HG22	1.83	0.59
2:C:134:ARG:HB2	2:C:175:TRP:CE3	2.38	0.59
1:A:375:SER:HB3	1:A:436:HIS:NE2	2.18	0.59
2:C:67:ASP:OD1	2:C:68:HIS:N	2.35	0.59
2:C:30:ALA:HB2	2:C:62:PRO:HD3	1.84	0.58
2:C:83:ILE:HB	2:C:87:ARG:HB2	1.84	0.58
1:A:250:ARG:NH1	1:A:378:ASP:OD2	2.36	0.58
1:A:358:GLU:HG2	1:A:365:VAL:HG12	1.85	0.58
1:A:382:ARG:HH21	1:A:392:ARG:HH21	1.51	0.58
2:C:18:VAL:HG23	2:C:69:MET:HG2	1.86	0.57
2:C:175:TRP:CD1	2:C:183:TRP:NE1	2.69	0.57
1:A:282:THR:CB	1:A:283:PRO:HD3	2.35	0.57
2:C:159:LEU:HB3	2:C:162:VAL:HG22	1.85	0.57
1:A:377:GLU:HB2	1:A:400:SER:OG	2.04	0.57
2:C:38:TRP:HB2	2:C:80:ARG:HB3	1.87	0.57
2:C:188:ASN:OD1	2:C:189:ALA:N	2.38	0.57
1:A:347:PRO:HD3	1:A:436:HIS:CD2	2.40	0.56
1:A:366:THR:OG1	1:A:418:ARG:NH2	2.38	0.56
2:C:100:GLY:HA2	2:C:185:PHE:CD1	2.40	0.56
2:C:153:HIS:CG	2:C:154:PRO:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:O	1:A:272:LYS:C	2.44	0.56
1:A:326:ASN:HB2	1:A:333:PRO:HB3	1.86	0.56
2:C:10:ILE:HG13	2:C:94:LEU:HD13	1.85	0.56
1:A:273:ASP:HB3	1:A:328:PRO:HG2	1.87	0.56
2:C:150:SER:HB2	2:C:157:PHE:HE1	1.70	0.56
2:C:12:THR:HG23	2:C:94:LEU:HD11	1.88	0.55
1:A:257:LEU:HD23	1:A:443:PHE:CE2	2.42	0.55
1:A:295:LYS:O	1:A:297:ASP:N	2.40	0.54
2:C:111:ARG:HD2	2:C:115:LEU:CD1	2.36	0.54
2:C:158:SER:CB	4:C:704:NAG:H61	2.37	0.54
1:A:271:LEU:CD2	1:A:329:GLU:CB	2.86	0.53
1:A:251:PRO:HD3	1:A:264:LEU:HD12	1.89	0.53
2:C:122:SER:HB2	2:C:158:SER:HB2	1.90	0.53
2:C:120:ASN:OD1	2:C:120:ASN:N	2.42	0.53
2:C:41:MET:HA	2:C:76:ARG:O	2.08	0.52
2:C:38:TRP:HB3	2:C:40:MET:CE	2.39	0.52
2:C:162:VAL:HG13	2:C:166:VAL:HB	1.92	0.52
2:C:116:MET:SD	2:C:117:PRO:HD2	2.50	0.52
1:A:395:TYR:HB3	1:A:417:LEU:HD13	1.92	0.51
1:A:282:THR:CB	1:A:283:PRO:CD	2.88	0.51
2:C:19:PRO:O	2:C:22:GLY:N	2.44	0.51
2:C:171:ARG:HE	2:C:189:ALA:HB2	1.74	0.51
2:C:145:LEU:HG	2:C:146:PRO:HD2	1.93	0.51
1:A:261:GLU:O	1:A:261:GLU:HG2	2.11	0.51
1:A:301:CYS:O	1:A:302:TYR:O	2.29	0.50
2:C:8:PRO:HB2	2:C:29:GLN:HB3	1.93	0.50
1:A:270:GLY:HA2	1:A:301:CYS:C	2.32	0.50
2:C:69:MET:HG3	2:C:98:VAL:HG12	1.92	0.50
2:C:114:VAL:HG23	2:C:193:VAL:C	2.32	0.50
2:C:5:PHE:HE1	2:C:7:THR:HB	1.76	0.49
1:A:329:GLU:OE1	1:A:330:LEU:N	2.43	0.49
1:A:326:ASN:CB	1:A:333:PRO:HB3	2.42	0.49
1:A:382:ARG:NH2	1:A:392:ARG:HH21	2.10	0.49
1:A:281:TRP:CD2	1:A:308:LEU:HD23	2.48	0.49
2:C:5:PHE:CE1	2:C:7:THR:HB	2.47	0.49
1:A:424:TRP:CZ2	1:A:450:ARG:HB3	2.48	0.49
1:A:282:THR:CG2	1:A:322:THR:H	2.26	0.48
1:A:297:ASP:OD1	1:A:298:PRO:HD2	2.12	0.48
1:A:387:THR:O	1:A:387:THR:HG22	2.13	0.48
2:C:17:VAL:HG22	2:C:99:THR:HG23	1.94	0.48
2:C:27:GLN:HA	2:C:63:GLU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:PRO:CB	2:C:162:VAL:HB	2.32	0.48
2:C:26:ILE:CD1	2:C:96:LEU:HD11	2.38	0.48
1:A:385:LYS:CB	1:A:390:LEU:HD11	2.43	0.47
2:C:134:ARG:HD3	2:C:175:TRP:CZ3	2.48	0.47
2:C:141:GLY:O	2:C:143:LEU:HD12	2.15	0.47
2:C:101:LEU:CD2	2:C:182:LEU:HB3	2.44	0.47
1:A:270:GLY:HA2	1:A:301:CYS:O	2.14	0.47
1:A:277:ALA:O	1:A:278:THR:HG23	2.15	0.47
2:C:6:SER:O	2:C:7:THR:HG22	2.15	0.47
2:C:21:GLY:N	2:C:69:MET:O	2.45	0.47
2:C:111:ARG:HD2	2:C:115:LEU:HD12	1.95	0.47
2:C:167:SER:HA	2:C:192:LEU:HD22	1.96	0.47
2:C:175:TRP:NE1	2:C:180:PRO:HA	2.30	0.47
1:A:271:LEU:O	1:A:271:LEU:HG	2.15	0.47
1:A:308:LEU:HD12	1:A:308:LEU:O	2.14	0.47
2:C:8:PRO:HA	2:C:29:GLN:OE1	2.15	0.47
2:C:120:ASN:OD1	4:C:703:NAG:N2	2.48	0.47
1:A:270:GLY:HA2	1:A:301:CYS:CB	2.45	0.46
2:C:158:SER:HB3	4:C:704:NAG:C6	2.45	0.46
1:A:270:GLY:O	1:A:271:LEU:CB	2.60	0.46
2:C:30:ALA:O	2:C:32:PRO:HD3	2.15	0.46
2:C:158:SER:HB3	4:C:704:NAG:H61	1.97	0.46
1:A:359:LEU:HA	1:A:365:VAL:HG11	1.97	0.46
1:A:431:SER:OG	1:A:447:THR:HG22	2.15	0.46
1:A:253:LEU:C	1:A:380:LEU:HD11	2.36	0.46
1:A:351:LEU:HD12	1:A:432:CYS:HB2	1.98	0.46
1:A:327:HIS:HD2	1:A:329:GLU:HB3	1.76	0.46
2:C:75:GLY:HA2	2:C:181:TYR:CE2	2.51	0.45
2:C:66:ILE:CG2	2:C:73:LYS:HD3	2.46	0.45
1:A:265:THR:HA	1:A:306:SER:O	2.16	0.45
2:C:8:PRO:HG2	2:C:91:SER:HB3	1.98	0.45
1:A:297:ASP:HB3	1:A:301:CYS:HB2	1.99	0.45
2:C:18:VAL:CG2	2:C:69:MET:HG2	2.46	0.45
1:A:435:GLY:HA2	1:A:443:PHE:HA	1.99	0.45
2:C:26:ILE:O	2:C:64:PHE:N	2.47	0.45
1:A:382:ARG:HH21	1:A:392:ARG:NH2	2.14	0.45
1:A:371:ALA:HB3	1:A:413:VAL:HB	1.98	0.44
1:A:398:TRP:HZ3	1:A:416:ILE:HG23	1.81	0.44
2:C:111:ARG:HD2	2:C:115:LEU:HD11	1.98	0.44
2:C:7:THR:OG1	2:C:8:PRO:HD2	2.17	0.44
2:C:37:ILE:HA	2:C:80:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:NH1	3:G:5:BMA:O2	2.51	0.44
2:C:190:LEU:CD2	2:C:192:LEU:HB2	2.48	0.44
2:C:29:GLN:O	2:C:81:TYR:OH	2.24	0.43
2:C:125:CYS:H	2:C:155:ALA:HB3	1.83	0.43
2:C:101:LEU:HD22	2:C:182:LEU:HB3	1.99	0.43
1:A:293:SER:O	1:A:295:LYS:N	2.51	0.43
2:C:70:ASP:HB2	2:C:73:LYS:HG3	2.01	0.43
2:C:152:GLU:HG3	2:C:154:PRO:O	2.18	0.43
1:A:273:ASP:HB3	1:A:328:PRO:CG	2.47	0.43
2:C:40:MET:SD	2:C:47:TYR:HD1	2.41	0.43
2:C:114:VAL:O	2:C:114:VAL:HG13	2.18	0.43
1:A:327:HIS:HB2	1:A:328:PRO:HD2	2.01	0.43
1:A:347:PRO:HD2	1:A:439:LEU:CG	2.47	0.43
1:A:379:VAL:CG2	1:A:413:VAL:HG21	2.46	0.43
2:C:39:LEU:HB2	2:C:64:PHE:CZ	2.53	0.43
2:C:89:ARG:HE	2:C:89:ARG:HB3	1.69	0.43
1:A:433:MET:CE	2:C:55:GLY:HA2	2.49	0.43
2:C:74:ALA:CB	2:C:181:TYR:HB3	2.49	0.43
1:A:282:THR:HG21	1:A:321:PHE:CA	2.27	0.42
2:C:132:PHE:CD1	2:C:174:GLY:HA3	2.54	0.42
1:A:267:THR:HA	1:A:305:SER:HA	2.00	0.42
2:C:102:TYR:CD2	2:C:132:PHE:HE1	2.37	0.42
1:A:254:GLU:N	1:A:380:LEU:HD11	2.35	0.41
2:C:43:LYS:HB3	2:C:48:GLU:OE1	2.21	0.41
2:C:75:GLY:HA2	2:C:181:TYR:CZ	2.55	0.41
2:C:117:PRO:HB2	2:C:162:VAL:O	2.20	0.41
1:A:436:HIS:HD2	1:A:438:ALA:HB3	1.86	0.41
1:A:320:THR:HA	1:A:339:SER:HB3	2.02	0.41
2:C:24:VAL:HG22	2:C:25:ARG:H	1.85	0.41
1:A:422:GLU:O	1:A:426:LYS:HB2	2.20	0.41
2:C:31:ILE:HD12	2:C:81:TYR:CG	2.56	0.41
2:C:38:TRP:NE1	2:C:52:GLU:HG3	2.36	0.41
2:C:39:LEU:HB2	2:C:64:PHE:CE1	2.55	0.41
2:C:117:PRO:O	2:C:161:PRO:HA	2.21	0.41
2:C:69:MET:CG	2:C:98:VAL:HG12	2.51	0.41
1:A:301:CYS:O	1:A:302:TYR:C	2.59	0.40
2:C:10:ILE:CG2	2:C:94:LEU:HB2	2.51	0.40
2:C:20:TRP:HE1	2:C:71:ALA:H	1.70	0.40
1:A:294:PRO:O	1:A:296:ARG:N	2.55	0.40
1:A:369:CYS:O	1:A:414:THR:HA	2.22	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	205/216 (95%)	158 (77%)	30 (15%)	17 (8%)	1	4
2	C	188/207 (91%)	153 (81%)	30 (16%)	5 (3%)	5	27
All	All	393/423 (93%)	311 (79%)	60 (15%)	22 (6%)	2	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	LEU
1	A	278	THR
1	A	282	THR
1	A	285	SER
1	A	296	ARG
1	A	319	GLU
1	A	345	PHE
1	A	375	SER
2	C	7	THR
1	A	286	GLY
1	A	295	LYS
1	A	362	ASN
1	A	386	GLY
2	C	42	LEU
1	A	270	GLY
1	A	264	LEU
1	A	302	TYR
2	C	44	ASN
2	C	86	SER
1	A	260	SER
2	C	161	PRO
1	A	294	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	181/187 (97%)	180 (99%)	1 (1%)	86	94
2	C	168/184 (91%)	165 (98%)	3 (2%)	59	81
All	All	349/371 (94%)	345 (99%)	4 (1%)	73	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	ARG
2	C	79	CYS
2	C	89	ARG
2	C	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	177	ASN

### 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](#)

5 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	G	1	3,1	14,14,15	1.69	1 (7%)	17,19,21	1.17	2 (11%)
3	NAG	G	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.71	0
3	MAN	G	3	3	11,11,12	0.92	1 (9%)	15,15,17	1.12	1 (6%)
3	MAN	G	4	3	11,11,12	1.18	1 (9%)	15,15,17	1.67	3 (20%)
3	BMA	G	5	3	11,11,12	0.84	1 (9%)	15,15,17	0.95	1 (6%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	MAN	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	BMA	G	5	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-6.08	1.34	1.43
3	G	4	MAN	C1-C2	3.21	1.59	1.52
3	G	5	BMA	C1-C2	2.41	1.57	1.52
3	G	3	MAN	O5-C1	-2.26	1.40	1.43
3	G	2	NAG	O5-C1	-2.17	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4	MAN	C1-O5-C5	4.23	117.92	112.19
3	G	1	NAG	C1-O5-C5	-3.72	107.16	112.19
3	G	4	MAN	C1-C2-C3	2.77	113.07	109.67
3	G	4	MAN	O5-C1-C2	2.52	114.66	110.77
3	G	5	BMA	O2-C2-C3	-2.26	105.60	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	O2-C2-C3	-2.20	105.72	110.14
3	G	1	NAG	C3-C4-C5	2.15	114.07	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

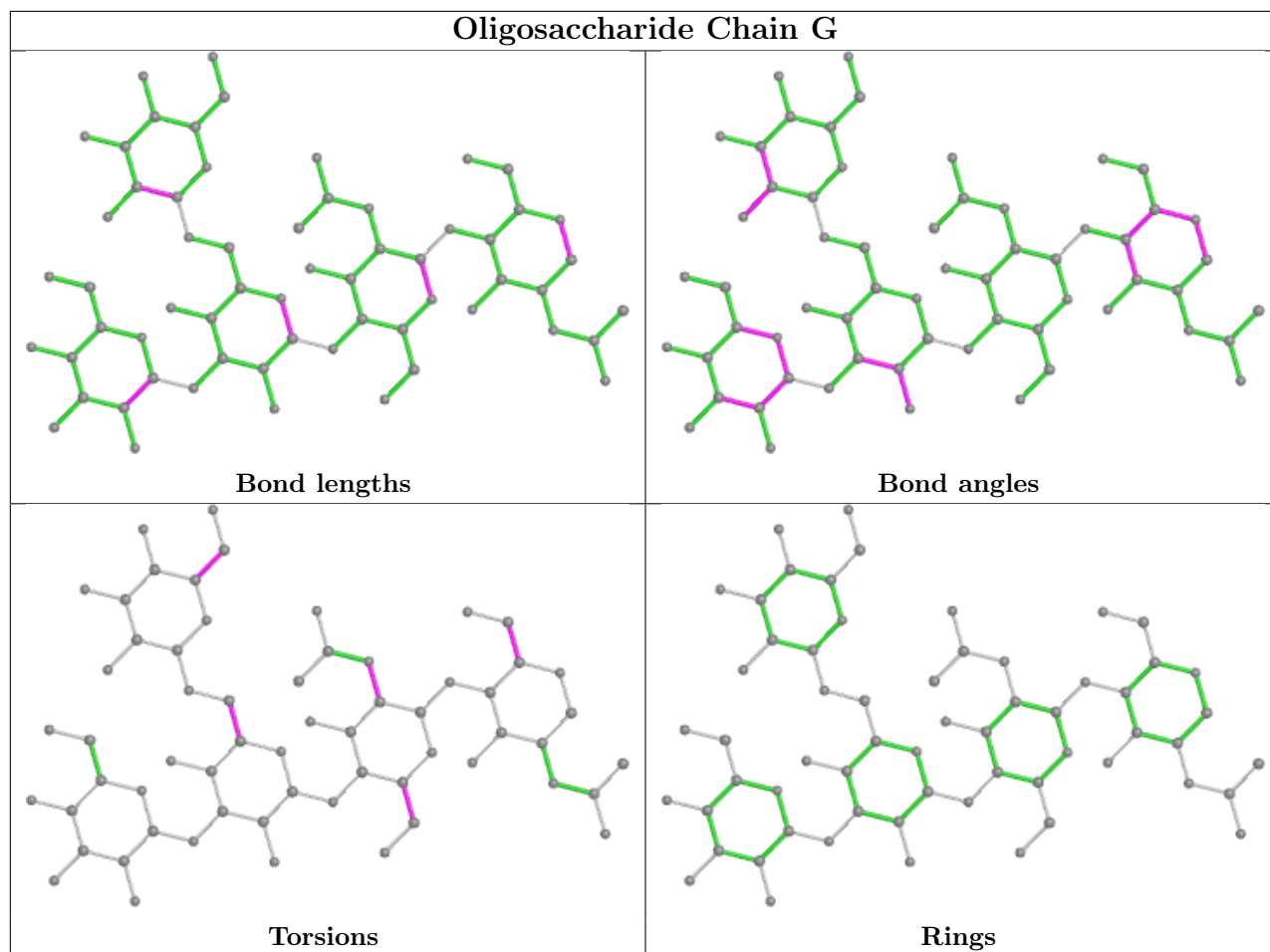
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	5	BMA	C4-C5-C6-O6
3	G	5	BMA	O5-C5-C6-O6
3	G	3	MAN	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	G	3	MAN	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5	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](#)

5 ligands 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$
4	NAG	C	701	2	14,14,15	0.39	0	17,19,21	0.63	0
4	NAG	C	704	2	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
4	NAG	C	702	2	14,14,15	0.20	0	17,19,21	0.41	0
5	SO4	C	705	-	4,4,4	0.29	0	6,6,6	0.68	0
4	NAG	C	703	2	14,14,15	0.29	0	17,19,21	0.58	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
4	NAG	C	703	2	-	4/6/23/26	0/1/1/1
4	NAG	C	701	2	-	3/6/23/26	0/1/1/1
4	NAG	C	704	2	-	2/6/23/26	0/1/1/1
4	NAG	C	702	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	704	NAG	O5-C1	-2.50	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	704	NAG	C4-C5-C6-O6
4	C	701	NAG	O5-C5-C6-O6
4	C	704	NAG	O5-C5-C6-O6
4	C	701	NAG	C4-C5-C6-O6
4	C	703	NAG	C8-C7-N2-C2
4	C	703	NAG	O7-C7-N2-C2
4	C	701	NAG	C1-C2-N2-C7
4	C	703	NAG	C4-C5-C6-O6
4	C	703	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	704	NAG	3	0
4	C	703	NAG	1	0

## 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, 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	207/216 (95%)	-0.18	8 (3%) 39 24	75, 133, 222, 358	0
2	C	190/207 (91%)	-0.18	3 (1%) 72 59	116, 156, 238, 318	0
All	All	397/423 (93%)	-0.18	11 (2%) 53 36	75, 146, 238, 358	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLY	4.1
1	A	271	LEU	2.6
1	A	296	ARG	2.5
1	A	272	LYS	2.5
1	A	368	THR	2.5
1	A	299	CYS	2.5
1	A	369	CYS	2.5
2	C	175	TRP	2.4
2	C	163	ASP	2.3
1	A	360	ALA	2.2
2	C	152	GLU	2.1

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

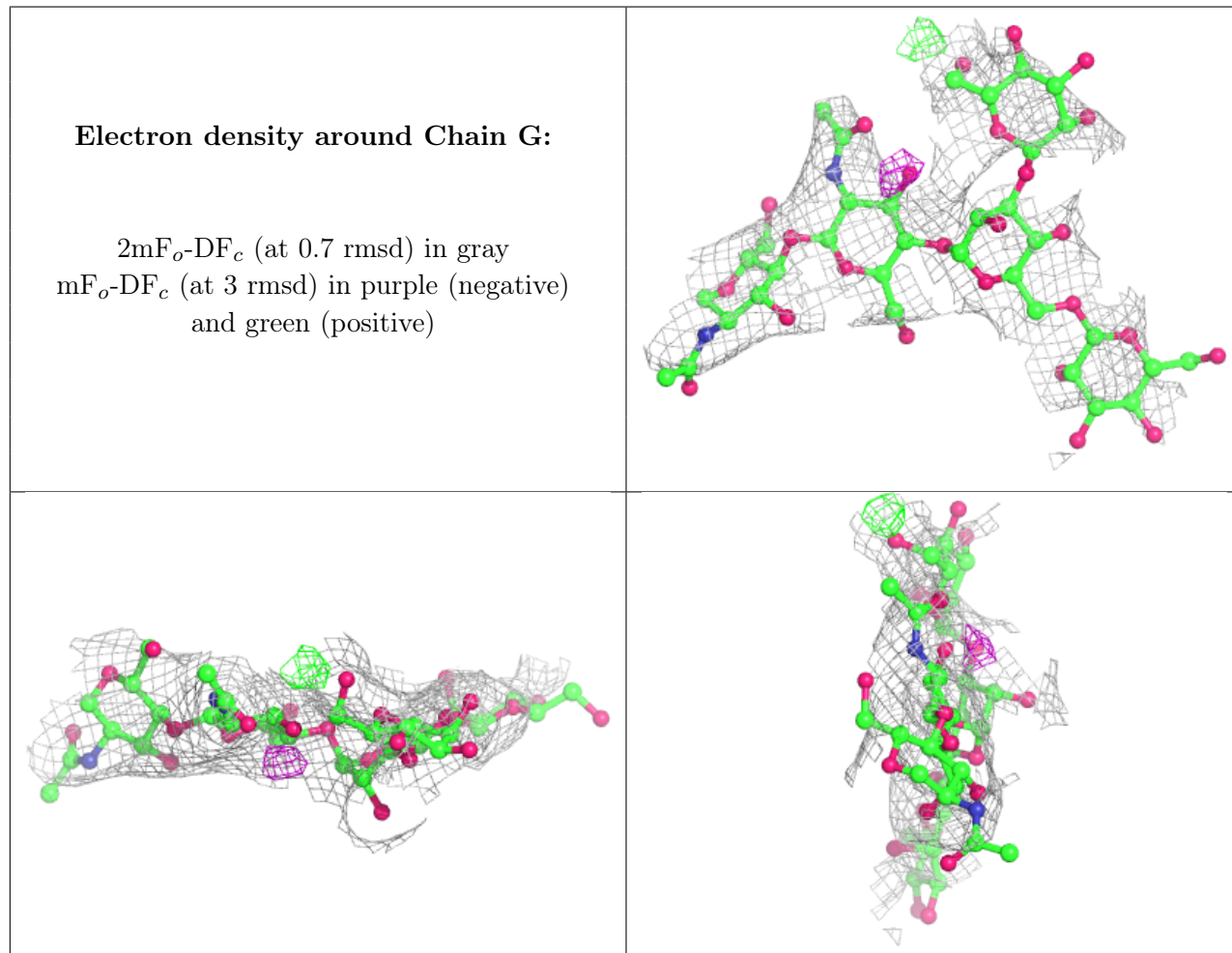
There are no non-standard protein/DNA/RNA residues in this entry.

### 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	G	4	11/12	0.31	0.45	258,292,304,306	0
3	BMA	G	5	11/12	0.65	0.37	267,275,291,292	0
3	MAN	G	3	11/12	0.73	0.25	254,263,272,278	0
3	NAG	G	2	14/15	0.80	0.31	198,216,257,266	0
3	NAG	G	1	14/15	0.95	0.29	171,190,209,214	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](#)

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
4	NAG	C	702	14/15	0.60	0.36	182,240,260,270	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	701	14/15	0.67	0.47	254,294,311,331	0
4	NAG	C	704	14/15	0.72	0.35	173,219,240,272	0
4	NAG	C	703	14/15	0.74	0.51	243,271,285,298	0
5	SO4	C	705	5/5	0.89	0.12	196,233,249,359	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.