



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:12 AM BST

PDB ID : 6MDV  
Title : Crystal structure of Streptococcus pyogenes endo-beta-N-acetylglucosaminidase (EndoS2) with high-mannose glycan  
Authors : Klontz, E.H.; Trastoy, B.; Orwenyo, J.; Wang, L.X.; Guerin, M.E.; Sundberg, E.J.  
Deposited on : 2018-09-05  
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](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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

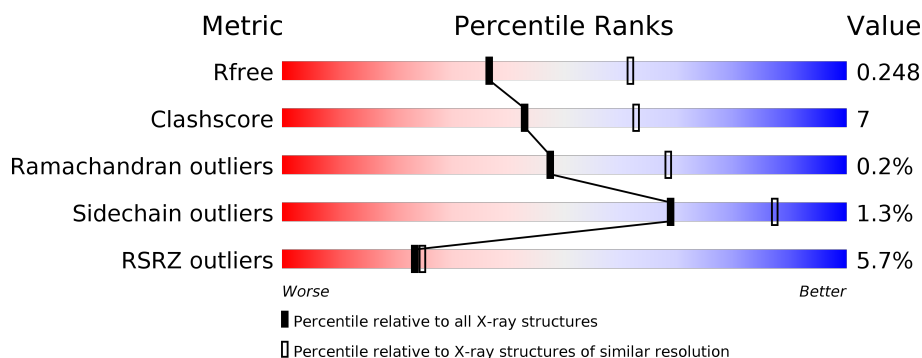
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	802	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	B	802	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div></div> </div> <div></div> </div>
2	C	8	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
3	D	7	<div> <div></div> <div> <div>57%</div> <div>43%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	C	7	-	-	-	X
2	MAN	C	8	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13060 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.

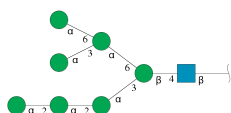
- Molecule 1 is a protein called Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6260	3925	1066	1254	15			
1	B	787	Total	C	N	O	S	0	0	0
			6254	3922	1066	1251	15			

There are 4 discrepancies between the modelled and reference sequences:

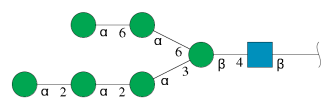
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP T1WGN1
A	844	LEU	-	expression tag	UNP T1WGN1
B	43	MET	-	initiating methionine	UNP T1WGN1
B	844	LEU	-	expression tag	UNP T1WGN1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			92	50	1	41			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			81	44	1	36			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

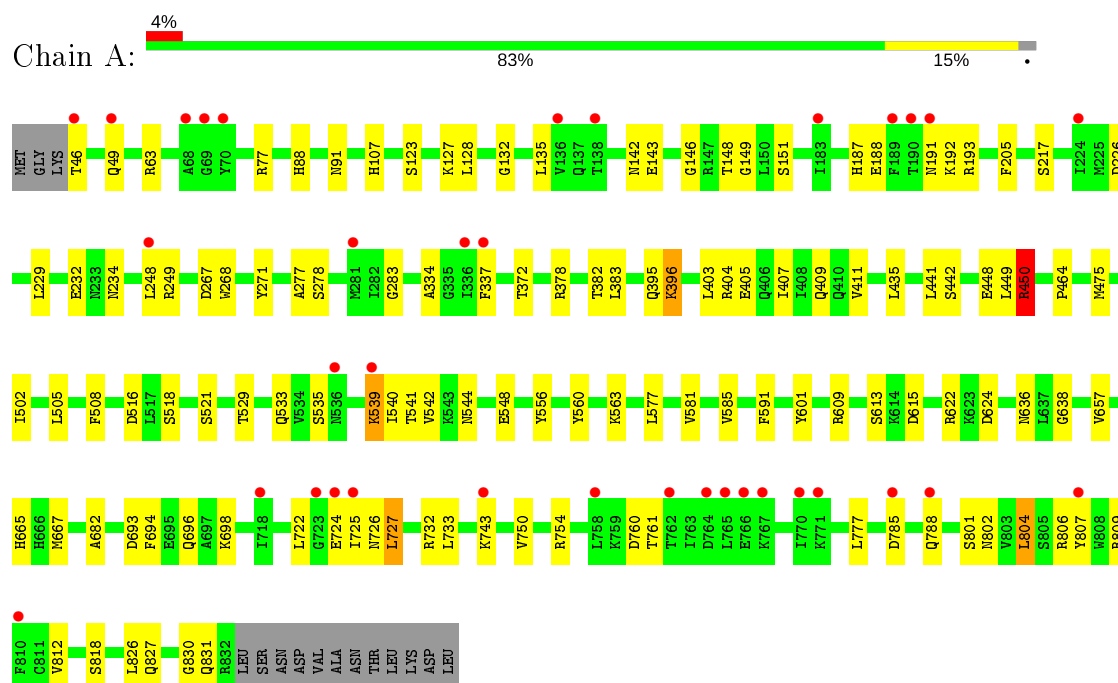
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total	O	0	0
			207	207		
5	B	164	Total	O	0	0
			164	164		

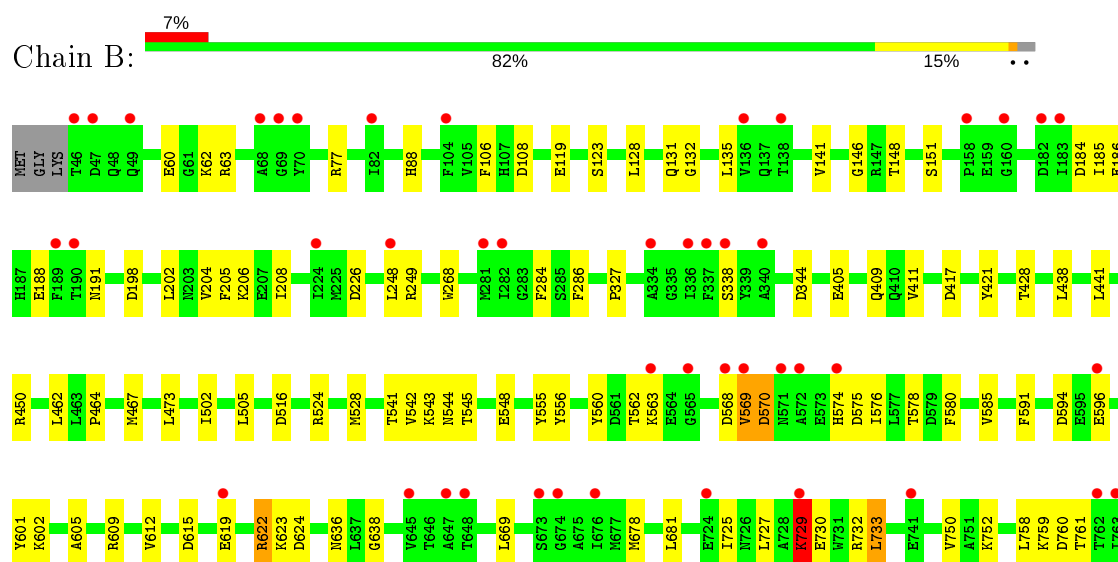
### 3 Residue-property plots

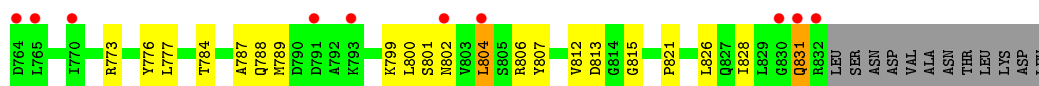
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endo-beta-N-acetylglucosaminidase



#### • Molecule 1: Endo-beta-N-acetylglucosaminidase





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

Chain C:  75% 25%



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

Chain D:  57% 43%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.97Å 105.35Å 257.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.50 29.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.63-2.50) 100.0 (29.63-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.198 , 0.248 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	4299 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	1/6378 (0.0%)	0.68	7/8621 (0.1%)
1	B	0.45	2/6371 (0.0%)	0.65	4/8612 (0.0%)
All	All	0.46	3/12749 (0.0%)	0.67	11/17233 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	LYS	CD-CE	6.44	1.67	1.51
1	B	729	LYS	CE-NZ	-6.36	1.33	1.49
1	B	729	LYS	CD-CE	-6.00	1.36	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	LEU	CA-CB-CG	8.03	133.77	115.30
1	A	396	LYS	CB-CG-CD	7.85	132.01	111.60
1	B	831	GLN	CA-CB-CG	-7.44	97.03	113.40
1	A	396	LYS	CG-CD-CE	-6.45	92.56	111.90
1	A	539	LYS	CA-CB-CG	-6.39	99.35	113.40
1	B	729	LYS	CA-CB-CG	6.02	126.64	113.40
1	A	450	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	B	569	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	A	217	SER	CB-CA-C	5.36	120.29	110.10
1	A	727	LEU	CA-CB-CG	-5.06	103.66	115.30
1	B	804	LEU	CA-CB-CG	5.03	126.86	115.30

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	6260	0	6056	77	0
1	B	6254	0	6058	93	0
2	C	92	0	78	3	0
3	D	81	0	69	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	207	0	0	2	0
5	B	164	0	0	3	0
All	All	13060	0	12261	170	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 (170) 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:576:ILE:HD11	1:B:669:LEU:HD22	1.52	0.90
1:A:192:LYS:HD3	1:A:193:ARG:H	1.42	0.85
1:B:727:LEU:CD1	1:B:729:LYS:HD2	2.08	0.82
1:A:405:GLU:O	1:A:409:GLN:HG3	1.82	0.80
1:A:724:GLU:OE1	1:A:726:ASN:ND2	2.16	0.78
1:A:448:GLU:OE2	1:A:450:ARG:NH2	2.17	0.77
1:A:785:ASP:OD2	1:A:788:GLN:NE2	2.18	0.76
1:B:541:THR:HG23	1:B:544:ASN:H	1.49	0.76
1:B:63:ARG:NH2	1:B:132:GLY:O	2.15	0.76
1:A:636:ASN:HB3	1:A:638:GLY:H	1.50	0.76
1:B:636:ASN:HB3	1:B:638:GLY:H	1.50	0.75
1:B:678:MET:HA	1:B:831:GLN:HE21	1.51	0.75
1:B:800:LEU:O	1:B:802:ASN:N	2.21	0.74
1:A:806:ARG:NH1	1:A:807:TYR:OH	2.21	0.73
1:B:560:TYR:O	1:B:563:LYS:NZ	2.23	0.71
1:B:541:THR:CG2	1:B:544:ASN:H	2.04	0.70
1:B:678:MET:HA	1:B:831:GLN:NE2	2.06	0.70
1:B:405:GLU:O	1:B:409:GLN:HG3	1.91	0.70
1:A:192:LYS:HD3	1:A:193:ARG:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:TYR:O	1:A:563:LYS:NZ	2.19	0.70
1:B:619:GLU:HG2	1:B:622:ARG:NH1	2.07	0.70
1:A:539:LYS:HG3	1:A:540:ILE:N	2.06	0.69
1:B:681:LEU:N	1:B:828:ILE:O	2.27	0.66
1:B:541:THR:HG22	1:B:544:ASN:CG	2.17	0.65
1:A:548:GLU:OE2	1:A:609:ARG:HD2	1.98	0.64
1:A:46:THR:HB	1:A:49:GLN:HG3	1.80	0.63
1:B:733:LEU:HD12	1:B:826:LEU:HD13	1.80	0.63
1:A:142:ASN:HB3	1:A:148:THR:HG22	1.81	0.63
1:B:417:ASP:OD2	5:B:1001:HOH:O	2.16	0.63
1:A:146:GLY:N	1:A:151:SER:OG	2.31	0.62
1:A:542:VAL:HG22	1:A:609:ARG:HD3	1.83	0.61
1:A:505:LEU:HD21	1:A:508:PHE:HB3	1.82	0.61
1:B:727:LEU:HD11	1:B:729:LYS:HZ2	1.65	0.60
1:B:619:GLU:HA	1:B:622:ARG:HG2	1.82	0.60
1:B:750:VAL:HG13	1:B:812:VAL:HG13	1.84	0.59
1:B:268:TRP:CD1	1:B:327:PRO:HB3	2.38	0.59
1:A:143:GLU:O	1:A:151:SER:HB2	2.02	0.59
1:B:732:ARG:NH1	5:B:1010:HOH:O	2.34	0.59
1:A:395:GLN:HA	1:A:404:ARG:NH1	2.17	0.58
1:A:777:LEU:O	1:A:809:ARG:NH1	2.36	0.58
1:B:555:TYR:HA	1:B:623:LYS:HE3	1.85	0.58
1:A:187:HIS:HD2	1:A:188:GLU:N	2.02	0.57
1:B:727:LEU:HD12	1:B:729:LYS:HD2	1.87	0.57
1:A:188:GLU:OE1	2:C:7:MAN:H62	2.05	0.56
1:A:63:ARG:NH2	1:A:132:GLY:O	2.25	0.55
1:A:283:GLY:HA3	1:A:337:PHE:CZ	2.42	0.55
1:B:542:VAL:HG22	1:B:609:ARG:HD3	1.87	0.55
1:B:727:LEU:HA	1:B:804:LEU:HD23	1.88	0.55
1:B:202:LEU:HG	1:B:206:LYS:HE2	1.89	0.55
1:A:142:ASN:ND2	2:C:7:MAN:H61	2.23	0.54
1:B:760:ASP:O	1:B:761:THR:OG1	2.24	0.54
1:B:568:ASP:HB2	1:B:570:ASP:OD1	2.08	0.54
1:B:806:ARG:HD3	1:B:807:TYR:CE2	2.43	0.54
1:A:107:HIS:CE1	2:C:8:MAN:H62	2.42	0.54
1:A:726:ASN:HB3	1:A:831:GLN:O	2.07	0.54
1:B:428:THR:HG22	1:B:450:ARG:HB2	1.90	0.53
1:A:725:ILE:HD11	1:A:804:LEU:HB2	1.91	0.53
1:B:615:ASP:N	1:B:615:ASP:OD1	2.38	0.53
1:A:806:ARG:HD3	1:A:807:TYR:CE2	2.45	0.52
1:A:806:ARG:HD3	1:A:807:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:GLU:OE2	1:B:609:ARG:HD2	2.10	0.52
1:B:188:GLU:HG2	1:B:191:ASN:O	2.10	0.52
1:A:556:TYR:OH	1:A:624:ASP:O	2.27	0.51
1:A:724:GLU:HG2	1:A:725:ILE:H	1.73	0.51
1:A:518:SER:OG	1:A:601:TYR:HE1	1.94	0.51
1:A:665:HIS:CD2	1:A:667:MET:HE2	2.45	0.51
1:B:198:ASP:OD2	5:B:1002:HOH:O	2.19	0.51
1:A:581:VAL:HG21	1:A:657:VAL:HG21	1.93	0.51
1:B:725:ILE:HG12	1:B:806:ARG:HB2	1.92	0.51
1:B:541:THR:HG23	1:B:543:LYS:N	2.26	0.51
1:A:187:HIS:CD2	1:A:188:GLU:N	2.79	0.50
1:A:383:LEU:C	1:A:383:LEU:HD23	2.31	0.50
1:B:60:GLU:OE1	1:B:62:LYS:HE2	2.11	0.50
1:A:694:PHE:CE2	1:A:698:LYS:HE3	2.47	0.50
1:B:467:MET:CE	1:B:473:LEU:HB2	2.42	0.50
1:B:570:ASP:OD2	1:B:574:HIS:NE2	2.38	0.50
1:B:602:LYS:HG2	1:B:612:VAL:HG11	1.94	0.50
1:B:773:ARG:O	1:B:777:LEU:HD12	2.12	0.49
1:B:146:GLY:N	1:B:151:SER:OG	2.42	0.49
1:A:727:LEU:HD11	1:A:802:ASN:HB3	1.92	0.49
1:B:502:ILE:HG22	1:B:505:LEU:HB2	1.95	0.49
1:A:541:THR:HG23	1:A:544:ASN:H	1.77	0.49
1:B:467:MET:HE1	1:B:473:LEU:HB2	1.94	0.49
1:A:188:GLU:HG2	1:A:191:ASN:O	2.13	0.48
1:B:284:PHE:CZ	1:B:338:SER:HB3	2.47	0.48
1:B:516:ASP:OD1	1:B:601:TYR:OH	2.18	0.48
1:B:108:ASP:OD2	3:D:2:BMA:H62	2.14	0.48
1:B:148:THR:HG21	3:D:7:MAN:H61	1.96	0.48
1:A:518:SER:OG	1:A:601:TYR:CE1	2.66	0.47
1:B:585:VAL:HG12	1:B:591:PHE:HA	1.95	0.47
1:B:815:GLY:HA3	1:B:821:PRO:HG3	1.96	0.47
1:B:752:LYS:HE2	1:B:788:GLN:NE2	2.30	0.47
1:B:594:ASP:CG	1:B:596:GLU:HG2	2.35	0.47
1:A:123:SER:O	1:A:127:LYS:HG3	2.15	0.47
1:A:585:VAL:HG12	1:A:591:PHE:HA	1.95	0.47
1:A:378:ARG:O	1:A:382:THR:HG23	2.14	0.47
1:B:141:VAL:HB	1:B:185:ILE:HG12	1.97	0.47
1:B:441:LEU:O	1:B:464:PRO:HB3	2.15	0.47
1:B:727:LEU:CD1	1:B:729:LYS:NZ	2.76	0.47
1:A:143:GLU:OE2	1:A:149:GLY:HA3	2.14	0.46
1:A:232:GLU:CD	1:A:232:GLU:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:OD1	1:B:186:GLU:HG3	2.15	0.46
1:B:562:THR:HG21	1:B:580:PHE:CE2	2.50	0.46
1:A:128:LEU:HD12	1:A:135:LEU:HD21	1.98	0.46
1:B:773:ARG:HG3	1:B:777:LEU:CD1	2.46	0.46
1:B:556:TYR:CE2	1:B:623:LYS:HD2	2.51	0.46
1:A:754:ARG:HG2	1:A:788:GLN:OE1	2.16	0.46
1:B:727:LEU:HD11	1:B:729:LYS:NZ	2.31	0.46
1:B:727:LEU:HD13	1:B:729:LYS:HD2	1.93	0.46
1:A:187:HIS:HD2	1:A:188:GLU:C	2.20	0.45
1:B:759:LYS:HG3	1:B:784:THR:OG1	2.17	0.45
1:A:226:ASP:HA	1:A:248:LEU:O	2.17	0.45
1:A:268:TRP:CH2	1:A:277:ALA:HA	2.51	0.45
1:A:502:ILE:HG22	1:A:505:LEU:HB2	1.97	0.45
1:A:727:LEU:O	1:A:830:GLY:HA3	2.17	0.45
1:B:636:ASN:O	1:B:732:ARG:NH2	2.50	0.45
1:B:787:ALA:HB2	1:B:800:LEU:CD2	2.47	0.45
1:A:403:LEU:HD22	1:A:435:LEU:HA	1.98	0.45
1:A:726:ASN:O	1:A:804:LEU:HB2	2.16	0.45
1:B:467:MET:HE2	1:B:473:LEU:HD22	1.99	0.45
1:B:727:LEU:HD21	1:B:802:ASN:HB3	2.00	0.44
1:A:529:THR:O	1:A:533:GLN:HG2	2.18	0.44
1:B:555:TYR:CA	1:B:623:LYS:HE3	2.47	0.44
1:A:407:ILE:O	1:A:411:VAL:HG22	2.18	0.44
1:A:732:ARG:HB3	1:A:827:GLN:HB2	1.99	0.44
1:B:727:LEU:HD13	1:B:727:LEU:C	2.38	0.44
1:B:788:GLN:HG3	1:B:789:MET:N	2.32	0.43
1:B:730:GLU:CD	1:B:799:LYS:HG2	2.38	0.43
1:A:516:ASP:O	1:A:521:SER:OG	2.27	0.43
1:B:286:PHE:CE1	1:B:344:ASP:HA	2.54	0.43
1:A:267:ASP:HB3	1:A:271:TYR:CE2	2.54	0.43
1:B:752:LYS:HG3	1:B:813:ASP:HB2	2.00	0.43
1:A:750:VAL:HG13	1:A:812:VAL:HG13	2.00	0.43
1:A:449:LEU:O	1:A:475:MET:HA	2.19	0.43
1:B:411:VAL:HG13	1:B:421:TYR:HB2	2.01	0.43
1:B:106:PHE:CE2	3:D:1:NAG:H82	2.54	0.43
1:B:562:THR:HG21	1:B:580:PHE:CD2	2.54	0.43
1:B:727:LEU:CD1	1:B:729:LYS:HZ2	2.28	0.43
1:B:605:ALA:HA	1:B:609:ARG:O	2.19	0.42
1:B:148:THR:O	1:B:151:SER:HB3	2.19	0.42
1:B:467:MET:HB3	1:B:467:MET:HE3	1.74	0.42
1:A:278:SER:O	1:A:334:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLU:HG2	1:A:725:ILE:N	2.34	0.42
1:B:524:ARG:O	1:B:528:MET:HG3	2.20	0.42
1:B:438:LEU:HB3	1:B:462:LEU:O	2.20	0.42
1:B:545:THR:OG1	1:B:609:ARG:NH2	2.48	0.42
1:B:758:LEU:HD12	1:B:758:LEU:O	2.19	0.42
1:B:428:THR:HA	1:B:450:ARG:O	2.20	0.41
1:A:77:ARG:HA	1:A:88:HIS:O	2.20	0.41
1:A:91:ASN:OD1	1:A:372:THR:HG22	2.21	0.41
1:B:128:LEU:O	1:B:131:GLN:HG2	2.20	0.41
1:B:226:ASP:HA	1:B:248:LEU:O	2.20	0.41
1:A:383:LEU:HD23	1:A:383:LEU:O	2.21	0.41
1:B:77:ARG:HA	1:B:88:HIS:O	2.21	0.41
1:B:773:ARG:O	1:B:776:TYR:HB3	2.21	0.41
1:A:682:ALA:HA	1:A:722:LEU:HD22	2.02	0.41
1:A:77:ARG:NH1	5:A:1018:HOH:O	2.44	0.41
1:A:396:LYS:CE	5:A:1001:HOH:O	2.65	0.41
1:B:119:GLU:O	1:B:123:SER:HB3	2.20	0.40
1:B:575:ASP:HB3	1:B:578:THR:HB	2.02	0.40
1:A:229:LEU:HB2	1:A:234:ASN:ND2	2.36	0.40
1:A:441:LEU:O	1:A:464:PRO:HB3	2.20	0.40
1:A:760:ASP:O	1:A:761:THR:OG1	2.23	0.40
1:B:204:VAL:O	1:B:208:ILE:HG13	2.21	0.40
1:B:541:THR:HG23	1:B:543:LYS:H	1.84	0.40
1:B:556:TYR:OH	1:B:624:ASP:O	2.35	0.40
1:A:577:LEU:HA	1:A:577:LEU:HD23	1.96	0.40
1:A:693:ASP:OD2	1:A:696:GLN:HG2	2.21	0.40
1:A:541:THR:HG22	1:A:544:ASN:CG	2.41	0.40
1:A:733:LEU:HD12	1:A:826:LEU:HD13	2.03	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	785/802 (98%)	758 (97%)	26 (3%)	1 (0%)	51 73
1	B	785/802 (98%)	754 (96%)	29 (4%)	2 (0%)	41 61
All	All	1570/1604 (98%)	1512 (96%)	55 (4%)	3 (0%)	47 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	801	SER
1	A	801	SER
1	B	569	VAL

### 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	679/699 (97%)	669 (98%)	10 (2%)	65 85
1	B	678/699 (97%)	671 (99%)	7 (1%)	76 90
All	All	1357/1398 (97%)	1340 (99%)	17 (1%)	69 87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	PHE
1	A	249	ARG
1	A	442	SER
1	A	450	ARG
1	A	535	SER
1	A	613	SER
1	A	615	ASP
1	A	622	ARG
1	A	743	LYS
1	A	818	SER
1	B	135	LEU
1	B	205	PHE
1	B	249	ARG

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Mol	Chain	Res	Type
1	B	570	ASP
1	B	622	ARG
1	B	729	LYS
1	B	733	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	782	ASN
1	B	445	GLN
1	B	571	ASN
1	B	802	ASN
1	B	831	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 ⓘ

15 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	15,15,15	1.21	2 (13%)	21,21,21	1.46	3 (14%)
2	BMA	C	2	2	11,11,12	1.16	1 (9%)	15,15,17	1.20	2 (13%)
2	MAN	C	3	2	11,11,12	1.02	1 (9%)	15,15,17	1.33	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	C	4	2	11,11,12	1.40	1 (9%)	15,15,17	1.20	1 (6%)
2	MAN	C	5	2	11,11,12	1.49	2 (18%)	15,15,17	1.28	1 (6%)
2	MAN	C	6	2	11,11,12	1.91	2 (18%)	15,15,17	1.41	2 (13%)
2	MAN	C	7	2	11,11,12	2.07	3 (27%)	15,15,17	1.14	1 (6%)
2	MAN	C	8	2	11,11,12	2.00	2 (18%)	15,15,17	1.22	3 (20%)
3	NAG	D	1	3	15,15,15	0.98	1 (6%)	21,21,21	0.65	0
3	BMA	D	2	3	11,11,12	1.29	2 (18%)	15,15,17	2.02	3 (20%)
3	MAN	D	3	3	11,11,12	1.29	1 (9%)	15,15,17	1.38	2 (13%)
3	MAN	D	4	3	11,11,12	1.45	2 (18%)	15,15,17	1.19	1 (6%)
3	MAN	D	5	3	11,11,12	1.53	3 (27%)	15,15,17	1.33	2 (13%)
3	MAN	D	6	3	11,11,12	1.49	2 (18%)	15,15,17	1.47	4 (26%)
3	MAN	D	7	3	11,11,12	1.56	3 (27%)	15,15,17	1.23	2 (13%)

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	-	1/6/26/26	0/1/1/1
2	BMA	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	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	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	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	MAN	C	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3	-	4/6/26/26	0/1/1/1
3	BMA	D	2	3	-	0/2/19/22	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	1/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C2-C3	4.70	1.59	1.52
2	C	8	MAN	C2-C3	4.22	1.58	1.52
2	C	8	MAN	O5-C5	4.17	1.51	1.43
2	C	7	MAN	C4-C5	4.14	1.61	1.53
2	C	1	NAG	C1-C2	3.88	1.57	1.52
2	C	7	MAN	O4-C4	3.44	1.51	1.43
3	D	1	NAG	O5-C1	3.44	1.51	1.42
3	D	4	MAN	C2-C3	3.08	1.57	1.52
2	C	5	MAN	C2-C3	3.05	1.57	1.52
2	C	7	MAN	C1-C2	2.90	1.58	1.52
3	D	7	MAN	C2-C3	2.86	1.56	1.52
2	C	6	MAN	O5-C5	2.73	1.49	1.43
2	C	4	MAN	C2-C3	2.70	1.56	1.52
3	D	5	MAN	C2-C3	2.70	1.56	1.52
2	C	5	MAN	C4-C3	2.67	1.59	1.52
3	D	7	MAN	C1-C2	2.64	1.58	1.52
3	D	6	MAN	C2-C3	2.60	1.56	1.52
3	D	5	MAN	C4-C3	2.55	1.58	1.52
3	D	4	MAN	O5-C5	2.53	1.48	1.43
2	C	2	BMA	C4-C3	2.52	1.58	1.52
3	D	2	BMA	O5-C5	2.34	1.48	1.43
3	D	6	MAN	C4-C3	2.32	1.58	1.52
3	D	7	MAN	O5-C5	2.28	1.48	1.43
2	C	3	MAN	O5-C5	2.21	1.47	1.43
3	D	2	BMA	C2-C3	2.16	1.55	1.52
3	D	3	MAN	C4-C5	2.16	1.57	1.53
2	C	1	NAG	O5-C1	2.16	1.48	1.42
3	D	5	MAN	C1-C2	2.15	1.57	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	BMA	C1-O5-C5	6.26	120.67	112.19
2	C	6	MAN	O3-C3-C2	3.96	117.58	109.99
2	C	1	NAG	C1-C2-N2	3.76	115.09	110.73
2	C	5	MAN	C1-O5-C5	3.76	117.29	112.19
2	C	4	MAN	C1-O5-C5	3.57	117.03	112.19
3	D	3	MAN	O2-C2-C3	-3.57	102.99	110.14
3	D	5	MAN	C1-O5-C5	3.48	116.91	112.19
3	D	4	MAN	C1-O5-C5	3.37	116.76	112.19
3	D	6	MAN	C1-O5-C5	3.30	116.66	112.19
2	C	3	MAN	C1-O5-C5	3.13	116.43	112.19
2	C	3	MAN	O2-C2-C3	-3.01	104.10	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	MAN	C1-O5-C5	2.91	116.13	112.19
3	D	2	BMA	C1-C2-C3	2.82	113.13	109.67
2	C	1	NAG	C1-O5-C5	2.82	118.98	113.66
3	D	7	MAN	C1-O5-C5	2.67	115.81	112.19
2	C	1	NAG	C1-C2-C3	2.64	114.14	110.54
2	C	2	BMA	C1-O5-C5	2.48	115.55	112.19
2	C	8	MAN	O3-C3-C2	2.36	114.52	109.99
3	D	2	BMA	O5-C1-C2	2.35	114.40	110.77
3	D	5	MAN	O5-C1-C2	2.26	114.26	110.77
2	C	8	MAN	O5-C5-C6	2.17	110.61	107.20
2	C	6	MAN	O6-C6-C5	-2.15	103.90	111.29
2	C	2	BMA	C1-C2-C3	2.15	112.31	109.67
3	D	6	MAN	O5-C1-C2	2.11	114.03	110.77
2	C	8	MAN	O5-C1-C2	2.11	114.03	110.77
3	D	6	MAN	O2-C2-C3	-2.09	105.96	110.14
3	D	7	MAN	O2-C2-C1	2.08	113.40	109.15
3	D	6	MAN	C1-C2-C3	2.01	112.14	109.67
2	C	7	MAN	C1-C2-C3	2.01	112.13	109.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

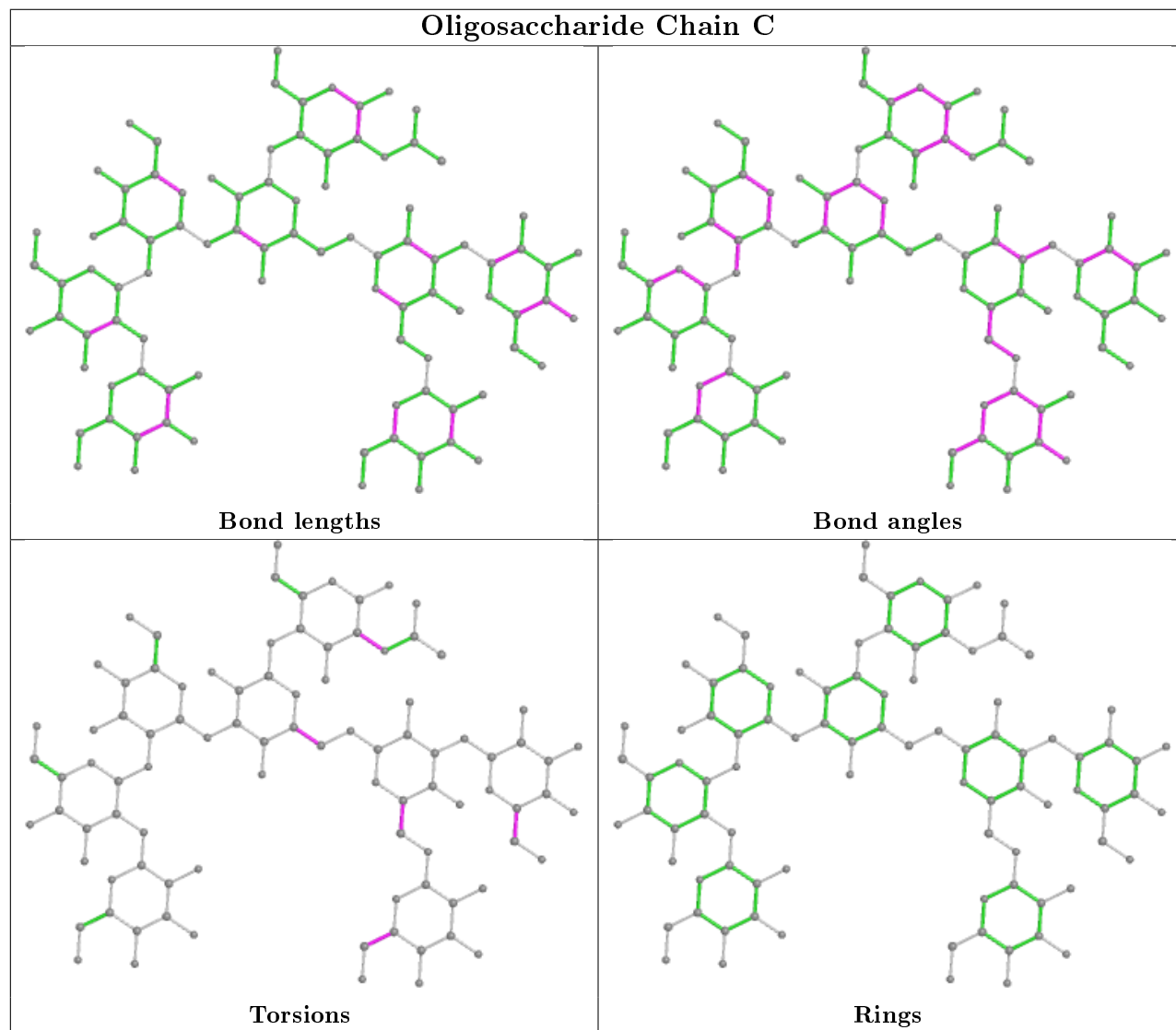
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
2	C	8	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
2	C	2	BMA	C4-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
2	C	2	BMA	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6

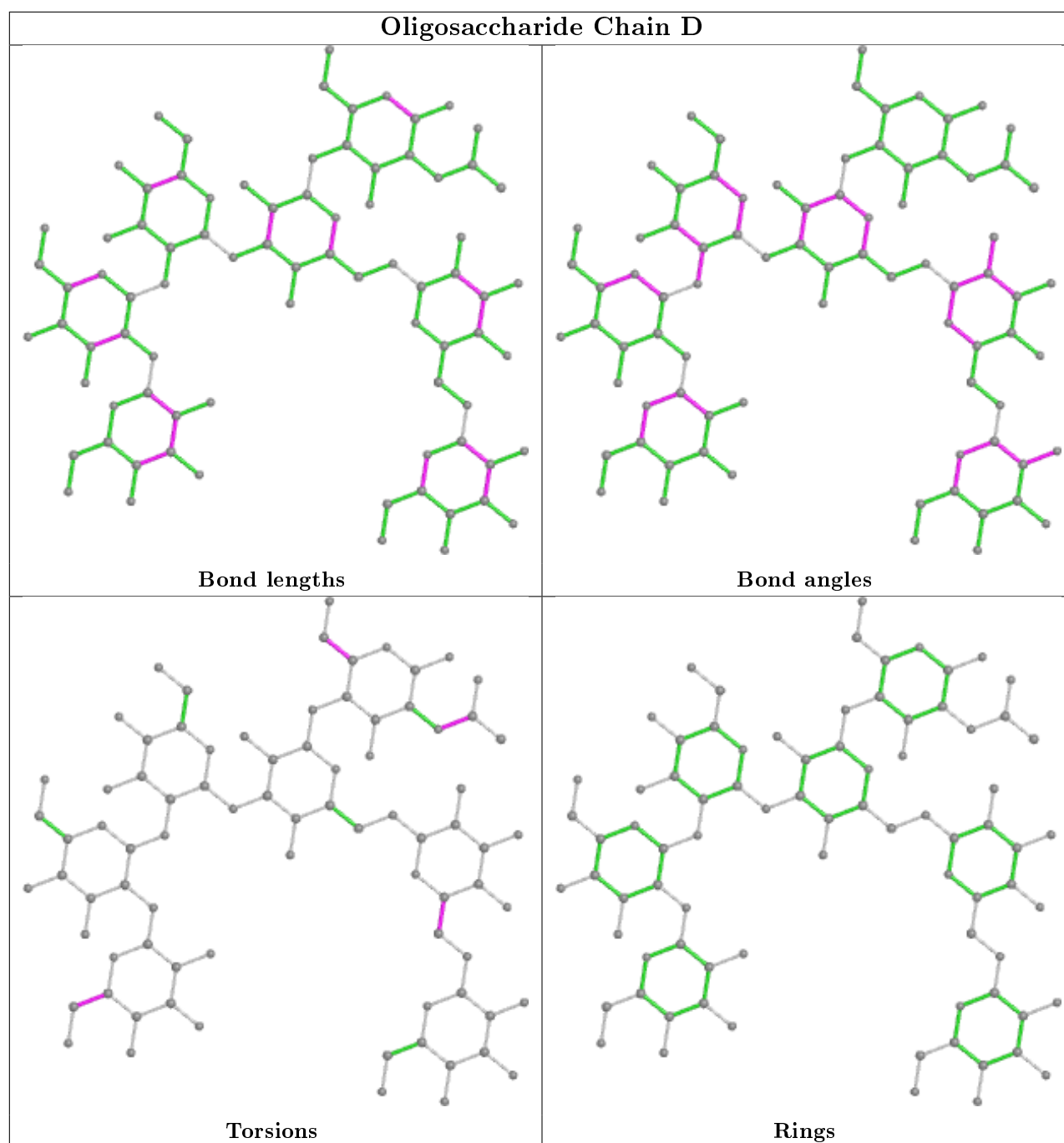
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	MAN	2	0
3	D	7	MAN	1	0
3	D	2	BMA	1	0
3	D	1	NAG	1	0
2	C	8	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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

### 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	787/802 (98%)	0.07	35 (4%) 34 37	30, 48, 72, 99	0
1	B	787/802 (98%)	0.25	55 (6%) 16 16	34, 53, 81, 92	0
All	All	1574/1604 (98%)	0.16	90 (5%) 23 25	30, 51, 78, 99	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	ALA	7.6
1	B	189	PHE	5.2
1	B	190	THR	4.7
1	B	764	ASP	4.6
1	B	46	THR	4.4
1	A	764	ASP	4.4
1	A	770	ILE	4.3
1	A	539	LYS	4.0
1	A	765	LEU	3.9
1	B	676	ILE	3.8
1	B	248	LEU	3.8
1	B	674	GLY	3.7
1	A	189	PHE	3.6
1	B	793	LYS	3.5
1	A	767	LYS	3.5
1	B	70	TYR	3.4
1	B	571	ASN	3.3
1	B	337	PHE	3.3
1	B	47	ASP	3.3
1	A	724	GLU	3.2
1	A	758	LEU	3.2
1	A	762	THR	3.1
1	B	182	ASP	3.1
1	A	723	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	762	THR	3.0
1	B	224	ILE	2.9
1	B	336	ILE	2.9
1	B	831	GLN	2.8
1	B	69	GLY	2.8
1	B	802	ASN	2.7
1	A	70	TYR	2.7
1	B	574	HIS	2.7
1	A	190	THR	2.7
1	B	104	PHE	2.7
1	B	596	GLU	2.7
1	B	673	SER	2.7
1	B	82	ILE	2.7
1	A	224	ILE	2.6
1	A	725	ILE	2.6
1	B	334	ALA	2.6
1	A	771	LYS	2.6
1	A	766	GLU	2.6
1	B	338	SER	2.6
1	B	645	VAL	2.6
1	B	49	GLN	2.5
1	A	337	PHE	2.5
1	B	281	MET	2.5
1	A	248	LEU	2.5
1	B	563	LYS	2.5
1	B	832	ARG	2.5
1	B	68	ALA	2.5
1	B	565	GLY	2.5
1	A	743	LYS	2.5
1	B	138	THR	2.5
1	A	68	ALA	2.4
1	B	136	VAL	2.4
1	B	158	PRO	2.4
1	B	770	ILE	2.4
1	A	788	GLN	2.4
1	B	804	LEU	2.4
1	B	568	ASP	2.4
1	B	830	GLY	2.4
1	B	569	VAL	2.4
1	B	763	ILE	2.3
1	A	138	THR	2.3
1	B	183	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	282	ILE	2.3
1	B	729	LYS	2.3
1	A	183	ILE	2.3
1	B	572	ALA	2.3
1	B	765	LEU	2.3
1	A	785	ASP	2.3
1	A	69	GLY	2.3
1	A	191	ASN	2.3
1	A	536	ASN	2.3
1	B	619	GLU	2.3
1	B	741	GLU	2.3
1	A	336	ILE	2.2
1	B	160	GLY	2.2
1	B	791	ASP	2.2
1	B	340	ALA	2.1
1	B	724	GLU	2.1
1	A	281	MET	2.1
1	A	136	VAL	2.1
1	A	46	THR	2.1
1	A	810	PHE	2.1
1	A	49	GLN	2.1
1	A	807	TYR	2.1
1	B	648	THR	2.0
1	A	718	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

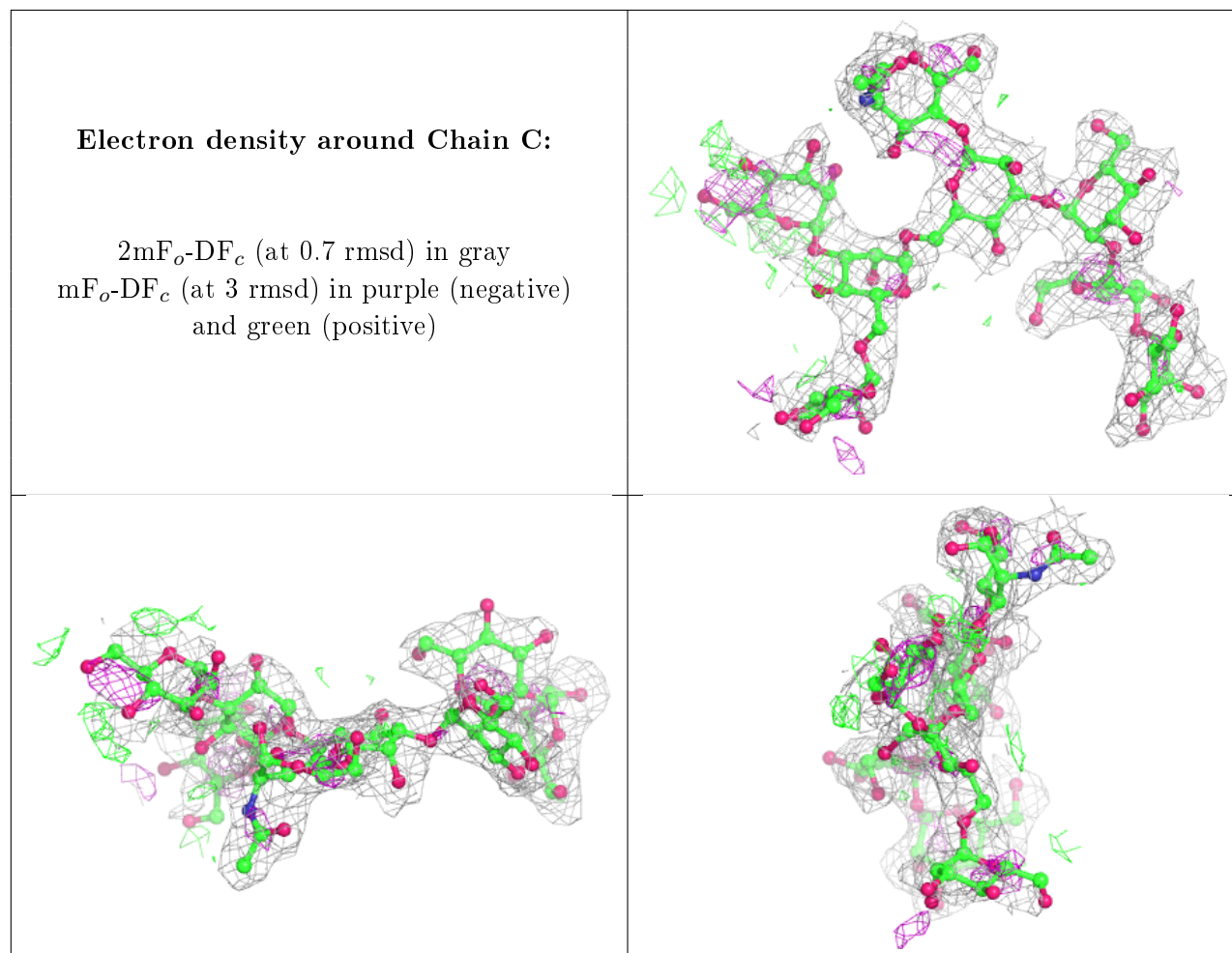
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	C	7	11/12	0.58	0.48	75,83,90,93	0
2	MAN	C	8	11/12	0.75	0.42	86,90,96,97	0
3	MAN	D	5	11/12	0.76	0.27	56,70,77,77	0
3	MAN	D	6	11/12	0.80	0.40	80,84,92,94	0

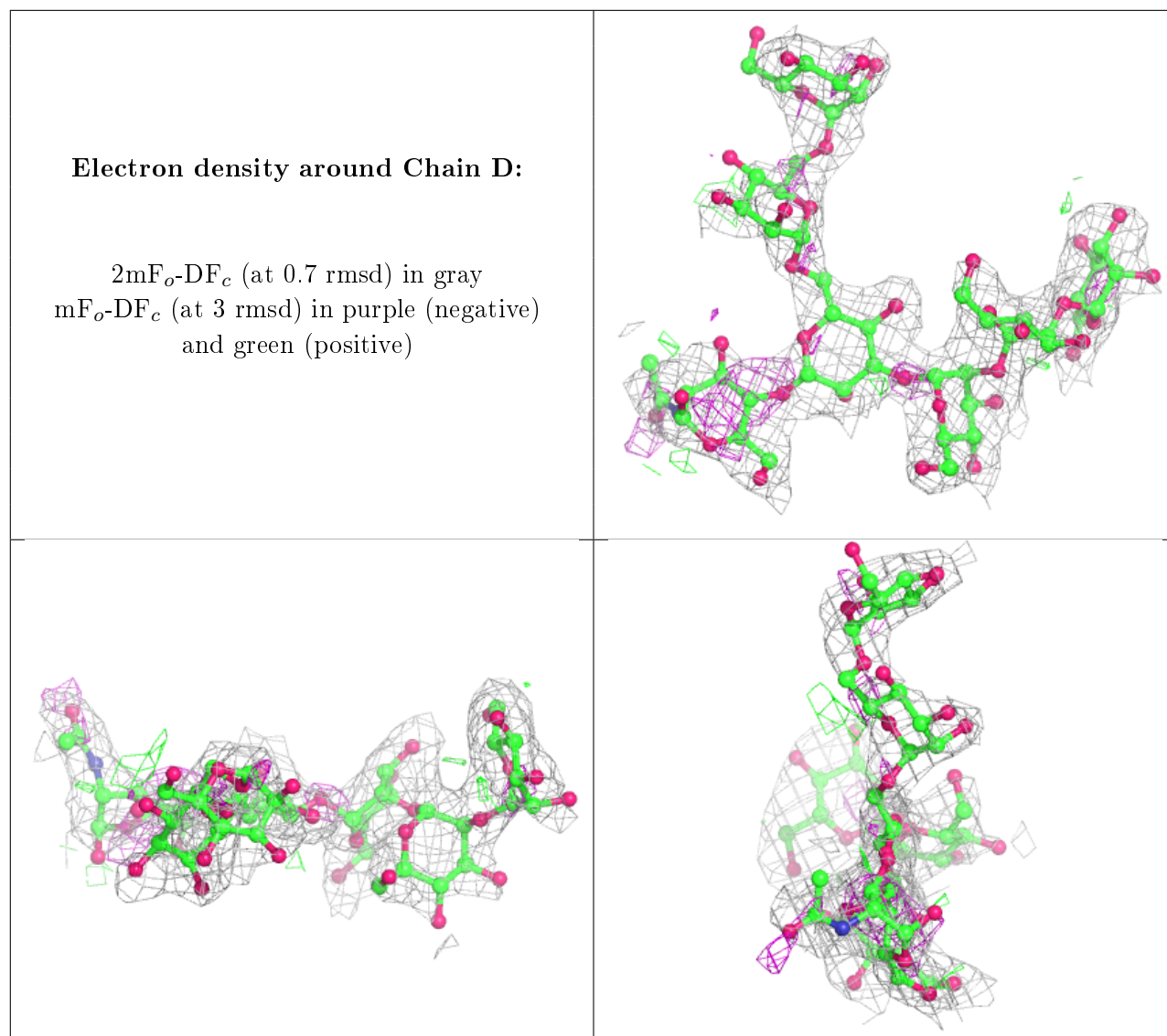
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	C	5	11/12	0.82	0.23	46,61,67,70	0
3	NAG	D	1	15/15	0.84	0.26	50,59,68,70	0
3	MAN	D	4	11/12	0.84	0.41	67,71,75,76	0
3	BMA	D	2	11/12	0.85	0.23	48,62,70,75	0
3	MAN	D	7	11/12	0.86	0.45	84,88,91,94	0
2	BMA	C	2	11/12	0.87	0.20	44,58,67,76	0
2	NAG	C	1	15/15	0.89	0.16	43,53,57,65	0
2	MAN	C	6	11/12	0.89	0.27	76,80,88,88	0
2	MAN	C	3	11/12	0.89	0.20	38,44,57,64	0
3	MAN	D	3	11/12	0.91	0.14	47,52,61,64	0
2	MAN	C	4	11/12	0.92	0.40	60,65,71,72	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(Å <sup>2</sup> )	Q<0.9
4	CA	B	901	1/1	0.91	0.05	75,75,75,75	0
4	CA	A	901	1/1	0.98	0.03	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.