



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2026 – 02:16 pm BST

PDB ID : 9QS0 / pdb\_00009qs0  
Title : Crystal Structure of the MAR1-FUS1 Gamete Adhesion Complex in Chlamydomonas reinhardtii  
Authors : Rey, F.A.; Baquero, E.  
Deposited on : 2025-04-04  
Resolution : 3.10 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

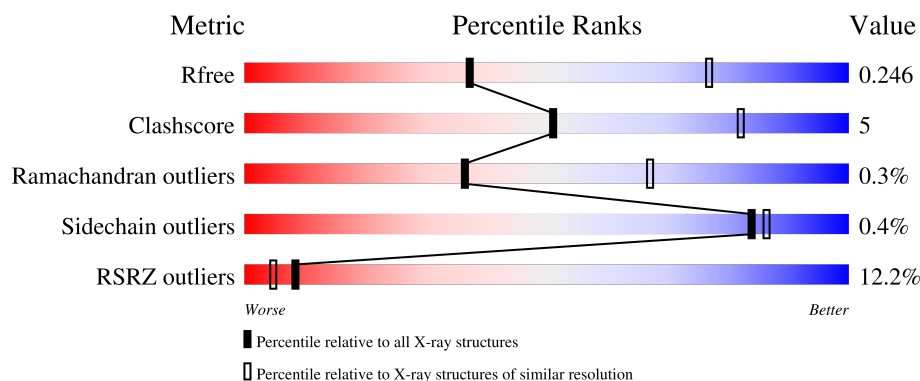
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



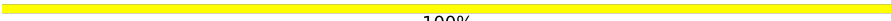
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	470	<div> <div>20%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	470	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>11%</div> <div>23%</div> </div> </div>
2	C	171	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>8%</div> <div>22%</div> </div> </div>
2	D	171	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>8%</div> <div>21%</div> </div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8532 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 FUS1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3553	2287	566	691	9			
1	B	364	Total	C	N	O	S	0	0	0
			2824	1818	453	544	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	GLY	-	expression tag	UNP Q39594
A	481	HIS	-	expression tag	UNP Q39594
A	482	HIS	-	expression tag	UNP Q39594
A	483	HIS	-	expression tag	UNP Q39594
A	484	HIS	-	expression tag	UNP Q39594
A	485	HIS	-	expression tag	UNP Q39594
A	486	HIS	-	expression tag	UNP Q39594
B	480	GLY	-	expression tag	UNP Q39594
B	481	HIS	-	expression tag	UNP Q39594
B	482	HIS	-	expression tag	UNP Q39594
B	483	HIS	-	expression tag	UNP Q39594
B	484	HIS	-	expression tag	UNP Q39594
B	485	HIS	-	expression tag	UNP Q39594
B	486	HIS	-	expression tag	UNP Q39594

- Molecule 2 is a protein called Minus adhesion receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	134	Total	C	N	O	S	0	0	0
			952	583	160	194	15			
2	D	135	Total	C	N	O	S	0	0	0
			961	588	162	196	15			

There are 78 discrepancies between the modelled and reference sequences:

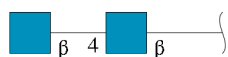
Chain	Residue	Modelled	Actual	Comment	Reference
C	56	GLN	ASN	engineered mutation	UNP A0A0U2YF84
C	64	GLN	ASN	engineered mutation	UNP A0A0U2YF84
C	72	GLN	ASN	engineered mutation	UNP A0A0U2YF84
C	75	GLN	ASN	engineered mutation	UNP A0A0U2YF84
C	162	ASP	-	expression tag	UNP A0A0U2YF84
C	163	ASP	-	expression tag	UNP A0A0U2YF84
C	164	ASP	-	expression tag	UNP A0A0U2YF84
C	165	ASP	-	expression tag	UNP A0A0U2YF84
C	166	LYS	-	expression tag	UNP A0A0U2YF84
C	167	ALA	-	expression tag	UNP A0A0U2YF84
C	168	GLY	-	expression tag	UNP A0A0U2YF84
C	169	TRP	-	expression tag	UNP A0A0U2YF84
C	170	SER	-	expression tag	UNP A0A0U2YF84
C	171	HIS	-	expression tag	UNP A0A0U2YF84
C	172	PRO	-	expression tag	UNP A0A0U2YF84
C	173	GLN	-	expression tag	UNP A0A0U2YF84
C	174	PHE	-	expression tag	UNP A0A0U2YF84
C	175	GLU	-	expression tag	UNP A0A0U2YF84
C	176	LYS	-	expression tag	UNP A0A0U2YF84
C	177	GLY	-	expression tag	UNP A0A0U2YF84
C	178	GLY	-	expression tag	UNP A0A0U2YF84
C	179	GLY	-	expression tag	UNP A0A0U2YF84
C	180	SER	-	expression tag	UNP A0A0U2YF84
C	181	GLY	-	expression tag	UNP A0A0U2YF84
C	182	GLY	-	expression tag	UNP A0A0U2YF84
C	183	GLY	-	expression tag	UNP A0A0U2YF84
C	184	SER	-	expression tag	UNP A0A0U2YF84
C	185	GLY	-	expression tag	UNP A0A0U2YF84
C	186	GLY	-	expression tag	UNP A0A0U2YF84
C	187	GLY	-	expression tag	UNP A0A0U2YF84
C	188	SER	-	expression tag	UNP A0A0U2YF84
C	189	TRP	-	expression tag	UNP A0A0U2YF84
C	190	SER	-	expression tag	UNP A0A0U2YF84
C	191	HIS	-	expression tag	UNP A0A0U2YF84
C	192	PRO	-	expression tag	UNP A0A0U2YF84
C	193	GLN	-	expression tag	UNP A0A0U2YF84
C	194	PHE	-	expression tag	UNP A0A0U2YF84
C	195	GLU	-	expression tag	UNP A0A0U2YF84
C	196	LYS	-	expression tag	UNP A0A0U2YF84
D	56	GLN	ASN	engineered mutation	UNP A0A0U2YF84
D	64	GLN	ASN	engineered mutation	UNP A0A0U2YF84
D	72	GLN	ASN	engineered mutation	UNP A0A0U2YF84
D	75	GLN	ASN	engineered mutation	UNP A0A0U2YF84

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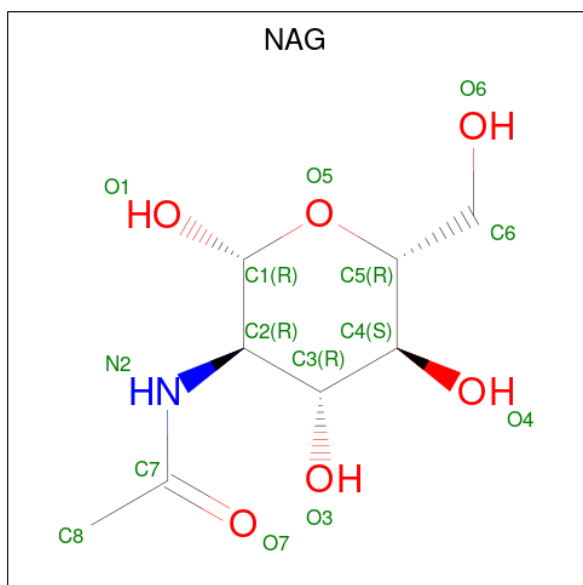
Chain	Residue	Modelled	Actual	Comment	Reference
D	162	ASP	-	expression tag	UNP A0A0U2YF84
D	163	ASP	-	expression tag	UNP A0A0U2YF84
D	164	ASP	-	expression tag	UNP A0A0U2YF84
D	165	ASP	-	expression tag	UNP A0A0U2YF84
D	166	LYS	-	expression tag	UNP A0A0U2YF84
D	167	ALA	-	expression tag	UNP A0A0U2YF84
D	168	GLY	-	expression tag	UNP A0A0U2YF84
D	169	TRP	-	expression tag	UNP A0A0U2YF84
D	170	SER	-	expression tag	UNP A0A0U2YF84
D	171	HIS	-	expression tag	UNP A0A0U2YF84
D	172	PRO	-	expression tag	UNP A0A0U2YF84
D	173	GLN	-	expression tag	UNP A0A0U2YF84
D	174	PHE	-	expression tag	UNP A0A0U2YF84
D	175	GLU	-	expression tag	UNP A0A0U2YF84
D	176	LYS	-	expression tag	UNP A0A0U2YF84
D	177	GLY	-	expression tag	UNP A0A0U2YF84
D	178	GLY	-	expression tag	UNP A0A0U2YF84
D	179	GLY	-	expression tag	UNP A0A0U2YF84
D	180	SER	-	expression tag	UNP A0A0U2YF84
D	181	GLY	-	expression tag	UNP A0A0U2YF84
D	182	GLY	-	expression tag	UNP A0A0U2YF84
D	183	GLY	-	expression tag	UNP A0A0U2YF84
D	184	SER	-	expression tag	UNP A0A0U2YF84
D	185	GLY	-	expression tag	UNP A0A0U2YF84
D	186	GLY	-	expression tag	UNP A0A0U2YF84
D	187	GLY	-	expression tag	UNP A0A0U2YF84
D	188	SER	-	expression tag	UNP A0A0U2YF84
D	189	TRP	-	expression tag	UNP A0A0U2YF84
D	190	SER	-	expression tag	UNP A0A0U2YF84
D	191	HIS	-	expression tag	UNP A0A0U2YF84
D	192	PRO	-	expression tag	UNP A0A0U2YF84
D	193	GLN	-	expression tag	UNP A0A0U2YF84
D	194	PHE	-	expression tag	UNP A0A0U2YF84
D	195	GLU	-	expression tag	UNP A0A0U2YF84
D	196	LYS	-	expression tag	UNP A0A0U2YF84

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



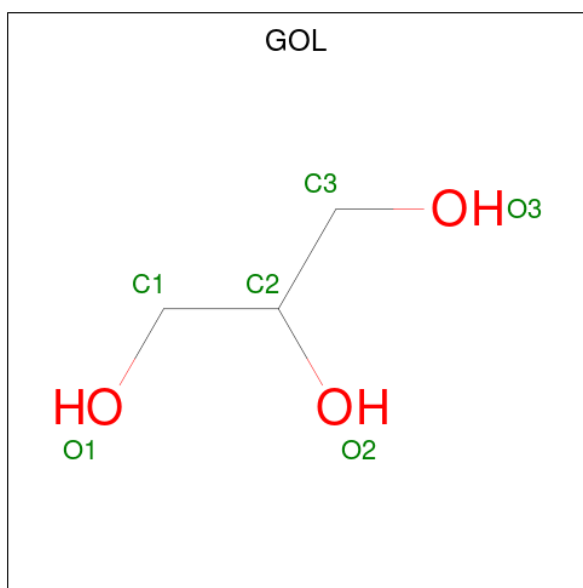
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



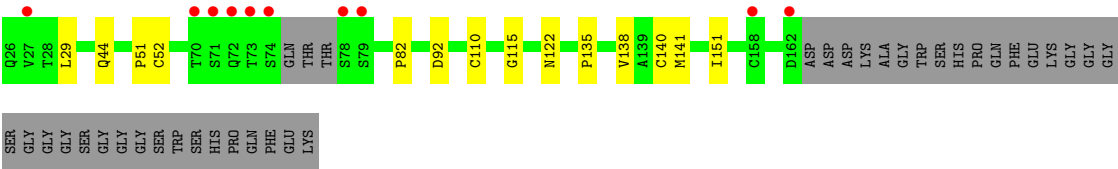
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

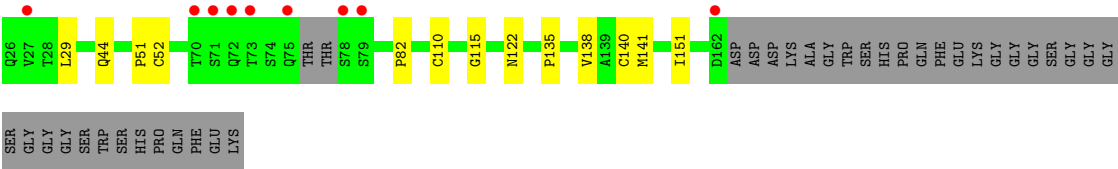
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	3	Total	O	0	0
			3	3		







• Molecule 2: Minus adhesion receptor 1



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	348.39Å 89.68Å 97.33Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	45.24 – 3.10 45.24 – 3.10	Depositor EDS
% Data completeness (in resolution range)	73.6 (45.24-3.10) 73.6 (45.24-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.216 , 0.246 0.216 , 0.246	Depositor DCC
$R_{free}$ test set	1891 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: GOL, 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	0.13	0/3652	0.29	0/5021
1	B	0.12	0/2904	0.28	0/3988
2	C	0.13	0/979	0.33	0/1349
2	D	0.13	0/988	0.35	0/1361
All	All	0.12	0/8523	0.30	0/11719

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	3553	0	3435	46	0
1	B	2824	0	2739	30	0
2	C	952	0	863	10	0
2	D	961	0	871	9	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	42	0	39	1	0
4	B	56	0	52	0	0
4	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	13	0	0
5	A	24	0	32	4	0
5	B	12	0	16	1	0
5	C	6	0	8	2	0
5	D	12	0	16	2	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
All	All	8532	0	8147	87	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 5.

All (87) 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:245:ARG:HH22	2:D:151:ILE:HG23	1.60	0.67
1:A:56:VAL:HG12	1:A:58:TYR:H	1.60	0.66
1:B:245:ARG:HH22	2:C:151:ILE:HG23	1.61	0.65
1:B:56:VAL:HG12	1:B:58:TYR:H	1.59	0.65
1:B:231:GLN:HG3	1:B:256:ASP:HB3	1.79	0.65
1:A:231:GLN:HG3	1:A:256:ASP:HB3	1.80	0.63
1:A:463:ILE:HD12	1:A:471:LEU:HD21	1.81	0.62
1:B:340:ILE:HD11	1:B:351:SER:HB2	1.82	0.62
1:A:177:TYR:HB3	1:A:215:TRP:HB3	1.83	0.60
1:A:340:ILE:HD11	1:A:351:SER:HB2	1.82	0.60
1:A:200:ALA:H	5:A:502:GOL:H12	1.68	0.59
1:B:177:TYR:HB3	1:B:215:TRP:HB3	1.84	0.59
1:A:430:THR:O	1:A:433:HIS:NE2	2.38	0.57
1:B:170:ARG:O	5:C:201:GOL:O1	2.24	0.56
1:A:170:ARG:O	5:D:201:GOL:O1	2.24	0.55
1:B:207:SER:HB2	1:B:219:TYR:HB2	1.89	0.54
1:A:207:SER:HB2	1:A:219:TYR:HB2	1.88	0.54
5:A:507:GOL:H11	2:C:92:ASP:HB3	1.90	0.53
1:A:408:ARG:HD2	4:A:506:NAG:H82	1.91	0.53
2:C:138:VAL:H	5:C:201:GOL:H32	1.74	0.52
2:D:138:VAL:H	5:D:201:GOL:H32	1.75	0.51
1:B:22:VAL:HG22	1:B:54:THR:HG21	1.93	0.51
1:A:317:ASN:HD22	1:A:320:LEU:HG	1.76	0.50
1:B:27:ILE:HD11	1:B:135:ILE:HD11	1.92	0.50
1:A:123:ASP:OD1	1:A:123:ASP:N	2.45	0.50
1:A:463:ILE:HB	1:A:471:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG22	1:A:54:THR:HG21	1.93	0.50
1:B:198:VAL:H	5:B:505:GOL:H11	1.77	0.49
2:C:44:GLN:HA	2:C:135:PRO:HG3	1.94	0.49
1:A:266:LEU:HD13	1:A:292:ALA:HB1	1.95	0.49
2:D:44:GLN:HA	2:D:135:PRO:HG3	1.94	0.49
1:A:428:GLY:H	1:A:433:HIS:CE1	2.31	0.48
1:A:106:PRO:HB3	2:D:141:MET:HE2	1.96	0.48
1:A:27:ILE:HD11	1:A:135:ILE:HD11	1.95	0.47
1:B:266:LEU:HD13	1:B:292:ALA:HB1	1.96	0.47
1:B:106:PRO:HB3	2:C:141:MET:HE2	1.96	0.47
1:A:281:GLU:HB3	1:A:284:ILE:HD12	1.97	0.46
2:D:29:LEU:HA	2:D:82:PRO:HA	1.95	0.46
1:B:162:PRO:HD3	2:C:122:ASN:HB3	1.98	0.46
1:B:295:ILE:HD12	1:B:295:ILE:H	1.80	0.45
2:C:29:LEU:HA	2:C:82:PRO:HA	1.97	0.45
1:A:161:VAL:O	2:D:140:CYS:HB2	2.16	0.45
1:A:64:VAL:HG12	1:A:79:LEU:HD22	1.98	0.45
1:B:179:ILE:O	1:B:186:TRP:HA	2.17	0.45
1:B:26:LYS:HB2	1:B:47:LEU:HD11	1.99	0.45
1:A:179:ILE:O	1:A:186:TRP:HA	2.17	0.45
1:A:276:LEU:HG	1:A:288:LEU:HD13	1.97	0.45
1:B:161:VAL:O	2:C:140:CYS:HB2	2.16	0.45
2:C:110:CYS:HA	2:C:115:GLY:HA3	1.99	0.45
1:A:295:ILE:H	1:A:295:ILE:HD12	1.82	0.45
1:A:26:LYS:HB2	1:A:47:LEU:HD11	1.99	0.44
1:A:340:ILE:HB	1:A:349:SER:HB2	2.00	0.44
1:A:162:PRO:HD3	2:D:122:ASN:HB3	2.00	0.44
1:A:199:SER:HA	5:A:502:GOL:H12	1.99	0.44
1:A:215:TRP:CD1	1:A:217:VAL:HG22	2.53	0.44
1:A:430:THR:HG21	1:A:455:GLU:HB3	1.99	0.43
1:A:433:HIS:CD2	1:A:459:TYR:HE2	2.36	0.43
1:B:276:LEU:HG	1:B:288:LEU:HD13	1.98	0.43
1:B:290:LEU:HB2	1:B:348:CYS:HB2	2.00	0.43
1:B:340:ILE:HB	1:B:349:SER:HB2	2.00	0.43
1:B:281:GLU:HB3	1:B:284:ILE:HD12	2.00	0.43
1:A:290:LEU:HB2	1:A:348:CYS:HB2	2.00	0.43
1:A:385:PRO:O	1:A:470:TRP:NE1	2.51	0.43
1:A:384:SER:N	1:A:408:ARG:O	2.50	0.43
1:B:84:LEU:HD11	1:B:90:ASN:HB2	2.00	0.43
1:B:166:VAL:O	1:B:169:SER:HB3	2.19	0.43
1:A:385:PRO:C	1:A:387:ASN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:CYS:HA	2:D:115:GLY:HA3	2.00	0.43
1:A:84:LEU:HD11	1:A:90:ASN:HB2	2.01	0.42
1:A:301:ARG:HB3	1:A:303:VAL:HG23	2.00	0.42
1:A:166:VAL:O	1:A:169:SER:HB3	2.20	0.42
1:B:215:TRP:CD1	1:B:217:VAL:HG22	2.54	0.42
2:C:51:PRO:O	2:C:52:CYS:HB2	2.20	0.42
2:D:51:PRO:O	2:D:52:CYS:HB2	2.20	0.42
1:A:337:VAL:HA	1:A:352:ILE:HG12	2.02	0.41
1:A:333:LEU:HB2	1:A:355:PHE:HB2	2.02	0.41
1:B:337:VAL:HA	1:B:352:ILE:HG12	2.02	0.41
1:A:200:ALA:N	5:A:502:GOL:H12	2.35	0.41
1:B:64:VAL:HG11	1:B:91:ILE:HD13	2.03	0.41
1:B:301:ARG:HB3	1:B:303:VAL:HG23	2.03	0.41
1:A:321:LEU:HD23	1:A:366:TYR:HB2	2.02	0.41
1:A:426:LEU:HD21	1:A:461:VAL:HG22	2.01	0.41
1:B:106:PRO:HA	1:B:107:PRO:HD3	1.95	0.40
1:A:41:ASN:HB3	1:A:90:ASN:HD21	1.86	0.40
1:B:64:VAL:HG12	1:B:79:LEU:HD22	2.04	0.40
1:A:424:ILE:HB	1:A:435:PHE:CZ	2.57	0.40
1:B:45:THR:HG23	1:B:88:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

## 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	460/470 (98%)	436 (95%)	22 (5%)	2 (0%)	30	61
1	B	362/470 (77%)	347 (96%)	14 (4%)	1 (0%)	36	67
2	C	130/171 (76%)	126 (97%)	4 (3%)	0	100	100
2	D	131/171 (77%)	128 (98%)	3 (2%)	0	100	100
All	All	1083/1282 (84%)	1037 (96%)	43 (4%)	3 (0%)	36	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	VAL
1	A	163	ALA
1	B	163	ALA

### 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	397/408 (97%)	395 (100%)	2 (0%)	81	85
1	B	317/408 (78%)	315 (99%)	2 (1%)	78	83
2	C	106/132 (80%)	106 (100%)	0	100	100
2	D	107/132 (81%)	107 (100%)	0	100	100
All	All	927/1080 (86%)	923 (100%)	4 (0%)	84	86

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	387	ASN
1	B	41	ASN
1	B	343	ASN

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	96	GLN
1	A	212	GLN
1	B	30	GLN
1	B	96	GLN
1	B	212	GLN
2	C	44	GLN
2	C	48	ASN
2	D	44	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 ⓘ

4 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	E	1	1,3	14,14,15	0.83	0	17,19,21	1.95	5 (29%)
3	NAG	E	2	3	14,14,15	0.80	0	17,19,21	2.47	5 (29%)
3	NAG	F	1	1,3	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
3	NAG	F	2	3	14,14,15	0.77	1 (7%)	17,19,21	1.06	1 (5%)

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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	2.07	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C1-C2	-5.82	102.09	111.29
3	E	2	NAG	C1-O5-C5	-5.25	105.08	112.19
3	E	1	NAG	C1-O5-C5	-4.50	106.09	112.19
3	E	2	NAG	C2-N2-C7	4.20	128.89	122.90
3	E	1	NAG	C2-N2-C7	2.98	127.15	122.90
3	E	1	NAG	C1-C2-N2	2.98	115.58	110.49
3	E	2	NAG	C3-C4-C5	2.64	114.95	110.24
3	E	1	NAG	O4-C4-C5	2.62	115.79	109.30
3	E	2	NAG	O4-C4-C3	-2.39	104.82	110.35
3	F	2	NAG	C2-N2-C7	2.29	126.16	122.90
3	F	1	NAG	O5-C1-C2	-2.03	108.08	111.29
3	E	1	NAG	C3-C4-C5	2.03	113.86	110.24

There are no chirality outliers.

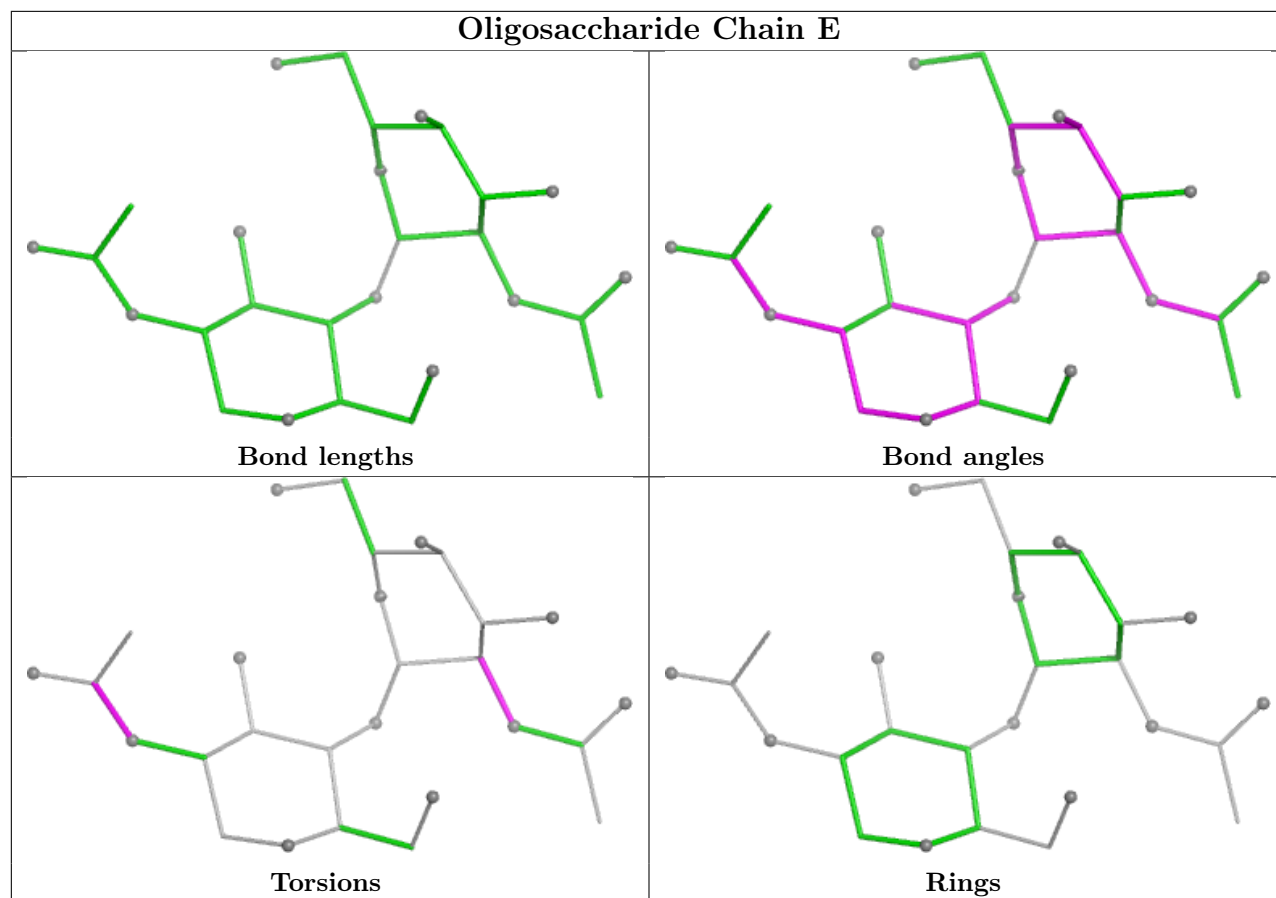
All (8) torsion outliers are listed below:

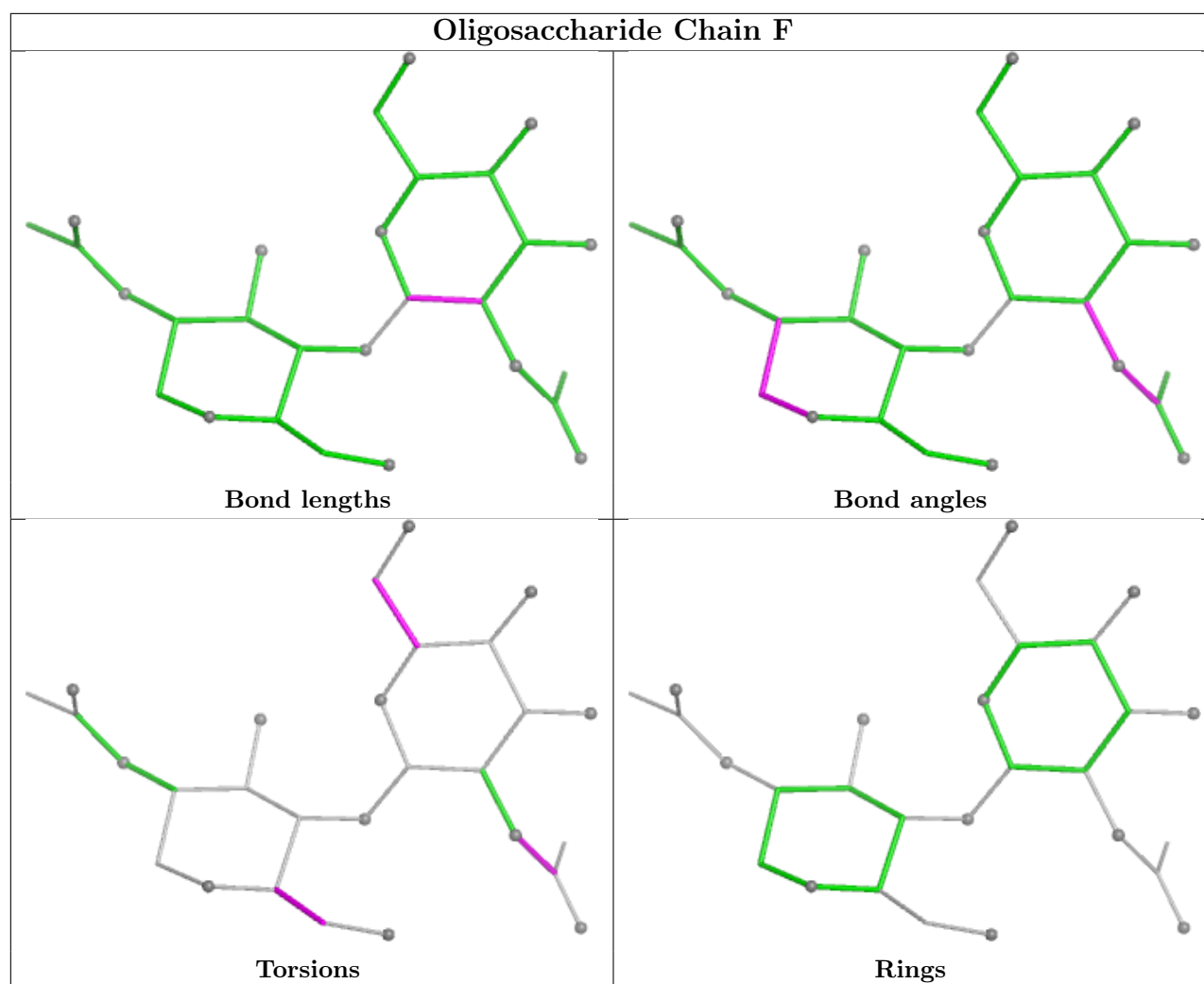
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

18 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	$\# Z  > 2$
5	GOL	B	503	-	5,5,5	0.36	0	5,5,5	0.43	0
4	NAG	A	503	1	14,14,15	0.78	0	17,19,21	2.88	4 (23%)
4	NAG	B	506	1	14,14,15	0.70	0	17,19,21	1.94	4 (23%)
4	NAG	A	506	1	14,14,15	0.66	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	501	1	14,14,15	0.76	0	17,19,21	1.08	1 (5%)
4	NAG	D	203	2	14,14,15	0.82	0	17,19,21	1.29	2 (11%)
5	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.48	0
5	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.39	0
4	NAG	B	504	1	14,14,15	0.79	0	17,19,21	1.16	1 (5%)
4	NAG	B	502	1	14,14,15	0.76	0	17,19,21	0.77	0
4	NAG	C	202	2	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
5	GOL	D	201	-	5,5,5	0.33	0	5,5,5	0.47	0
5	GOL	C	201	-	5,5,5	0.34	0	5,5,5	0.48	0
5	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.42	0
5	GOL	D	202	-	5,5,5	0.34	0	5,5,5	0.43	0
5	GOL	B	505	-	5,5,5	0.36	0	5,5,5	0.44	0
4	NAG	A	501	1	14,14,15	0.77	0	17,19,21	1.07	1 (5%)

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
5	GOL	B	503	-	-	2/4/4/4	-
4	NAG	A	503	1	-	5/6/23/26	0/1/1/1
4	NAG	B	506	1	-	1/6/23/26	0/1/1/1
4	NAG	A	506	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	203	2	-	2/6/23/26	0/1/1/1
5	GOL	A	507	-	-	0/4/4/4	-
5	GOL	A	502	-	-	0/4/4/4	-
5	GOL	A	505	-	-	0/4/4/4	-
4	NAG	B	504	1	-	2/6/23/26	0/1/1/1
4	NAG	B	502	1	-	2/6/23/26	0/1/1/1
4	NAG	C	202	2	-	0/6/23/26	0/1/1/1
5	GOL	D	201	-	-	0/4/4/4	-
5	GOL	C	201	-	-	0/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
5	GOL	D	202	-	-	0/4/4/4	-
5	GOL	B	505	-	-	0/4/4/4	-
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NAG	C2-N2-C7	9.34	136.20	122.90
4	B	506	NAG	C2-N2-C7	6.07	131.55	122.90
4	A	503	NAG	C1-O5-C5	4.26	117.96	112.19
4	A	503	NAG	C8-C7-N2	3.31	121.70	116.10
4	B	504	NAG	C2-N2-C7	3.24	127.51	122.90
4	A	503	NAG	C1-C2-N2	3.13	115.84	110.49
4	B	501	NAG	C1-O5-C5	3.02	116.28	112.19
4	A	501	NAG	C1-O5-C5	2.99	116.25	112.19
4	C	202	NAG	C1-O5-C5	2.82	116.02	112.19
4	D	203	NAG	C4-C3-C2	2.75	115.05	111.02
4	B	506	NAG	C1-C2-N2	2.66	115.03	110.49
4	B	506	NAG	O7-C7-N2	2.29	126.16	121.95
4	D	203	NAG	C2-N2-C7	2.21	126.05	122.90
4	B	506	NAG	C1-O5-C5	2.19	115.16	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	506	NAG	C1-C2-N2-C7
4	A	503	NAG	C8-C7-N2-C2
4	A	503	NAG	O7-C7-N2-C2
4	B	504	NAG	C8-C7-N2-C2
4	B	504	NAG	O7-C7-N2-C2
4	D	203	NAG	O5-C5-C6-O6
4	B	502	NAG	O5-C5-C6-O6
4	B	502	NAG	C4-C5-C6-O6
5	B	503	GOL	O1-C1-C2-C3
5	B	503	GOL	O1-C1-C2-O2
4	D	203	NAG	C4-C5-C6-O6
4	A	503	NAG	O5-C5-C6-O6
4	A	503	NAG	C3-C2-N2-C7
4	A	503	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	GOL	1	0
5	A	502	GOL	3	0
5	D	201	GOL	2	0
5	C	201	GOL	2	0
5	B	505	GOL	1	0

## 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	462/470 (98%)	1.00	94 (20%) 3 1	19, 65, 195, 209	0
1	B	364/470 (77%)	0.22	21 (5%) 29 16	21, 50, 128, 155	0
2	C	134/171 (78%)	0.10	10 (7%) 20 11	29, 45, 91, 112	0
2	D	135/171 (78%)	0.18	9 (6%) 24 13	27, 44, 92, 112	0
All	All	1095/1282 (85%)	0.53	134 (12%) 8 5	19, 51, 187, 209	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	LEU	10.5
1	A	392	LEU	10.3
1	A	436	ILE	9.3
1	A	390	ALA	8.3
1	A	438	VAL	8.0
1	A	425	GLY	7.8
1	B	326	VAL	7.8
1	A	479	ALA	7.6
1	A	326	VAL	7.6
1	A	424	ILE	7.4
1	A	395	ILE	7.0
1	A	449	TYR	7.0
1	A	473	LYS	6.8
1	A	437	PRO	6.7
1	A	427	THR	6.6
1	A	403	LEU	6.5
1	A	393	PRO	6.4
1	A	471	LEU	6.4
1	B	328	VAL	6.4
1	A	476	THR	6.2
1	A	423	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	402	LEU	6.1
1	A	461	VAL	6.0
1	A	458	LEU	5.9
1	A	462	SER	5.9
1	A	432	PHE	5.7
1	A	435	PHE	5.6
1	A	394	GLU	5.5
1	A	448	VAL	5.4
1	A	477	ILE	5.4
1	A	405	VAL	5.3
1	A	463	ILE	5.3
1	B	381	ALA	5.3
1	A	414	ILE	5.1
1	A	426	LEU	5.1
1	B	333	LEU	5.0
1	A	419	ASN	5.0
1	A	474	ASN	4.9
1	A	472	GLU	4.6
1	A	447	SER	4.6
2	D	70	THR	4.6
1	A	431	PHE	4.5
1	A	434	SER	4.5
1	A	454	THR	4.4
2	D	71	SER	4.3
1	A	401	THR	4.1
2	D	72	GLN	3.9
1	A	450	SER	3.9
1	A	404	TYR	3.9
1	A	406	THR	3.8
2	C	78	SER	3.8
1	A	328	VAL	3.8
1	A	475	ILE	3.8
1	A	407	PRO	3.7
1	A	327	THR	3.7
2	C	71	SER	3.7
1	A	422	LEU	3.7
1	A	389	THR	3.6
2	C	70	THR	3.6
1	A	418	ALA	3.5
1	A	420	ASN	3.5
1	A	452	THR	3.5
1	A	410	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	3.5
1	A	470	TRP	3.5
1	A	433	HIS	3.3
1	A	398	ALA	3.3
2	C	79	SER	3.3
1	A	421	ASP	3.3
1	A	460	VAL	3.2
1	B	357	SER	3.2
1	B	329	ASP	3.2
1	A	464	GLN	3.2
1	A	441	VAL	3.2
1	A	385	PRO	3.1
1	A	478	GLU	3.1
1	A	466	HIS	3.1
2	D	75	GLN	3.1
1	A	386	SER	3.1
1	A	396	GLY	3.1
1	B	327	THR	3.1
1	A	440	PRO	3.1
1	A	465	LEU	3.0
1	A	446	TYR	3.0
2	D	79	SER	3.0
1	A	397	GLN	3.0
1	A	439	GLU	2.9
2	D	162	ASP	2.9
1	A	360	TYR	2.9
1	A	416	PRO	2.8
2	C	27	VAL	2.8
1	B	354	PHE	2.8
1	A	469	SER	2.8
1	A	456	ALA	2.8
2	D	78	SER	2.8
1	B	355	PHE	2.8
1	A	333	LEU	2.8
1	A	399	GLY	2.6
2	C	72	GLN	2.6
1	A	411	TRP	2.6
1	B	282	ALA	2.5
1	B	379	ARG	2.5
2	C	162	ASP	2.5
1	A	417	LEU	2.5
1	A	443	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	27	VAL	2.5
2	C	158	CYS	2.4
1	A	331	GLY	2.4
1	A	442	ARG	2.4
1	B	353	THR	2.3
1	A	445	ASP	2.3
1	B	336	ASN	2.3
1	A	335	PRO	2.3
1	A	336	ASN	2.2
1	A	330	SER	2.2
1	A	334	GLN	2.2
1	B	236	ASP	2.2
1	A	332	ALA	2.2
1	A	428	GLY	2.2
1	B	283	GLY	2.2
2	D	73	THR	2.2
1	B	360	TYR	2.2
1	B	284	ILE	2.2
1	A	380	ASN	2.2
1	B	359	ASP	2.2
2	C	73	THR	2.1
1	B	356	THR	2.1
1	A	451	LEU	2.1
1	A	457	GLY	2.1
1	B	331	GLY	2.1
2	C	74	SER	2.1
1	A	355	PHE	2.1
1	A	354	PHE	2.0
1	B	352	ILE	2.0

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

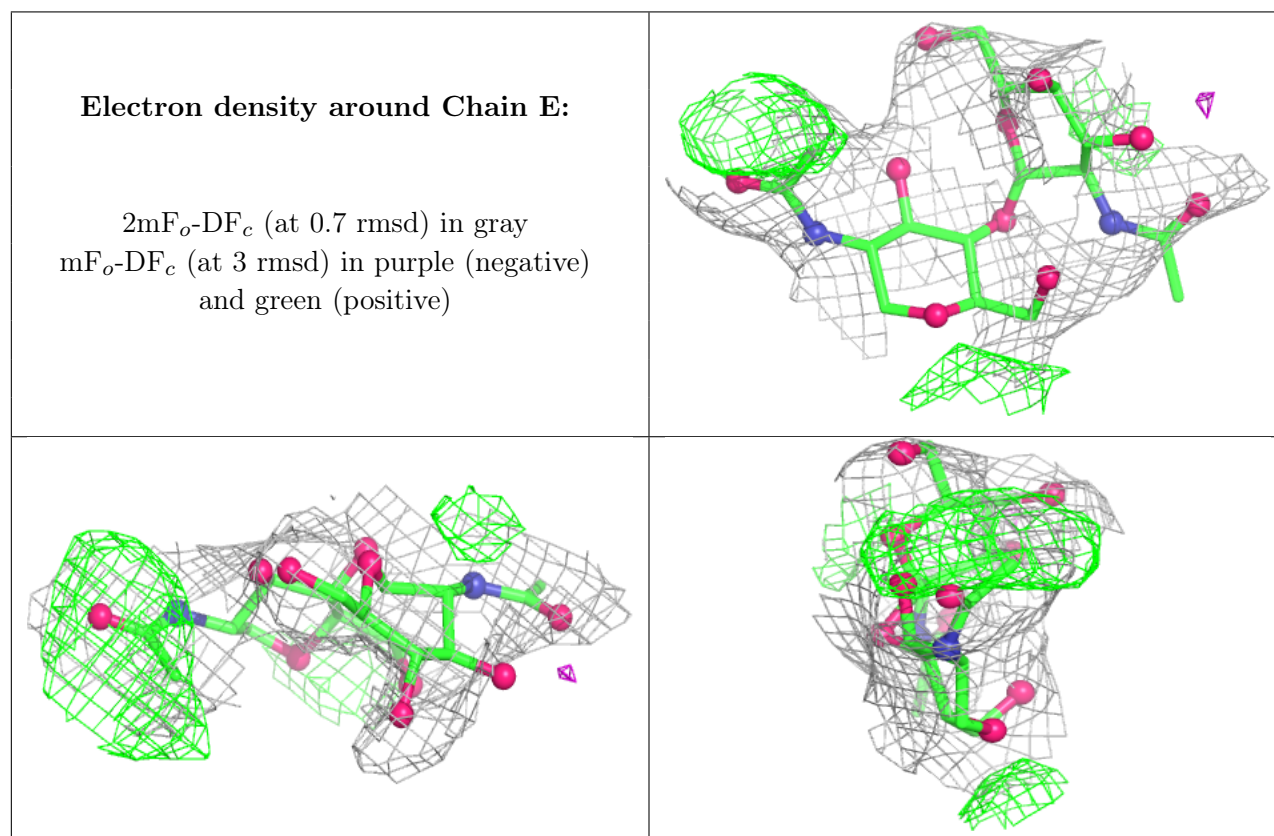
There are no non-standard protein/DNA/RNA residues in this entry.

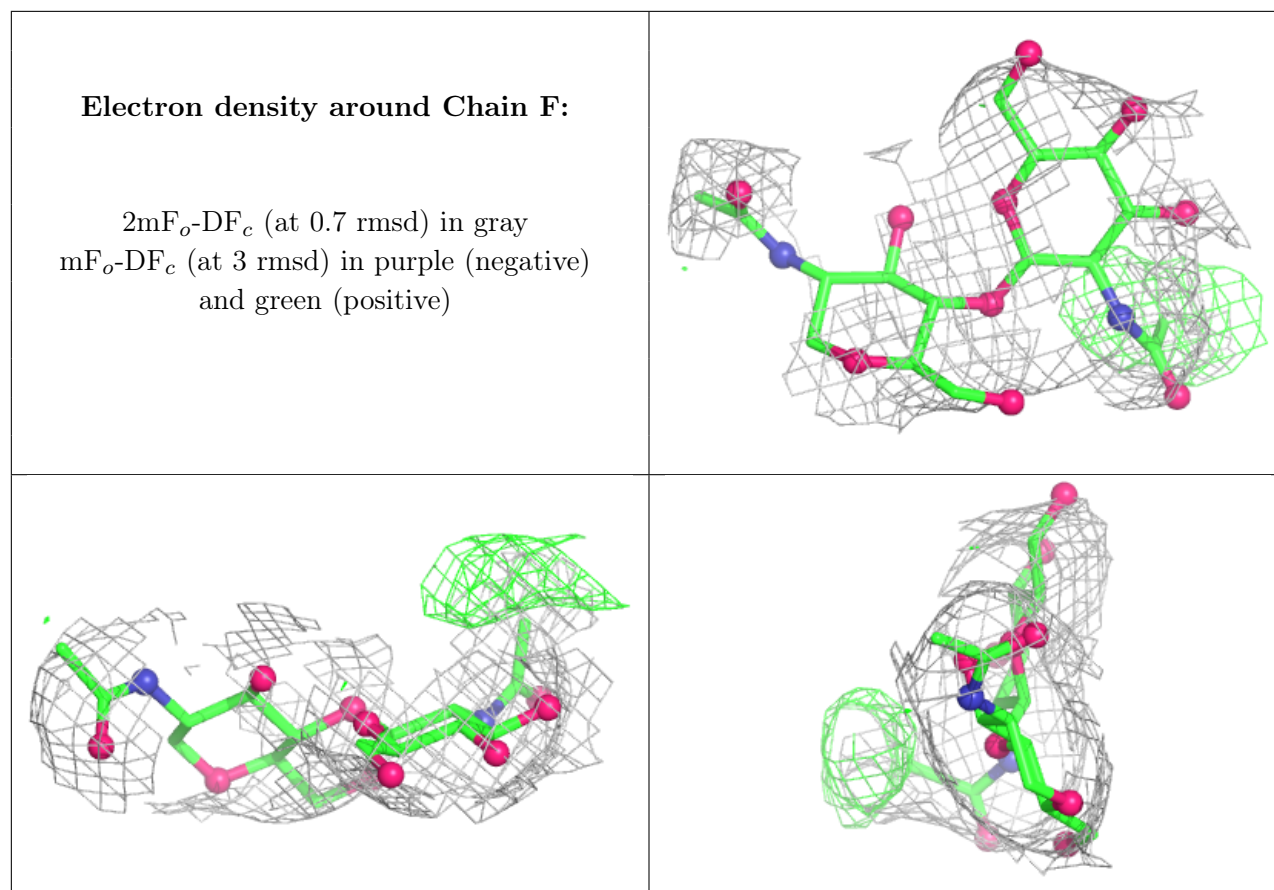
## 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	2	14/15	0.24	0.19	115,134,144,145	0
3	NAG	E	2	14/15	0.49	0.21	100,136,150,153	0
3	NAG	E	1	14/15	0.51	0.21	88,108,130,142	0
3	NAG	F	1	14/15	0.76	0.14	87,106,120,133	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	NAG	B	502	14/15	0.42	0.20	82,94,105,111	0
4	NAG	A	506	14/15	0.49	0.19	110,149,166,173	0
4	NAG	D	203	14/15	0.49	0.17	63,84,92,95	0
4	NAG	C	202	14/15	0.60	0.16	50,77,91,95	0
4	NAG	A	503	14/15	0.62	0.17	62,92,103,105	0
4	NAG	A	501	14/15	0.73	0.14	45,59,72,89	0
4	NAG	B	501	14/15	0.77	0.12	42,59,73,76	0
4	NAG	B	504	14/15	0.77	0.13	66,85,95,95	0
4	NAG	B	506	14/15	0.78	0.11	82,97,102,102	0
5	GOL	A	504	6/6	0.88	0.20	67,70,81,82	0
5	GOL	A	505	6/6	0.89	0.18	54,68,75,77	0
5	GOL	B	505	6/6	0.90	0.19	55,59,61,78	0
5	GOL	A	502	6/6	0.91	0.14	40,47,50,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	201	6/6	0.91	0.13	46,50,57,61	0
5	GOL	B	503	6/6	0.92	0.14	33,39,49,50	0
5	GOL	C	201	6/6	0.94	0.11	47,50,56,58	0
5	GOL	A	507	6/6	0.94	0.17	46,53,58,67	0
5	GOL	D	202	6/6	0.95	0.13	44,55,59,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.