



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:11 PM BST

PDB ID : 6U7F  
Title : HCoV-229E RBD Class IV in complex with human APN  
Authors : Tomlinson, A.C.A.; Li, Z.; Rini, J.M.  
Deposited on : 2019-09-02  
Resolution : 2.75 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

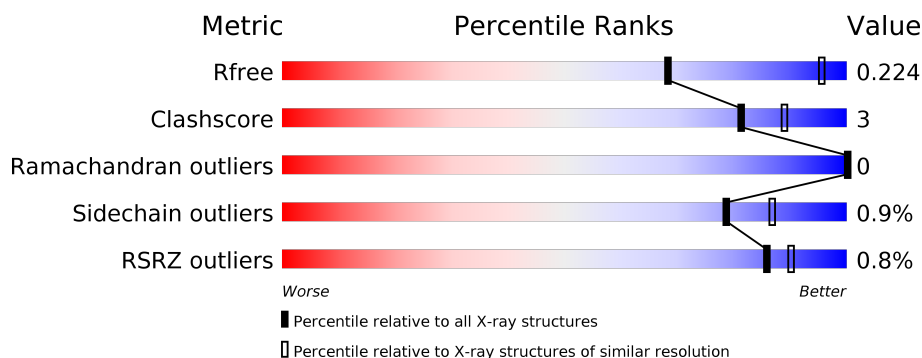
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	906	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	B	906	<div> <div style="width: 94%;"></div> <div>94%</div> <div style="width: 5%; background-color: yellow;"></div> <div>5%</div> </div>
2	C	145	<div> <div style="width: 6%; background-color: red;"></div> <div>6%</div> <div style="width: 50%; background-color: green;"></div> <div>50%</div> <div style="width: 16%; background-color: yellow;"></div> <div>16%</div> <div style="width: 34%; background-color: grey;"></div> <div>34%</div> </div>
2	D	145	<div> <div style="width: 3%; background-color: red;"></div> <div>3%</div> <div style="width: 53%; background-color: green;"></div> <div>53%</div> <div style="width: 17%; background-color: yellow;"></div> <div>17%</div> <div style="width: 29%; background-color: grey;"></div> <div>29%</div> </div>
3	E	2	<div> <div style="width: 50%; background-color: green;"></div> <div>50%</div> <div style="width: 50%; background-color: yellow;"></div> <div>50%</div> </div>
3	F	2	<div> <div style="width: 100%; background-color: yellow;"></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	H	2	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16575 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C	N	O	S	0	0	0
			7251	4623	1223	1381	24			
1	B	897	Total	C	N	O	S	0	0	0
			7251	4623	1223	1381	24			

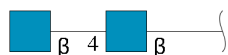
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	expression tag	UNP P15144
A	63	GLY	-	expression tag	UNP P15144
A	64	ARG	-	expression tag	UNP P15144
A	65	PRO	-	expression tag	UNP P15144
B	62	GLY	-	expression tag	UNP P15144
B	63	GLY	-	expression tag	UNP P15144
B	64	ARG	-	expression tag	UNP P15144
B	65	PRO	-	expression tag	UNP P15144

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	S	0	0	0
			736	474	126	129	7			
2	D	103	Total	C	N	O	S	0	0	0
			785	503	136	138	8			

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

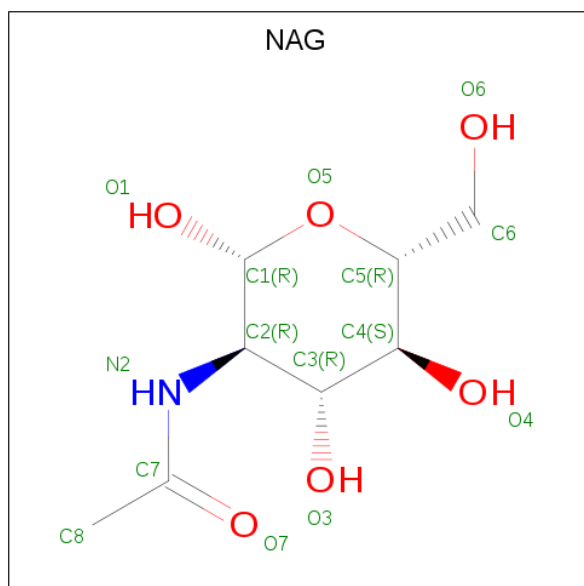


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

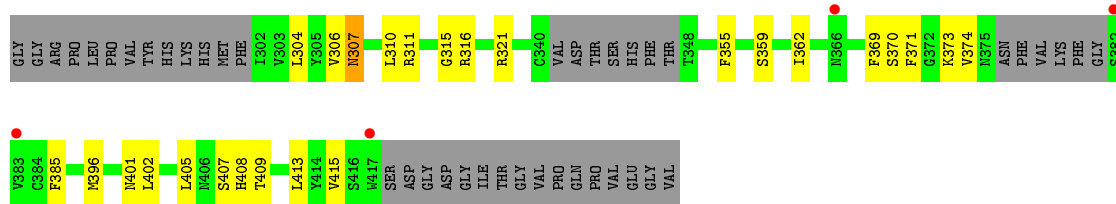
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	0
			126	126		
6	B	97	Total	O	0	0
			97	97		
6	C	1	Total	O	0	0
			1	1		
6	D	4	Total	O	0	0
			4	4		



- Molecule 1: Aminopeptidase N





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

Chain E: 50% 50%



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

Chain F: 100%



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

Chain G: 50% 50%



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

Chain H: 100%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.16 Å 98.57 Å 147.78 Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	49.38 – 2.75 49.38 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.38-2.75) 93.6 (49.38-2.55)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.54 Å)	Xtriage
Refinement program	PHENIX 1.16rc1_3535	Depositor
R, $R_{free}$	0.190 , 0.225 0.190 , 0.224	Depositor DCC
$R_{free}$ test set	4497 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: ZN, 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	0.29	0/7437	0.50	0/10128
1	B	0.30	0/7437	0.51	0/10128
2	C	0.42	0/752	0.72	0/1018
2	D	0.54	0/802	0.65	0/1086
All	All	0.32	0/16428	0.53	0/22360

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	7251	0	7014	22	0
1	B	7251	0	7015	25	0
2	C	736	0	726	20	0
2	D	785	0	773	17	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	84	0	78	2	0
5	B	70	0	65	1	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
6	A	126	0	0	0	0
6	B	97	0	0	0	0
6	C	1	0	0	0	0
6	D	4	0	0	0	0
All	All	16575	0	15823	82	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 3.

All (82) 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:495:VAL:HG22	1:B:528:ARG:HD3	1.76	0.66
2:C:395:ALA:HB1	2:C:412:THR:HG21	1.76	0.66
2:C:395:ALA:HB1	2:C:412:THR:CG2	2.27	0.65
1:A:349:PHE:H	1:A:857:GLN:NE2	1.96	0.64
2:D:374:VAL:HG12	2:D:374:VAL:O	2.01	0.61
1:B:624:LEU:HD21	3:H:1:NAG:H82	1.83	0.61
2:C:395:ALA:HB2	2:C:414:TYR:CD1	2.36	0.60
2:C:311:ARG:HG2	2:C:323:ALA:HB2	1.84	0.59
1:B:487:LEU:HA	1:B:490:PHE:CZ	2.37	0.59
1:A:502:SER:HB2	5:A:5007:NAG:H83	1.84	0.59
1:B:487:LEU:HA	1:B:490:PHE:CE1	2.38	0.58
2:D:311:ARG:O	2:D:316:ARG:HD2	2.04	0.57
2:D:321:ARG:NH1	2:D:409:THR:O	2.40	0.55
2:C:363:ASN:O	2:C:396:MET:HB2	2.06	0.54
1:A:492:SER:HB3	1:A:495:VAL:HG23	1.89	0.54
2:C:370:SER:O	2:C:370:SER:OG	2.27	0.52
2:C:303:VAL:HB	2:C:330:ALA:HB2	1.92	0.52
2:D:385:PHE:CD2	2:D:415:VAL:HG22	2.44	0.52
1:B:287:PHE:O	2:D:315:GLY:HA2	2.10	0.51
1:A:643:GLN:O	1:A:647:GLN:HG2	2.11	0.51
2:D:402:LEU:HD23	2:D:405:LEU:HD23	1.93	0.51
1:A:935:ARG:HG3	1:A:935:ARG:O	2.10	0.51
2:C:346:PHE:C	2:C:346:PHE:CD2	2.84	0.51
1:B:844:TYR:O	1:B:848:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:395:ALA:HB2	2:C:414:TYR:CE1	2.46	0.50
1:A:488:SER:HB2	1:A:496:PHE:CD2	2.47	0.50
2:C:347:THR:OG1	2:C:347:THR:O	2.24	0.49
2:D:370:SER:HB2	2:D:373:LYS:HG2	1.94	0.49
1:B:369:PHE:CZ	1:B:379:LYS:HE3	2.48	0.49
1:B:104:LYS:HG2	1:B:183:GLU:HG2	1.93	0.48
2:C:371:PHE:HB2	2:C:396:MET:HE1	1.95	0.48
1:A:720:ASN:HB3	1:A:966:SER:CB	2.43	0.48
1:B:123:HIS:HB3	1:B:218:ARG:HB3	1.94	0.48
1:A:809:TRP:CE2	1:A:832:LEU:HD22	2.49	0.48
1:B:490:PHE:CD2	1:B:491:LEU:HD13	2.49	0.47
2:C:396:MET:HE2	2:C:413:LEU:HD23	1.96	0.47
1:B:215:ALA:HB1	1:B:218:ARG:CZ	2.44	0.47
1:B:867:THR:HG21	1:B:905:VAL:HA	1.97	0.47
2:D:321:ARG:HA	2:D:408:HIS:CD2	2.50	0.47
2:C:371:PHE:HB2	2:C:396:MET:CE	2.46	0.46
2:D:362:ILE:O	2:D:362:ILE:HG23	2.16	0.46
2:D:369:PHE:HZ	2:D:415:VAL:HG11	1.81	0.46
1:A:844:TYR:O	1:A:848:THR:HG23	2.15	0.46
2:C:302:ILE:HG12	2:C:385:PHE:CD2	2.51	0.46
1:B:350:ASN:HD21	1:B:857:GLN:HG2	1.81	0.45
1:A:455:LEU:HA	1:A:455:LEU:HD12	1.79	0.45
1:B:290:VAL:HG13	1:B:309:ILE:HG23	1.98	0.45
1:A:283:ILE:HD13	1:A:344:ILE:HD13	1.98	0.45
1:A:864:ILE:O	1:A:867:THR:HG22	2.16	0.45
1:A:882:SER:HB3	1:B:913:TYR:CD1	2.51	0.45
1:B:498:GLN:OE1	1:B:528:ARG:HD2	2.17	0.45
1:B:257:PRO:HD3	5:B:5005:NAG:H62	1.99	0.44
1:A:487:LEU:HA	1:A:490:PHE:CE1	2.53	0.44
1:B:250:LEU:HG	1:B:340:LYS:HG2	1.99	0.44
2:C:346:PHE:CD2	2:C:346:PHE:O	2.70	0.44
1:A:488:SER:O	1:A:488:SER:OG	2.36	0.43
1:B:913:TYR:O	1:B:916:GLN:HG3	2.18	0.43
1:B:362:TYR:HE2	1:B:385:VAL:HG12	1.84	0.43
1:B:726:VAL:HG21	1:B:759:THR:HB	1.99	0.43
2:C:346:PHE:HD2	2:C:346:PHE:O	2.01	0.43
1:A:213:GLN:HA	1:A:214:ALA:HA	1.76	0.43
2:D:304:LEU:HD22	2:D:413:LEU:HD22	2.00	0.43
1:B:172:LYS:HG2	1:B:173:ASP:OD1	2.19	0.43
2:C:349:GLN:O	2:C:371:PHE:HE1	2.01	0.43
2:D:310:LEU:HD21	2:D:355:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:369:PHE:N	2:D:369:PHE:CD2	2.87	0.42
1:A:149:ASP:HB2	1:A:167:LYS:HD2	2.01	0.42
1:A:502:SER:CB	5:A:5007:NAG:H83	2.46	0.42
1:B:399:VAL:HG21	1:B:504:LEU:HD23	2.02	0.42
2:D:371:PHE:HB2	2:D:396:MET:HE3	2.01	0.42
1:A:356:ASN:HB2	1:A:359:LEU:O	2.19	0.42
1:A:720:ASN:HB3	1:A:966:SER:HB2	2.01	0.42
2:C:327:ILE:HD13	2:C:411:GLY:HA3	2.01	0.42
2:D:371:PHE:HB2	2:D:396:MET:CE	2.50	0.42
2:D:306:VAL:C	2:D:307:ASN:HD22	2.23	0.42
1:A:601:TRP:HB3	1:A:603:ILE:HD11	2.02	0.41
2:C:394:CYS:O	2:C:394:CYS:SG	2.78	0.41
2:D:310:LEU:HD21	2:D:355:PHE:CZ	2.56	0.41
1:A:221:PHE:CE2	1:A:223:CYS:HB3	2.56	0.41
1:B:340:LYS:NZ	1:B:342:ASP:OD2	2.49	0.40
1:B:710:ASP:HA	1:B:715:TYR:CG	2.57	0.40
2:C:367:CYS:HA	2:C:368:PRO:HD3	1.95	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	893/906 (99%)	874 (98%)	19 (2%)	0	100	100
1	B	893/906 (99%)	876 (98%)	17 (2%)	0	100	100
2	C	90/145 (62%)	86 (96%)	4 (4%)	0	100	100
2	D	97/145 (67%)	94 (97%)	3 (3%)	0	100	100
All	All	1973/2102 (94%)	1930 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	798/802 (100%)	791 (99%)	7 (1%)	78	87
1	B	798/802 (100%)	794 (100%)	4 (0%)	88	92
2	C	81/122 (66%)	80 (99%)	1 (1%)	71	82
2	D	87/122 (71%)	83 (95%)	4 (5%)	27	46
All	All	1764/1848 (96%)	1748 (99%)	16 (1%)	78	87

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

Mol	Chain	Res	Type
1	A	340	LYS
1	A	357	TRP
1	A	528	ARG
1	A	672	HIS
1	A	720	ASN
1	A	842	ASN
1	A	867	THR
1	B	190	LEU
1	B	203	VAL
1	B	340	LYS
1	B	935	ARG
2	C	407	SER
2	D	307	ASN
2	D	359	SER
2	D	401	ASN
2	D	407	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	598	GLN
1	A	691	GLN
1	A	720	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	815	GLN
1	A	842	ASN
1	A	857	GLN
1	A	889	ASN
1	A	903	GLN
1	A	960	GLN
1	B	213	GLN
1	B	541	ASN
1	B	643	GLN
1	B	803	GLN
1	B	889	ASN
1	B	900	ASN
2	C	349	GLN
2	C	408	HIS
2	D	307	ASN

### 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 ⓘ

8 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	0.23	0	17,19,21	0.41	0
3	NAG	E	2	3	14,14,15	0.44	0	17,19,21	0.91	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	2	3	14,14,15	1.24	2 (14%)	17,19,21	1.22	2 (11%)
3	NAG	G	1	1,3	14,14,15	0.46	0	17,19,21	0.85	0
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.38	0	17,19,21	0.84	0
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	0.70	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	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-2.48	1.39	1.43
3	F	2	NAG	C2-N2	-2.26	1.42	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	3.41	116.81	112.19
3	G	2	NAG	C1-O5-C5	3.15	116.45	112.19
3	F	2	NAG	C2-N2-C7	-2.89	118.79	122.90
3	F	1	NAG	O5-C1-C2	-2.44	107.44	111.29
3	H	2	NAG	C1-O5-C5	2.43	115.49	112.19
3	F	1	NAG	C3-C4-C5	2.29	114.33	110.24
3	F	2	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:



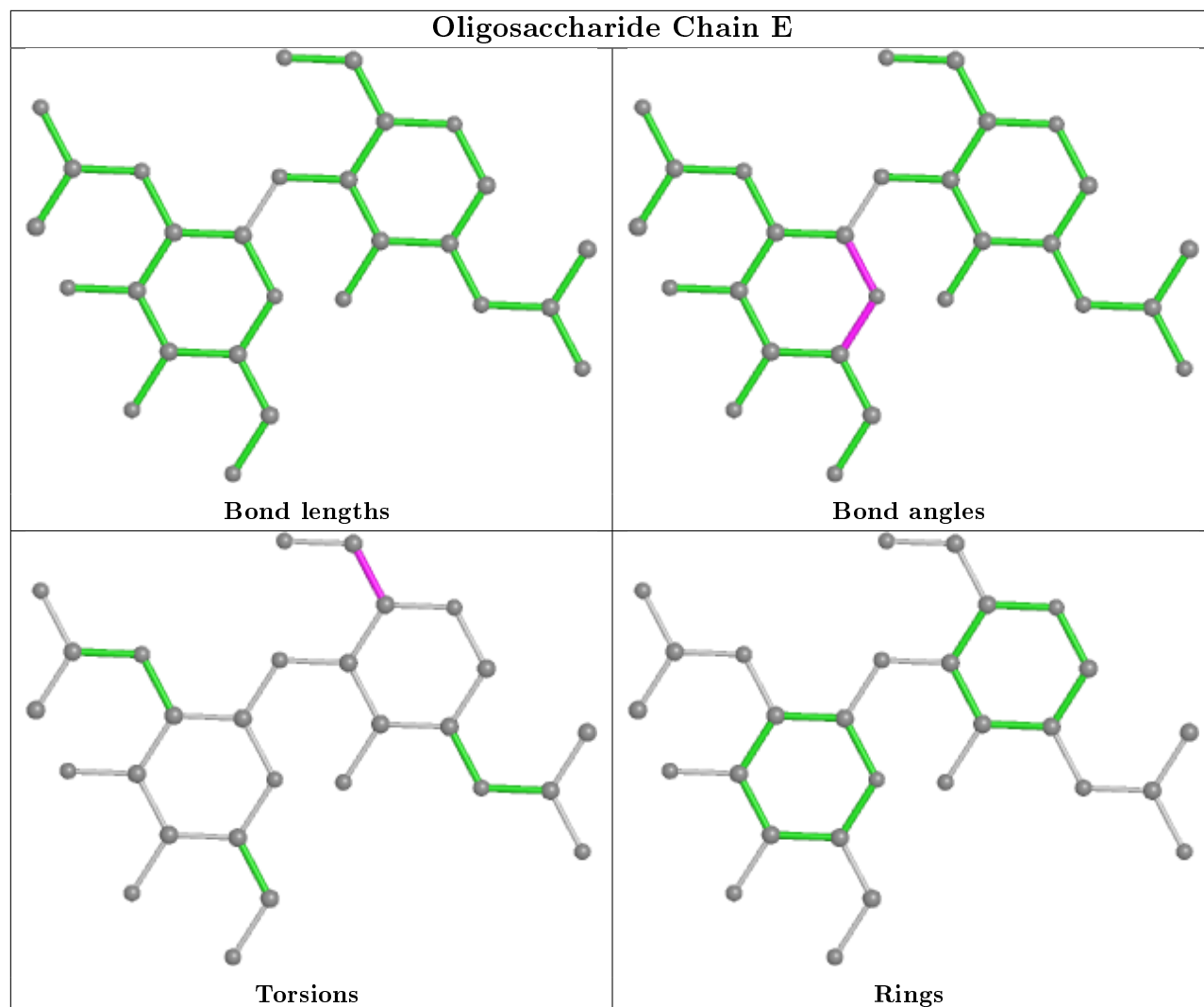
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

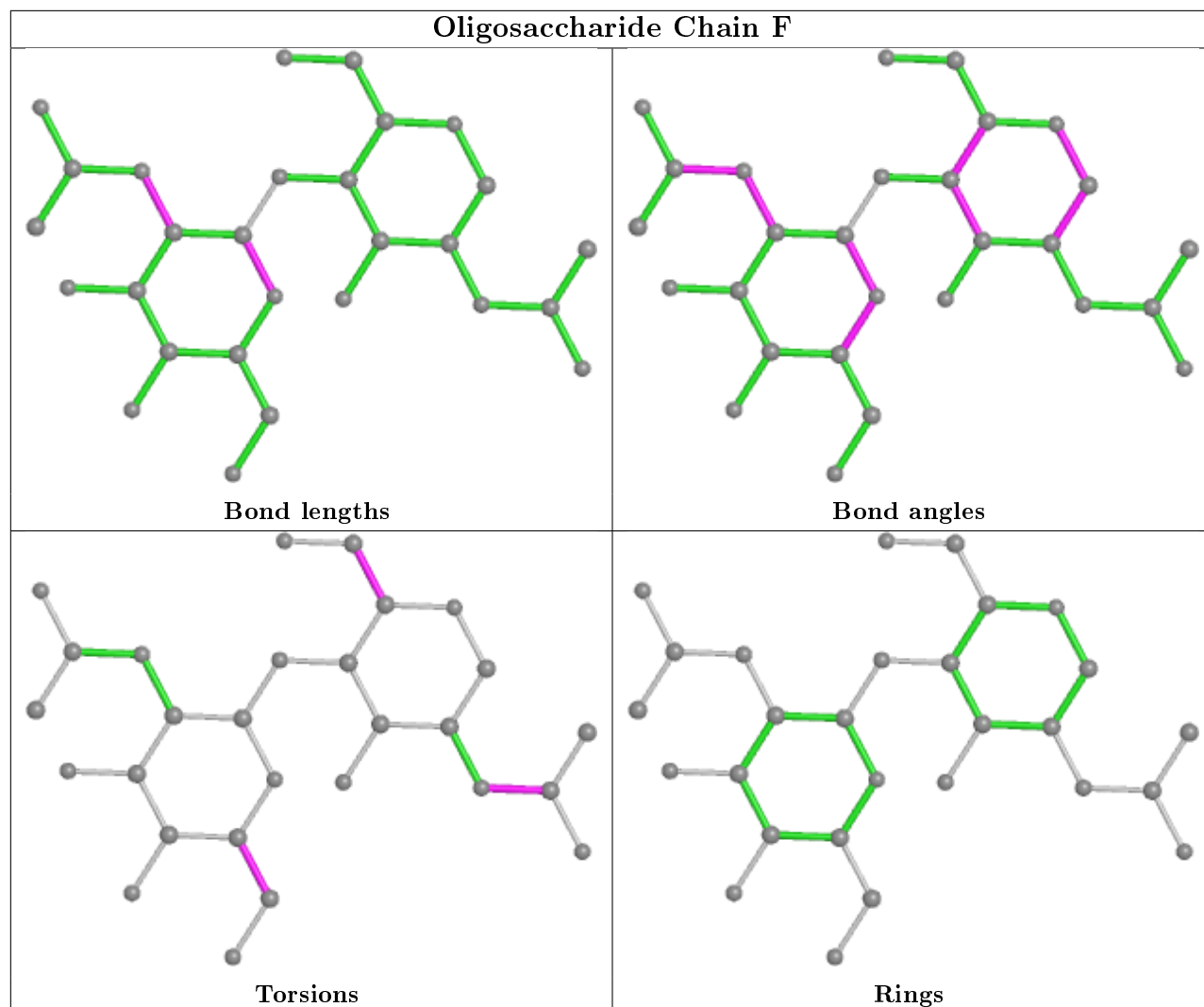
There are no ring outliers.

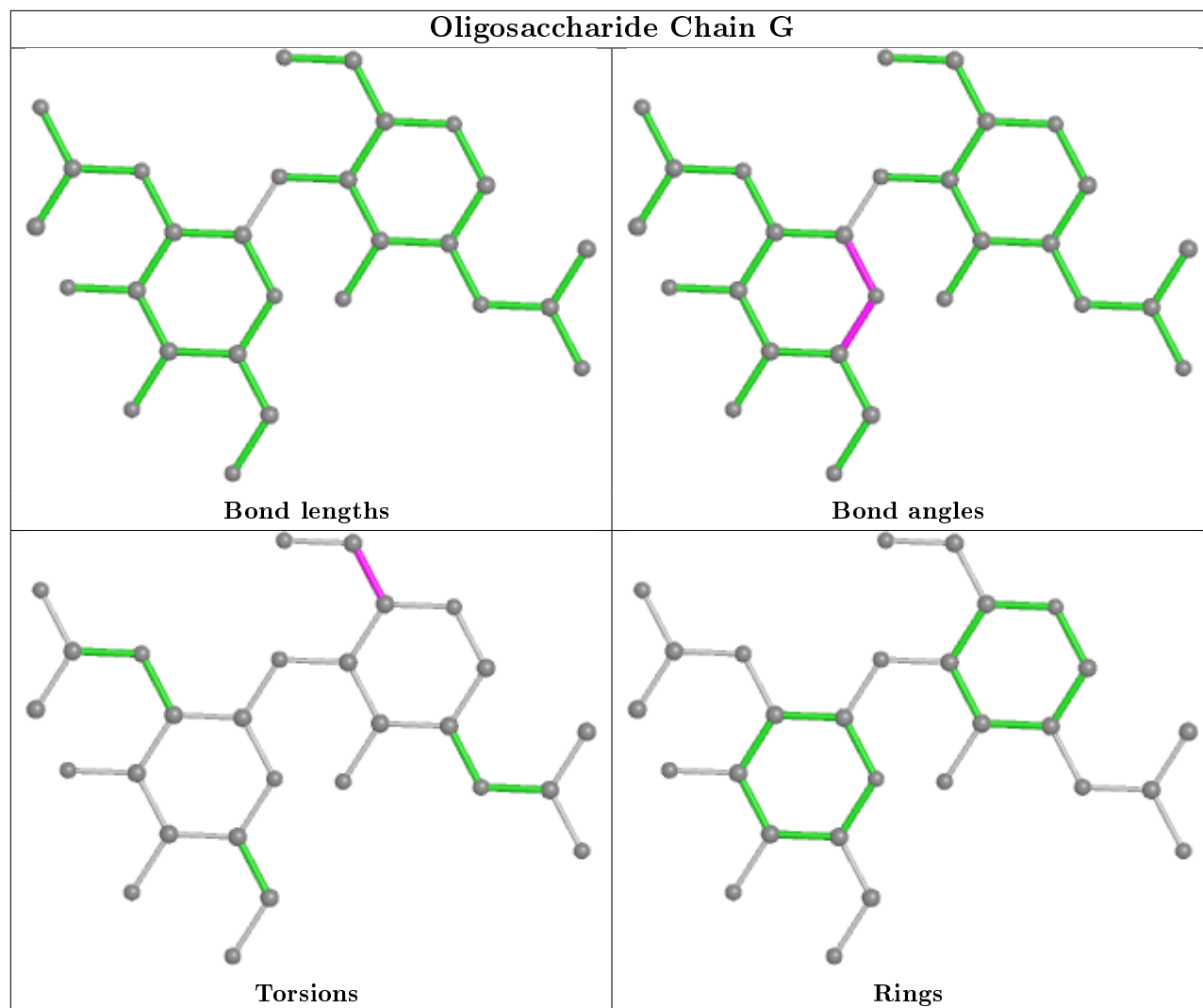
1 monomer is involved in 1 short contact:

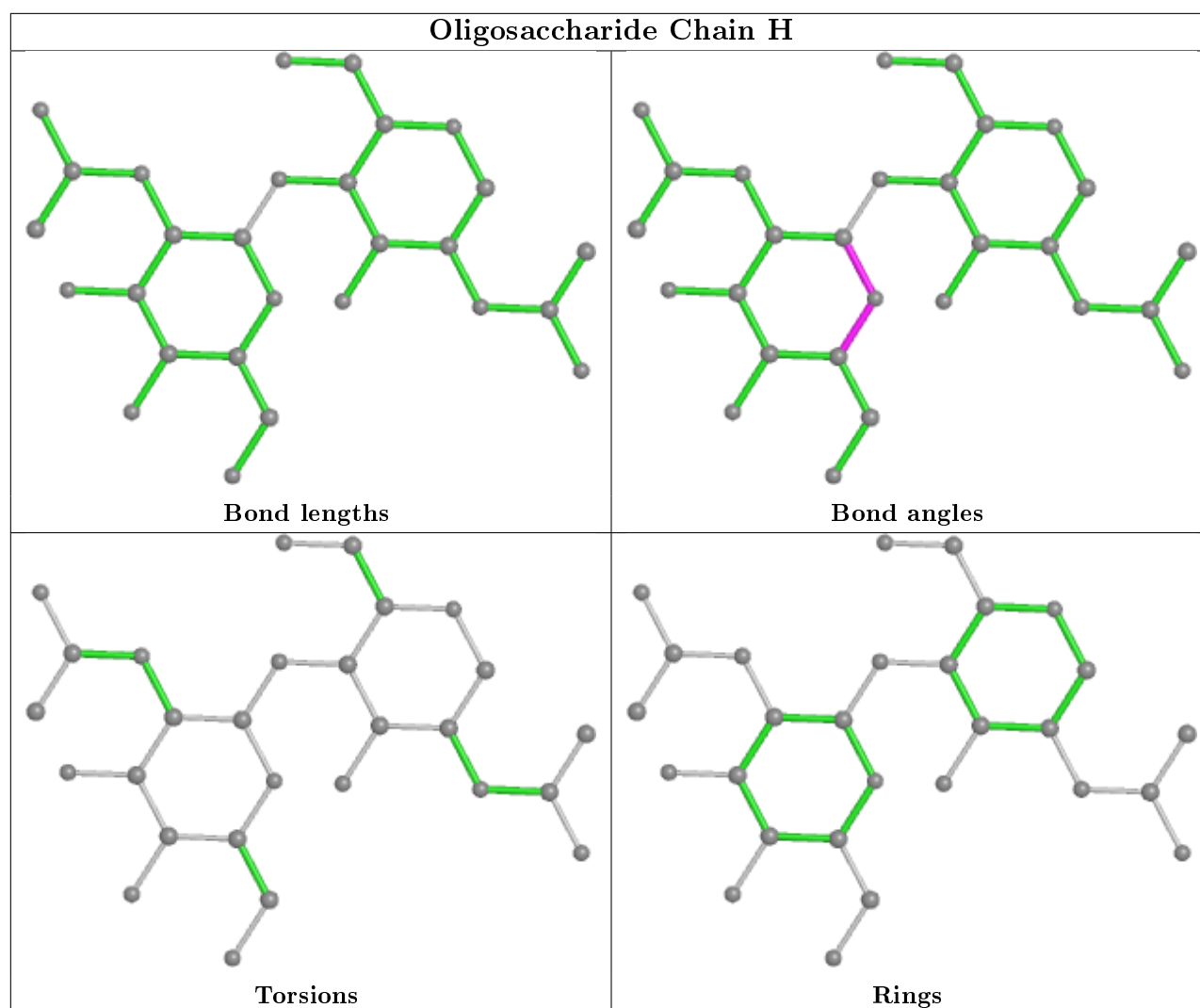
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0

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 ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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	NAG	B	5010	1	14,14,15	0.38	0	17,19,21	1.02	1 (5%)
5	NAG	A	5010	1	14,14,15	0.34	0	17,19,21	0.78	0
5	NAG	B	5007	1	14,14,15	0.38	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	5007	1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
5	NAG	A	5011	1	14,14,15	0.38	0	17,19,21	0.66	0
5	NAG	D	2001	2	14,14,15	0.39	0	17,19,21	0.74	0
5	NAG	B	5006	1	14,14,15	0.46	0	17,19,21	0.73	0
5	NAG	D	2002	2	14,14,15	0.42	0	17,19,21	1.21	2 (11%)
5	NAG	A	5005	1	14,14,15	0.38	0	17,19,21	0.67	0
5	NAG	B	5005	1	14,14,15	0.32	0	17,19,21	0.80	1 (5%)
5	NAG	B	5002	1	14,14,15	0.18	0	17,19,21	0.53	0
5	NAG	A	5002	1	14,14,15	0.16	0	17,19,21	0.41	0
5	NAG	A	5006	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)
5	NAG	C	2002	2	14,14,15	1.32	2 (14%)	17,19,21	2.26	8 (47%)
5	NAG	C	2001	2	14,14,15	0.32	0	17,19,21	0.48	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
5	NAG	B	5010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5010	1	-	4/6/23/26	0/1/1/1
5	NAG	B	5007	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5007	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5011	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2001	2	-	2/6/23/26	0/1/1/1
5	NAG	B	5006	1	-	1/6/23/26	0/1/1/1
5	NAG	D	2002	2	-	4/6/23/26	0/1/1/1
5	NAG	A	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5002	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5002	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5006	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2002	2	-	0/6/23/26	0/1/1/1
5	NAG	C	2001	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2002	NAG	O5-C1	-2.22	1.40	1.43
5	C	2002	NAG	C2-N2	-2.11	1.42	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2002	NAG	O5-C1-C2	-4.74	103.80	111.29
5	C	2002	NAG	C4-C3-C2	-3.28	106.21	111.02
5	B	5010	NAG	O5-C1-C2	-3.11	106.38	111.29
5	C	2002	NAG	O6-C6-C5	-2.96	101.15	111.29
5	C	2002	NAG	C6-C5-C4	-2.94	106.11	113.00
5	A	5007	NAG	C1-O5-C5	2.85	116.06	112.19
5	B	5005	NAG	C1-O5-C5	2.56	115.66	112.19
5	C	2002	NAG	O5-C5-C6	-2.49	103.30	107.20
5	D	2002	NAG	O5-C5-C6	2.42	111.00	107.20
5	D	2002	NAG	O5-C1-C2	-2.37	107.54	111.29
5	C	2002	NAG	C1-O5-C5	2.32	115.34	112.19
5	A	5006	NAG	C1-O5-C5	2.28	115.28	112.19
5	C	2002	NAG	O4-C4-C5	-2.25	103.72	109.30
5	C	2002	NAG	C2-N2-C7	-2.18	119.79	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5011	NAG	C8-C7-N2-C2
5	A	5011	NAG	O7-C7-N2-C2
5	D	2001	NAG	O5-C5-C6-O6
5	A	5010	NAG	C8-C7-N2-C2
5	D	2002	NAG	C8-C7-N2-C2
5	D	2002	NAG	O7-C7-N2-C2
5	D	2001	NAG	C4-C5-C6-O6
5	B	5010	NAG	C8-C7-N2-C2
5	A	5010	NAG	O7-C7-N2-C2
5	B	5010	NAG	O7-C7-N2-C2
5	D	2002	NAG	O5-C5-C6-O6
5	D	2002	NAG	C4-C5-C6-O6
5	A	5010	NAG	C4-C5-C6-O6
5	B	5007	NAG	O5-C5-C6-O6
5	A	5011	NAG	C4-C5-C6-O6
5	A	5010	NAG	O5-C5-C6-O6
5	B	5006	NAG	O5-C5-C6-O6
5	A	5011	NAG	O5-C5-C6-O6
5	B	5007	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5007	NAG	2	0
5	B	5005	NAG	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	897/906 (99%)	-0.26	1 (0%) 95 97	28, 47, 73, 98	0
1	B	897/906 (99%)	-0.21	3 (0%) 94 96	29, 50, 77, 102	0
2	C	96/145 (66%)	0.50	8 (8%) 11 13	40, 68, 97, 121	0
2	D	103/145 (71%)	0.35	4 (3%) 39 46	48, 66, 91, 113	0
All	All	1993/2102 (94%)	-0.17	16 (0%) 86 90	28, 50, 78, 121	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	395	ALA	4.5
2	C	394	CYS	3.3
2	C	369	PHE	3.2
1	B	202	ASN	2.8
2	D	382	SER	2.7
1	B	174	SER	2.6
2	C	302	ILE	2.3
2	C	330	ALA	2.3
2	C	392	GLY	2.3
1	A	595	ARG	2.2
2	D	417	TRP	2.2
2	C	347	THR	2.2
2	C	332	PHE	2.2
2	D	366	ASN	2.2
1	B	927	GLU	2.2
2	D	383	VAL	2.1

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

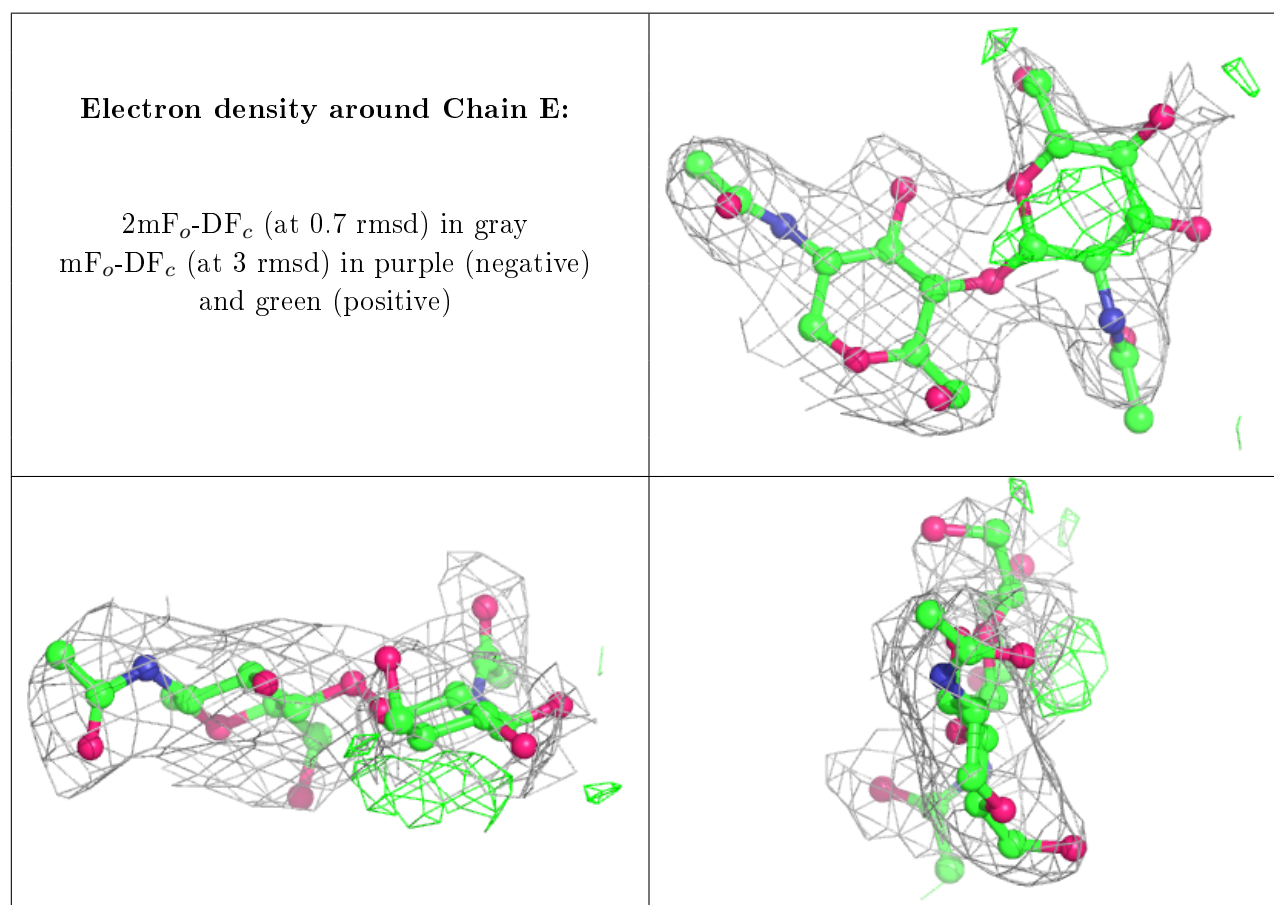
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

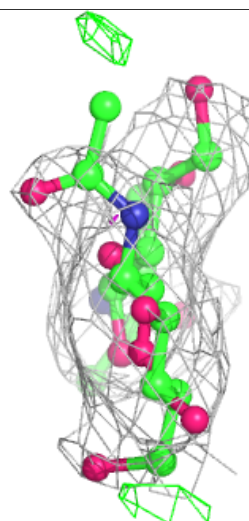
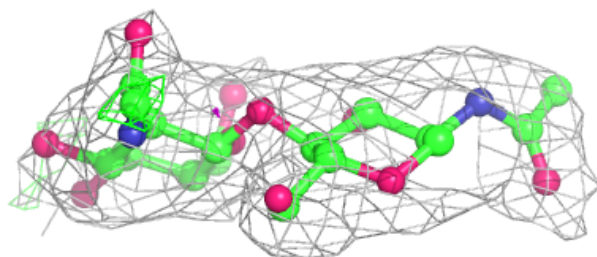
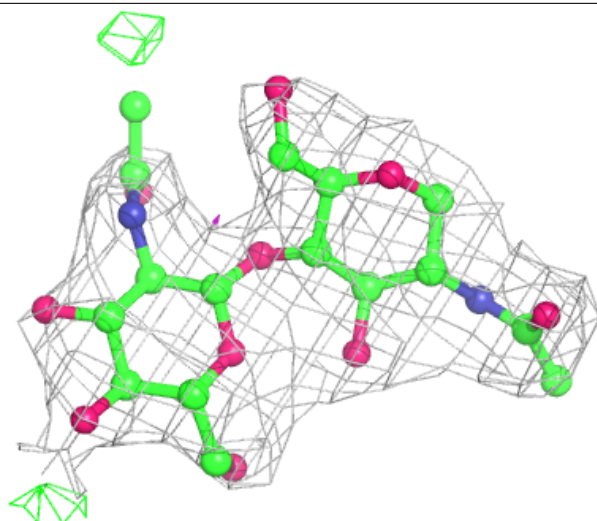
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.80	0.23	72,85,89,91	0
3	NAG	G	2	14/15	0.81	0.29	84,91,97,99	0
3	NAG	H	2	14/15	0.81	0.27	74,104,110,110	0
3	NAG	F	2	14/15	0.89	0.23	82,92,98,101	0
3	NAG	F	1	14/15	0.92	0.14	61,66,71,82	0
3	NAG	G	1	14/15	0.94	0.15	43,61,66,76	0
3	NAG	H	1	14/15	0.94	0.14	57,65,76,89	0
3	NAG	E	1	14/15	0.97	0.12	47,53,65,69	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



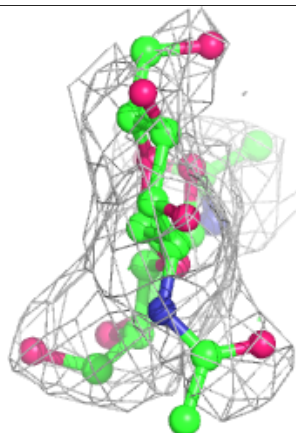
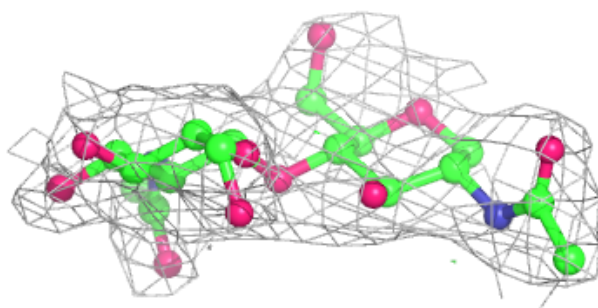
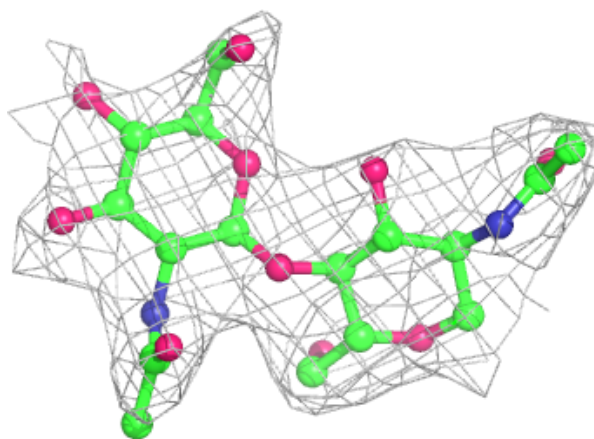
**Electron density around Chain F:**

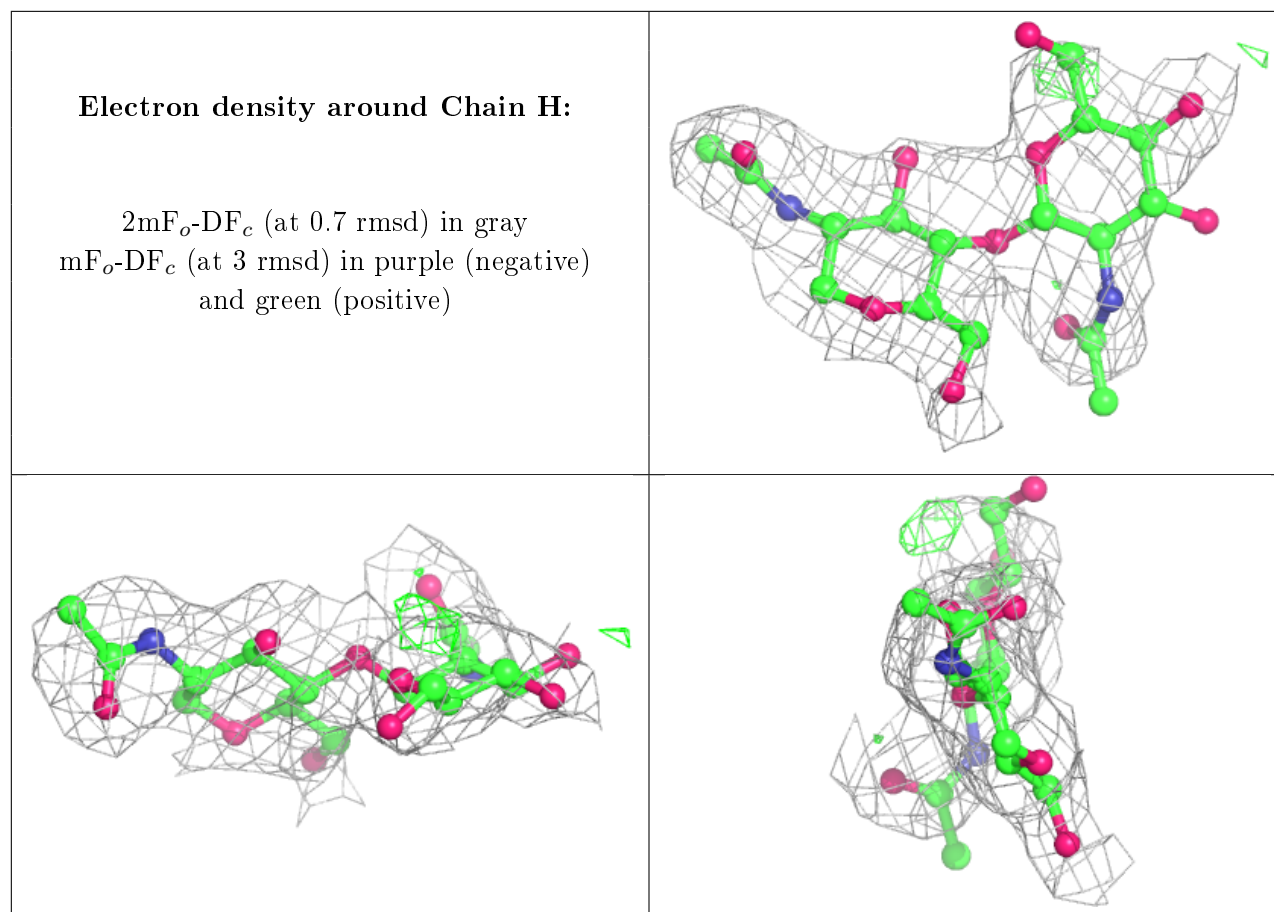
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands ⓘ

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
5	NAG	A	5010	14/15	0.82	0.24	89,99,107,108	0
5	NAG	B	5005	14/15	0.84	0.18	77,87,89,89	0
5	NAG	A	5011	14/15	0.85	0.23	95,100,105,107	0
5	NAG	B	5007	14/15	0.86	0.27	83,90,98,100	0
5	NAG	A	5005	14/15	0.87	0.15	70,79,84,85	0
5	NAG	B	5010	14/15	0.90	0.17	72,77,83,84	0
5	NAG	D	2002	14/15	0.91	0.21	63,72,77,77	0
5	NAG	A	5007	14/15	0.91	0.17	55,65,69,73	0
5	NAG	C	2002	14/15	0.92	0.15	55,65,72,76	0
5	NAG	A	5002	14/15	0.93	0.16	41,47,53,57	0
5	NAG	A	5006	14/15	0.93	0.13	51,57,61,65	0
5	NAG	B	5002	14/15	0.94	0.17	59,76,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	2001	14/15	0.94	0.13	65,73,75,76	0
5	NAG	D	2001	14/15	0.95	0.22	75,81,89,94	0
5	NAG	B	5006	14/15	0.96	0.13	48,57,63,64	0
4	ZN	A	5001	1/1	0.99	0.21	43,43,43,43	0
4	ZN	B	5001	1/1	0.99	0.17	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.