



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 12:05 PM EDT

PDB ID : 7U0N  
Title : Crystal structure of chimeric omicron RBD (strain BA.1) complexed with human ACE2  
Authors : Geng, Q.; Shi, K.; Ye, G.; Zhang, W.; Aihara, H.; Li, F.  
Deposited on : 2022-02-18  
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

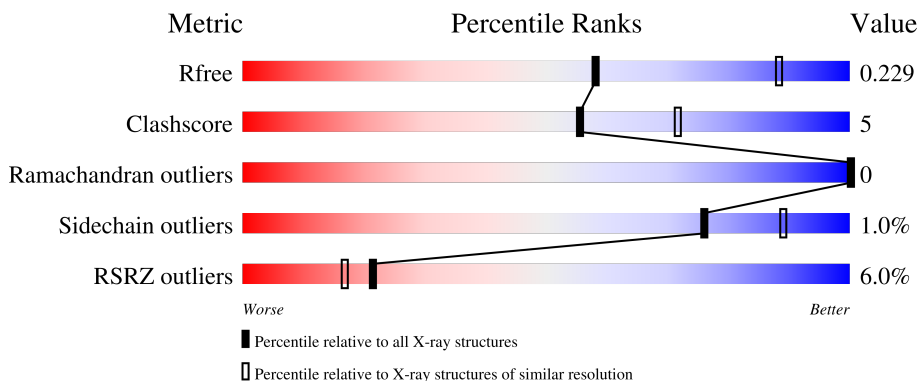
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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.




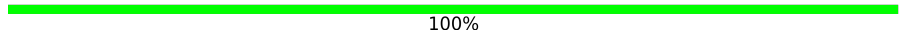
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	597	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">5%      87%      12%</p>
1	B	597	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">4%      84%      16%</p>
2	E	217	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">7%      76%      11%      13%</p>
2	F	217	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">11%      77%      11%      12%</p>
3	C	3	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">100%</p>

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Mol	Chain	Length	Quality of chain
3	D	3	 67% 33%
3	G	3	 100%
3	I	3	 33% 33% 33%
3	J	3	 100%
4	K	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	701	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13116 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	Total 4862	C 3111	N 805	O 917	S 29	0	0	0
1	B	596	Total 4871	C 3116	N 806	O 920	S 29	0	1	0

- Molecule 2 is a protein called Spike protein S1.

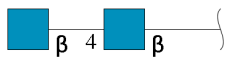
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	188	Total 1500	C 966	N 247	O 278	S 9	0	0	0
2	F	190	Total 1515	C 975	N 250	O 281	S 9	0	0	0

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



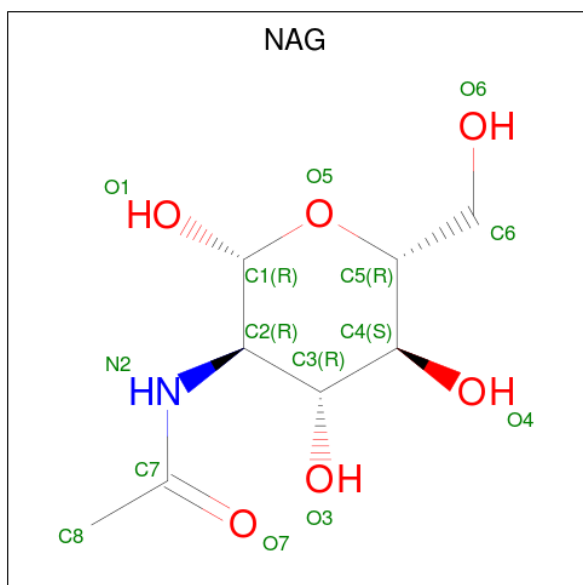
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	Total 39	C 22	N 2	O 15	0	0	0
3	D	3	Total 39	C 22	N 2	O 15	0	0	0
3	G	3	Total 39	C 22	N 2	O 15	0	0	0
3	I	3	Total 39	C 22	N 2	O 15	0	0	0
3	J	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	K	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

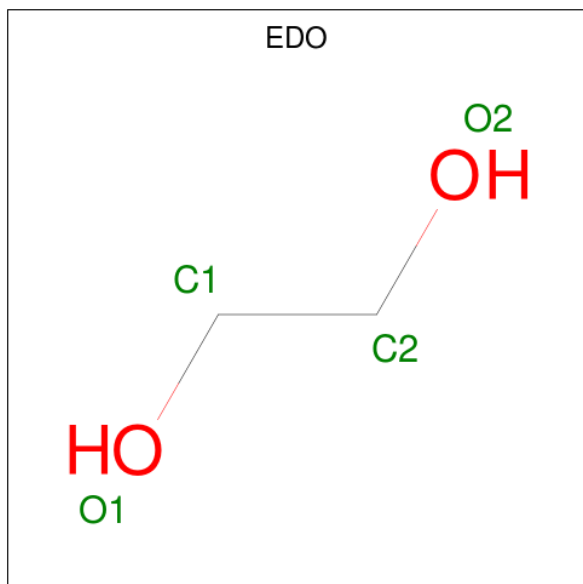
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	B	2	Total	Cl	0	0
			2	2		
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0

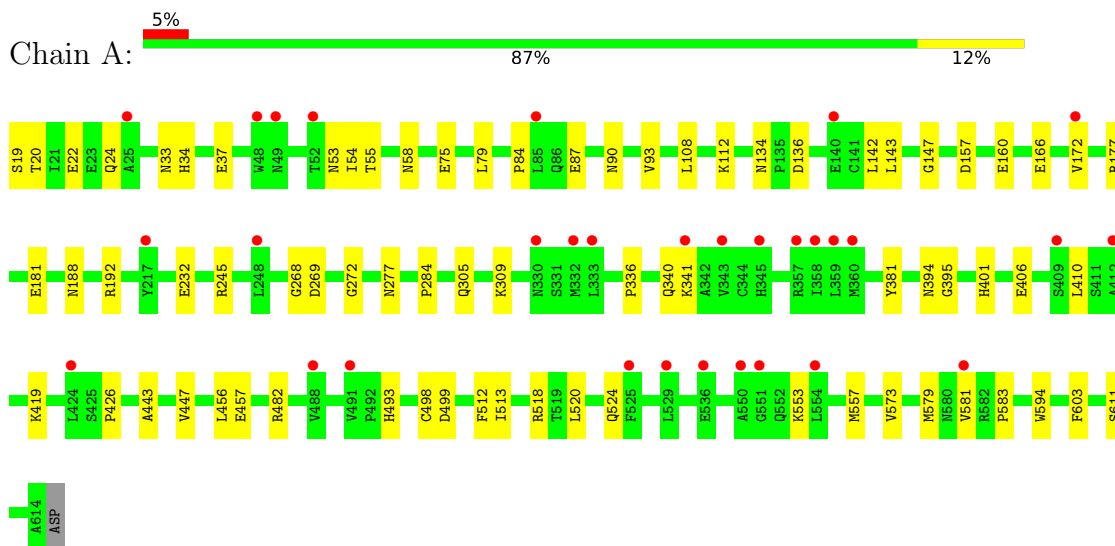
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total O 4 4	0	0
10	B	6	Total O 6 6	0	0
10	E	2	Total O 2 2	0	0
10	F	1	Total O 1 1	0	0

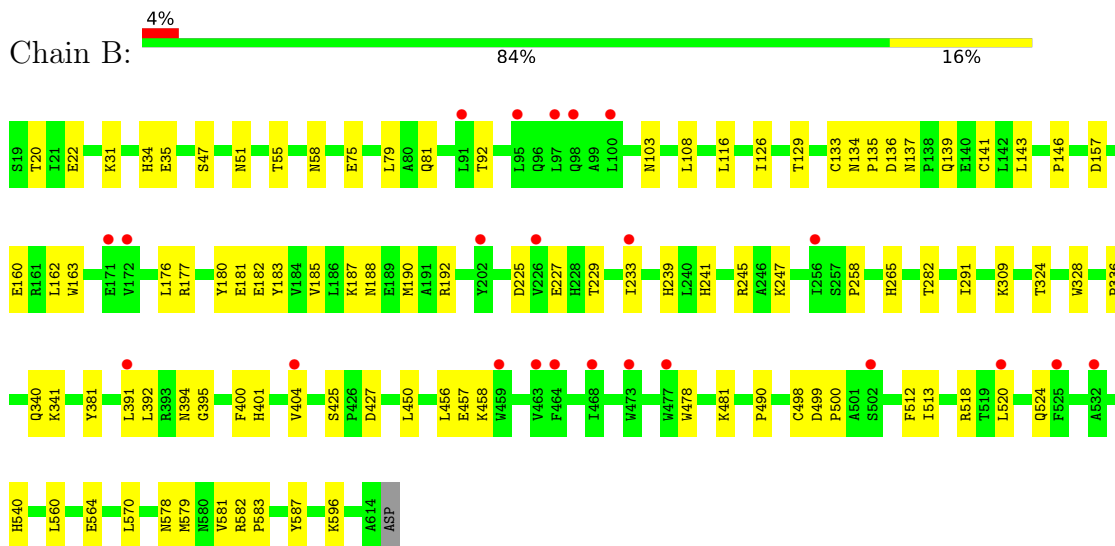
### 3 Residue-property plots

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.

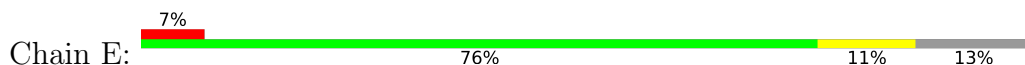
- Molecule 1: Angiotensin-converting enzyme 2



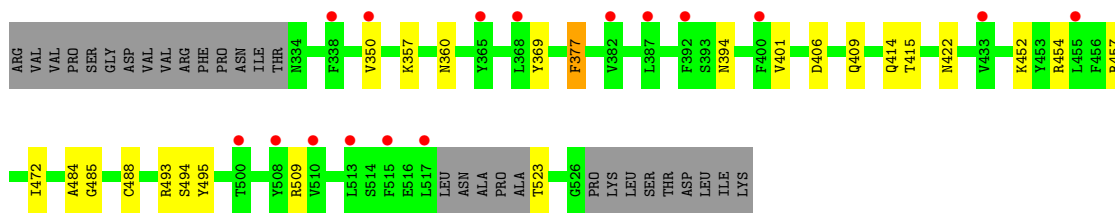
- Molecule 1: Angiotensin-converting enzyme 2



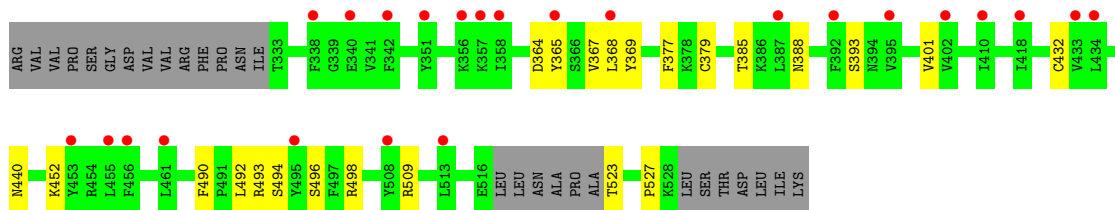
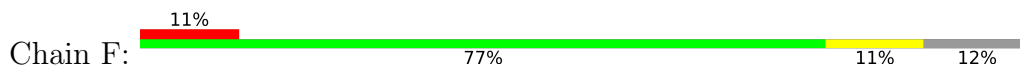
- Molecule 2: Spike protein S1







- Molecule 2: Spike protein S1



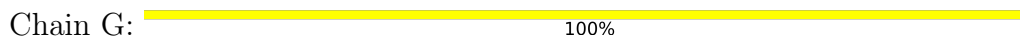
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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

Chain J:  100%

MAG1  
MAG2  
EMM3

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

Chain K:  50%  50%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.13Å 120.18Å 113.33Å 90.00° 92.44° 90.00°	Depositor
Resolution (Å)	30.11 – 2.61 113.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	54.9 (30.11-2.61) 54.9 (113.22-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.62Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.188 , 0.235 0.188 , 0.229	Depositor DCC
$R_{free}$ test set	1734 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.7	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: CL, ZN, NAG, BMA, MG, EDO

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	0.24	0/4999	0.45	0/6792
1	B	0.24	0/5008	0.46	0/6804
2	E	0.26	0/1542	0.54	0/2094
2	F	0.25	0/1558	0.53	0/2116
All	All	0.24	0/13107	0.48	0/17806

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	4862	0	4633	42	0
1	B	4871	0	4638	54	0
2	E	1500	0	1424	15	0
2	F	1515	0	1442	16	0
3	C	39	0	34	0	0
3	D	39	0	34	1	0
3	G	39	0	34	1	0
3	I	39	0	34	1	0
3	J	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	28	0	25	0	0
5	A	56	0	52	9	0
5	B	28	0	26	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	F	1	0	0	1	0
8	B	12	0	18	1	0
9	B	1	0	0	0	0
10	A	4	0	0	0	0
10	B	6	0	0	0	0
10	E	2	0	0	0	0
10	F	1	0	0	2	0
All	All	13116	0	12454	129	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 (129) 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:53:ASN:ND2	5:A:701:NAG:C1	1.72	1.49
5:A:701:NAG:O3	5:A:701:NAG:H82	1.24	1.31
5:A:701:NAG:O3	5:A:701:NAG:C8	2.03	1.05
1:A:53:ASN:ND2	5:A:701:NAG:C2	2.21	1.04
5:A:701:NAG:H82	5:A:701:NAG:HO3	1.16	0.96
1:A:53:ASN:ND2	5:A:701:NAG:H2	1.99	0.77
2:E:485:GLY:H	2:E:488:CYS:HB2	1.50	0.77
1:A:53:ASN:CG	5:A:701:NAG:C1	2.54	0.73
2:F:385:THR:O	2:F:388:ASN:ND2	2.24	0.71
2:E:369:TYR:HA	2:E:377:PHE:HE2	1.56	0.70
1:B:177:ARG:HD3	1:B:498:CYS:HB2	1.73	0.70
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.26	0.67
1:A:245:ARG:NH2	1:A:603:PHE:O	2.28	0.66
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.78	0.66
2:F:493:ARG:NH1	10:F:701:HOH:O	2.31	0.64
1:B:146:PRO:HD2	8:B:707:EDO:H12	1.79	0.63
1:A:55:THR:OG1	1:A:58:ASN:ND2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:364:ASP:HA	2:F:527:PRO:HD3	1.81	0.62
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.81	0.62
1:B:126:ILE:HD11	1:B:176:LEU:HG	1.81	0.61
1:B:55:THR:OG1	1:B:58:ASN:ND2	2.31	0.60
1:B:75:GLU:O	1:B:79:LEU:HD13	2.02	0.59
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.85	0.58
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.85	0.58
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.85	0.58
2:E:415:THR:HG21	3:D:3:BMA:H4	1.87	0.56
1:B:126:ILE:HA	1:B:129:THR:HG22	1.87	0.56
1:A:166:GLU:OE1	1:A:493:HIS:NE2	2.31	0.55
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.87	0.55
1:A:336:PRO:HB2	1:A:340:GLN:HB3	1.89	0.54
1:B:425:SER:OG	1:B:427:ASP:OD1	2.24	0.54
1:B:324:THR:HB	7:F:602:CL:CL	2.45	0.54
1:B:245:ARG:NH1	1:B:258:PRO:O	2.40	0.53
1:A:34:HIS:CE1	2:E:493:ARG:HB3	2.44	0.53
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.91	0.52
2:E:452:LYS:HA	2:E:494:SER:HA	1.90	0.52
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.74	0.52
1:B:34:HIS:CE1	2:F:493:ARG:HB3	2.44	0.52
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.92	0.51
1:A:53:ASN:ND2	5:A:701:NAG:O5	2.38	0.51
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.91	0.51
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.75	0.51
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.93	0.51
1:A:406:GLU:O	1:A:410:LEU:HD13	2.11	0.50
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.94	0.50
1:A:75:GLU:O	1:A:79:LEU:HD13	2.12	0.50
1:A:134:ASN:HD21	1:A:136:ASP:HB2	1.76	0.49
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.93	0.49
2:F:393:SER:O	2:F:523:THR:OG1	2.26	0.49
1:A:53:ASN:HD22	5:A:701:NAG:H2	1.75	0.49
1:B:239:HIS:CE1	1:B:596:LYS:HG2	2.48	0.49
1:B:336:PRO:HB2	1:B:340:GLN:HB3	1.95	0.48
2:E:350:VAL:HG22	2:E:422:ASN:HB3	1.95	0.48
1:A:54:ILE:HD12	1:A:341:LYS:HG2	1.94	0.48
1:B:108:LEU:HD11	1:B:190:MET:HB2	1.96	0.48
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.96	0.48
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.95	0.47
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PHE:HZ	1:B:570:LEU:HB2	1.79	0.47
2:E:409:GLN:HA	2:E:414:GLN:HG3	1.95	0.47
1:B:81:GLN:NE2	1:B:103:ASN:OD1	2.33	0.47
1:A:336:PRO:HG2	1:A:340:GLN:O	2.14	0.47
2:E:454:ARG:HD3	2:E:457:ARG:HB2	1.97	0.47
1:A:268:GLY:O	1:A:277:ASN:ND2	2.34	0.46
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.79	0.46
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.48	0.46
1:B:20:THR:HG22	1:B:22:GLU:H	1.80	0.46
1:B:225:ASP:O	1:B:229:THR:HG22	2.15	0.46
1:B:229:THR:OG1	1:B:581:VAL:HB	2.15	0.46
1:B:31:LYS:HD2	2:F:493:ARG:HH12	1.81	0.46
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.97	0.46
1:B:188:ASN:HB3	1:B:192:ARG:HE	1.81	0.45
3:I:1:NAG:HO6	3:I:2:NAG:HN2	1.59	0.45
1:A:443:ALA:HA	1:A:447:VAL:HG13	1.97	0.45
1:B:134:ASN:ND2	1:B:136:ASP:HB2	2.31	0.45
1:B:478:TRP:HA	1:B:481:LYS:HB2	1.99	0.45
1:A:482:ARG:HH21	1:A:611:SER:HB3	1.81	0.45
1:B:227:GLU:OE2	1:B:458:LYS:HE2	2.17	0.45
1:B:116:LEU:HD11	1:B:187:LYS:HE2	1.98	0.45
1:B:582:ARG:HB3	1:B:583:PRO:HD3	1.98	0.45
2:E:493:ARG:HD3	2:E:493:ARG:HA	1.82	0.45
2:F:367:VAL:C	2:F:369:TYR:H	2.19	0.45
2:F:452:LYS:HG2	2:F:494:SER:HB3	1.99	0.44
1:B:247:LYS:HB2	1:B:282:THR:HG22	2.00	0.44
1:A:394:ASN:OD1	1:A:395:GLY:N	2.51	0.44
1:A:20:THR:HG22	1:A:22:GLU:H	1.82	0.43
1:B:578:ASN:OD1	1:B:579:MET:N	2.50	0.43
2:F:490:PHE:CE2	2:F:492:LEU:HB2	2.54	0.43
1:A:269:ASP:OD1	1:A:272:GLY:N	2.51	0.43
1:B:241:HIS:CE1	1:B:245:ARG:HH21	2.37	0.43
1:B:133:CYS:HA	1:B:141:CYS:HA	2.01	0.43
1:B:92:THR:HG23	1:B:392:LEU:HD21	2.01	0.43
1:B:180:TYR:HA	1:B:183:TYR:HB3	2.00	0.42
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.51	0.42
1:B:265:HIS:CE1	1:B:490:PRO:HB3	2.54	0.42
1:A:108:LEU:HD23	1:A:112:LYS:HB3	2.01	0.42
1:A:188:ASN:HB3	1:A:192:ARG:HE	1.84	0.42
2:F:440:ASN:OD1	2:F:440:ASN:N	2.50	0.42
1:B:35:GLU:HB2	10:F:701:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ASN:OD1	1:B:395:GLY:N	2.51	0.42
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.55	0.42
1:A:305:GLN:O	1:A:309:LYS:HB2	2.19	0.42
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.55	0.42
1:A:553:LYS:HE2	1:A:573:VAL:O	2.20	0.42
2:F:365:TYR:HD2	2:F:388:ASN:HA	1.84	0.42
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.55	0.41
2:E:472:ILE:HD12	2:E:484:ALA:HB2	2.02	0.41
2:F:367:VAL:O	2:F:368:LEU:HB2	2.19	0.41
3:G:1:NAG:O6	3:G:2:NAG:N2	2.44	0.41
1:B:560:LEU:HD13	1:B:564:GLU:HG3	2.01	0.41
1:A:33:ASN:O	1:A:37:GLU:HB2	2.20	0.41
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.55	0.41
1:B:47:SER:O	1:B:51:ASN:ND2	2.40	0.41
1:B:291:ILE:H	1:B:291:ILE:HG13	1.68	0.41
1:A:84:PRO:HG2	1:A:87:GLU:HB2	2.02	0.41
1:B:391:LEU:H	1:B:391:LEU:HD12	1.86	0.41
2:E:360:ASN:HA	2:E:523:THR:HB	2.03	0.41
2:F:496:SER:O	2:F:498:ARG:HG3	2.21	0.41
1:B:182:GLU:HA	1:B:185:VAL:HG12	2.03	0.41
2:F:379:CYS:HA	2:F:432:CYS:HA	2.03	0.41
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.56	0.40
2:E:369:TYR:HA	2:E:377:PHE:CE2	2.46	0.40
1:B:137:ASN:OD1	1:B:139:GLN:HG2	2.21	0.40
1:B:229:THR:OG1	1:B:520:LEU:HD21	2.21	0.40
1:B:499:ASP:N	1:B:500:PRO:HD2	2.36	0.40
2:E:406:ASP:OD2	2:E:495:TYR:OH	2.32	0.40
2:F:452:LYS:HG2	2:F:494:SER:HA	2.03	0.40
1:A:19:SER:HB2	1:A:24:GLN:HE21	1.86	0.40
1:B:400:PHE:O	1:B:404:VAL:HG23	2.22	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	594/597 (100%)	574 (97%)	20 (3%)	0	100	100
1	B	595/597 (100%)	575 (97%)	20 (3%)	0	100	100
2	E	184/217 (85%)	172 (94%)	12 (6%)	0	100	100
2	F	186/217 (86%)	170 (91%)	16 (9%)	0	100	100
All	All	1559/1628 (96%)	1491 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	526/527 (100%)	520 (99%)	6 (1%)	73	88
1	B	527/527 (100%)	521 (99%)	6 (1%)	73	88
2	E	164/190 (86%)	163 (99%)	1 (1%)	86	94
2	F	166/190 (87%)	165 (99%)	1 (1%)	86	94
All	All	1383/1434 (96%)	1369 (99%)	14 (1%)	76	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	172	VAL
1	A	381	TYR
1	A	401	HIS
1	A	518	ARG
1	A	557	MET
1	B	143	LEU
1	B	162	LEU
1	B	341	LYS
1	B	381	TYR

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Mol	Chain	Res	Type
1	B	401	HIS
1	B	518	ARG
2	E	377	PHE
2	F	377	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	340	GLN
1	B	34	HIS
1	B	58	ASN
1	B	96	GLN
1	B	194	ASN
1	B	340	GLN
1	B	522	GLN
1	B	535	HIS
2	E	370	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

17 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	C	1	1,3	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.57	0
3	BMA	C	3	3	11,11,12	0.64	0	15,15,17	0.77	0
3	NAG	D	1	1,3	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	BMA	D	3	3	11,11,12	0.58	0	15,15,17	0.67	0
3	NAG	G	1	1,3	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.43	0
3	BMA	G	3	3	11,11,12	0.76	0	15,15,17	1.21	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.43	0
3	BMA	I	3	3	11,11,12	0.66	0	15,15,17	0.82	0
3	NAG	J	1	1,3	14,14,15	0.33	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	BMA	J	3	3	11,11,12	0.60	0	15,15,17	0.73	0
4	NAG	K	1	1,4	14,14,15	0.42	0	17,19,21	0.66	1 (5%)
4	NAG	K	2	4	14,14,15	0.27	0	17,19,21	0.43	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-O5-C5	2.31	115.32	112.19
4	K	1	NAG	C1-O5-C5	2.18	115.15	112.19
3	G	3	BMA	C1-C2-C3	2.07	112.21	109.67
3	I	1	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

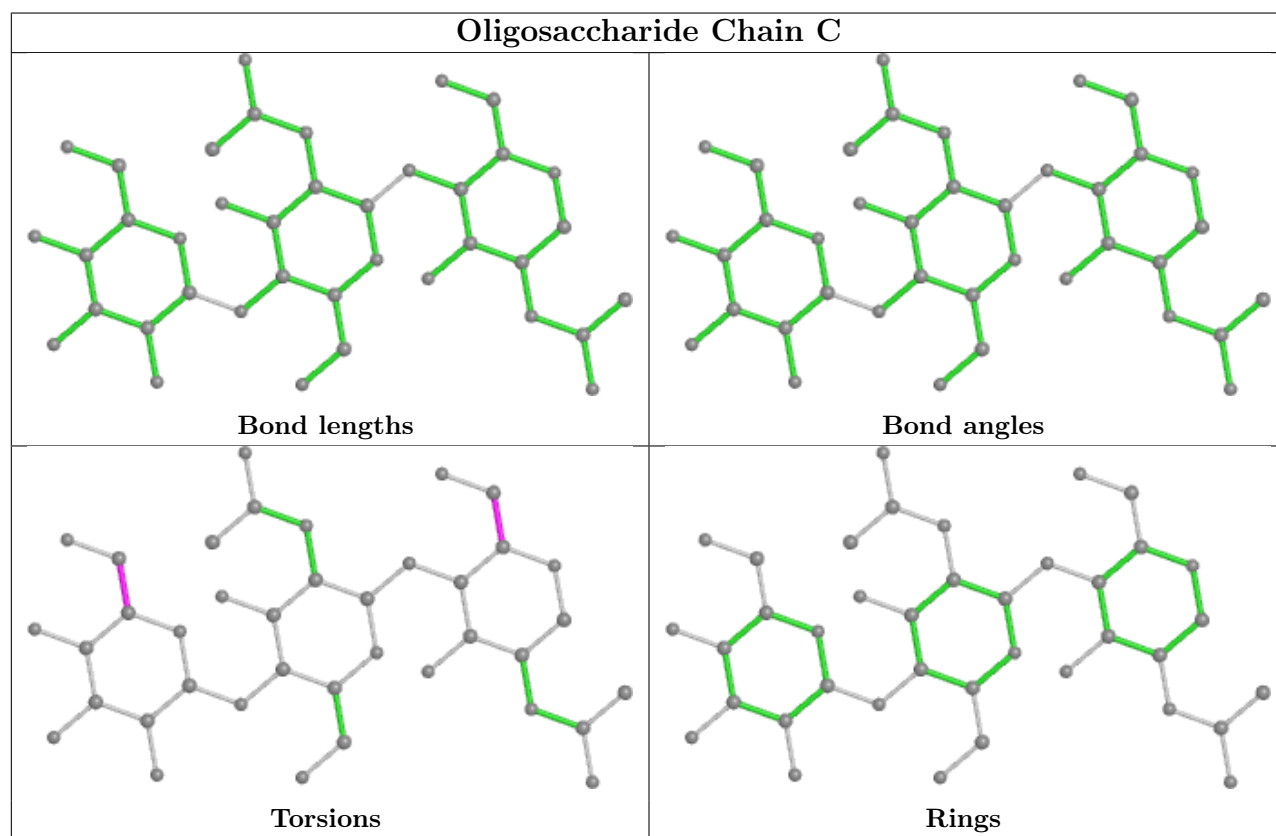
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	J	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

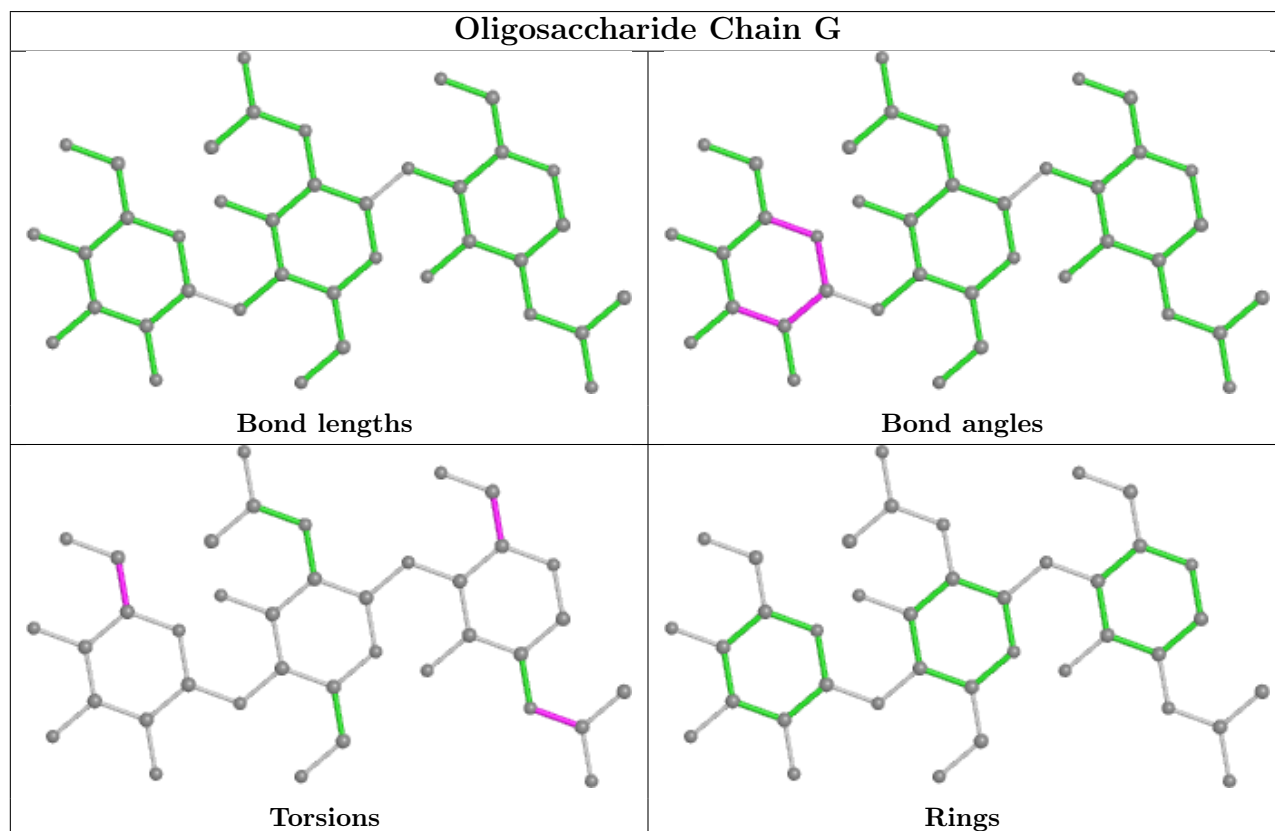
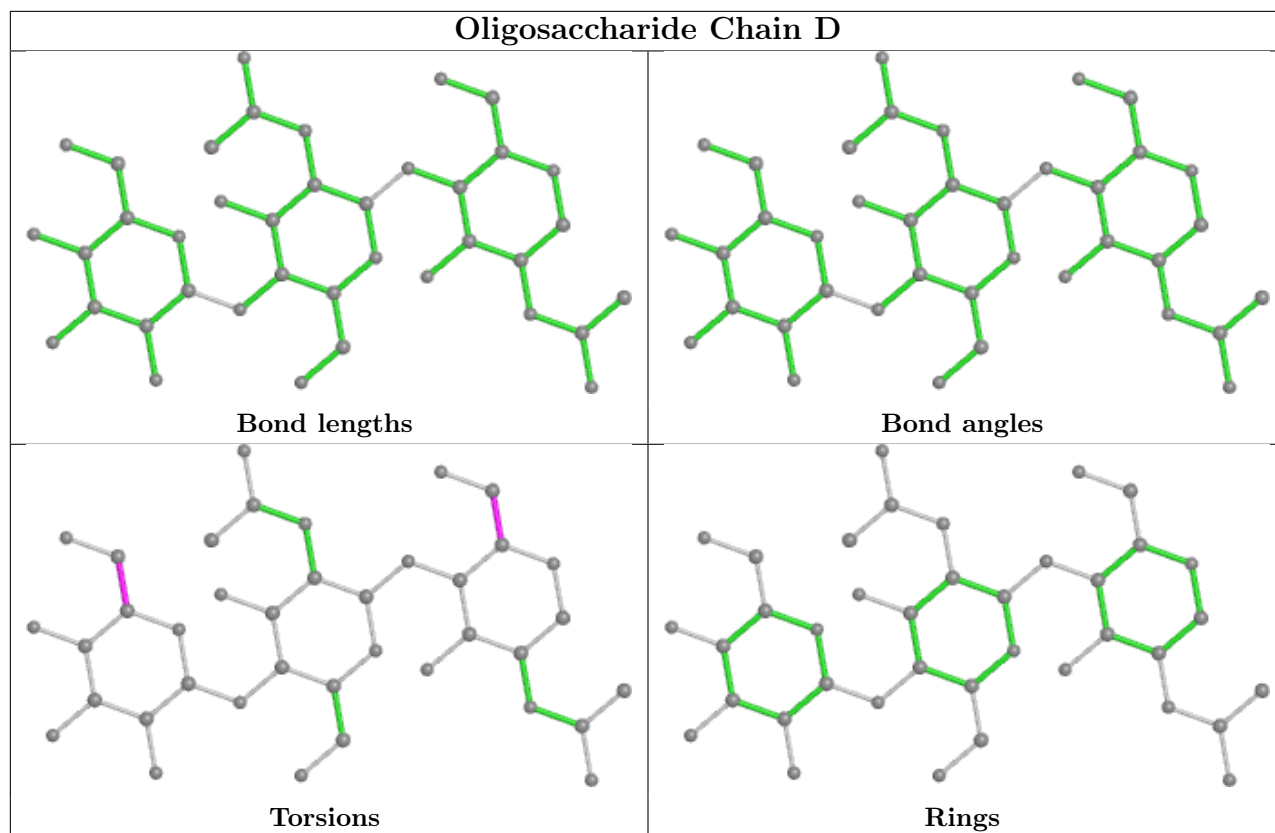
There are no ring outliers.

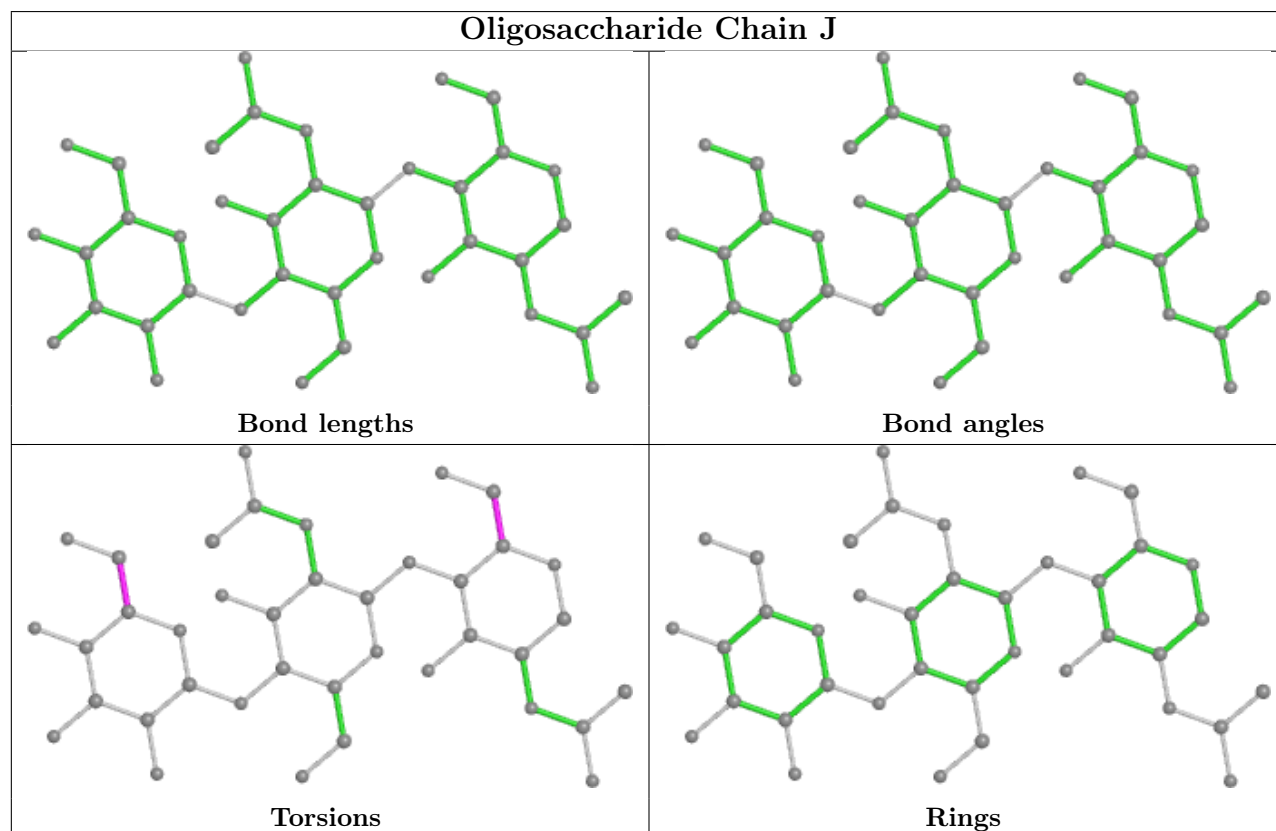
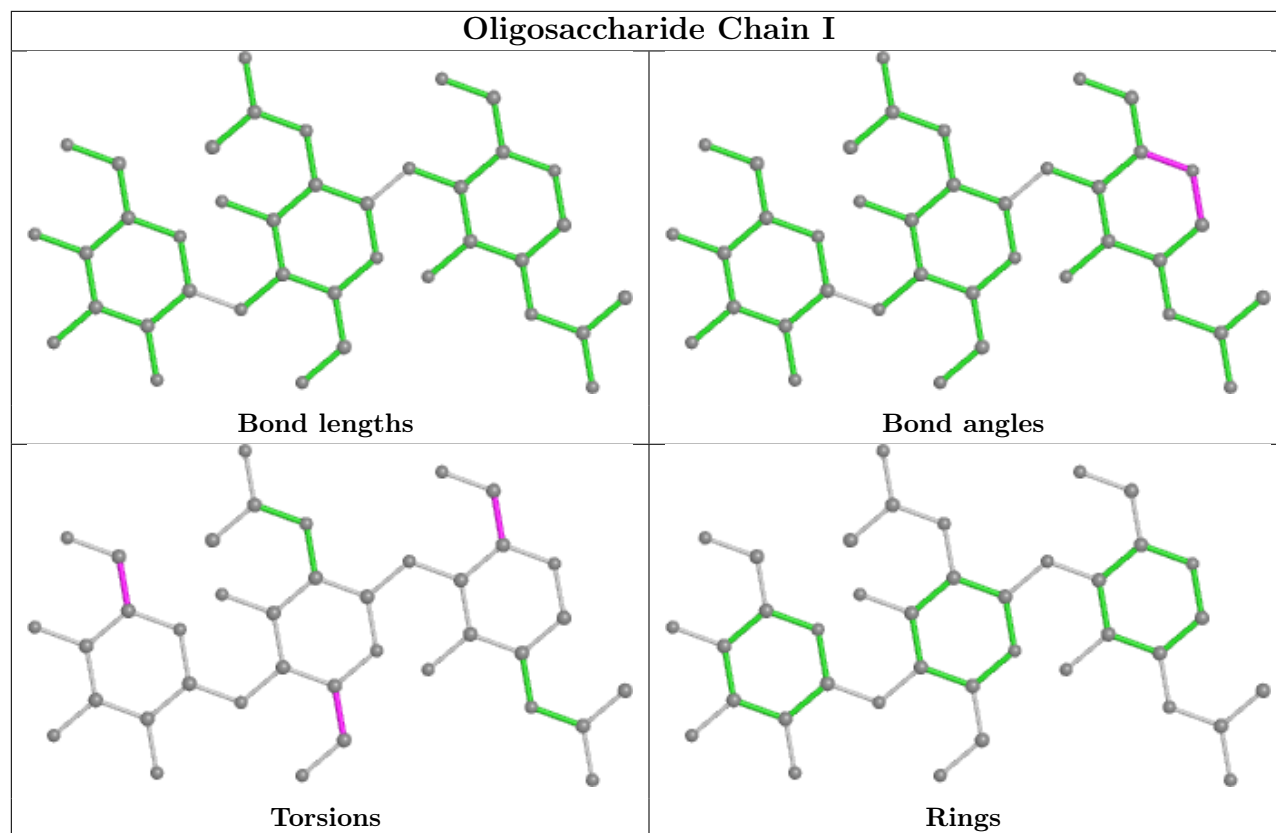
5 monomers are involved in 3 short contacts:

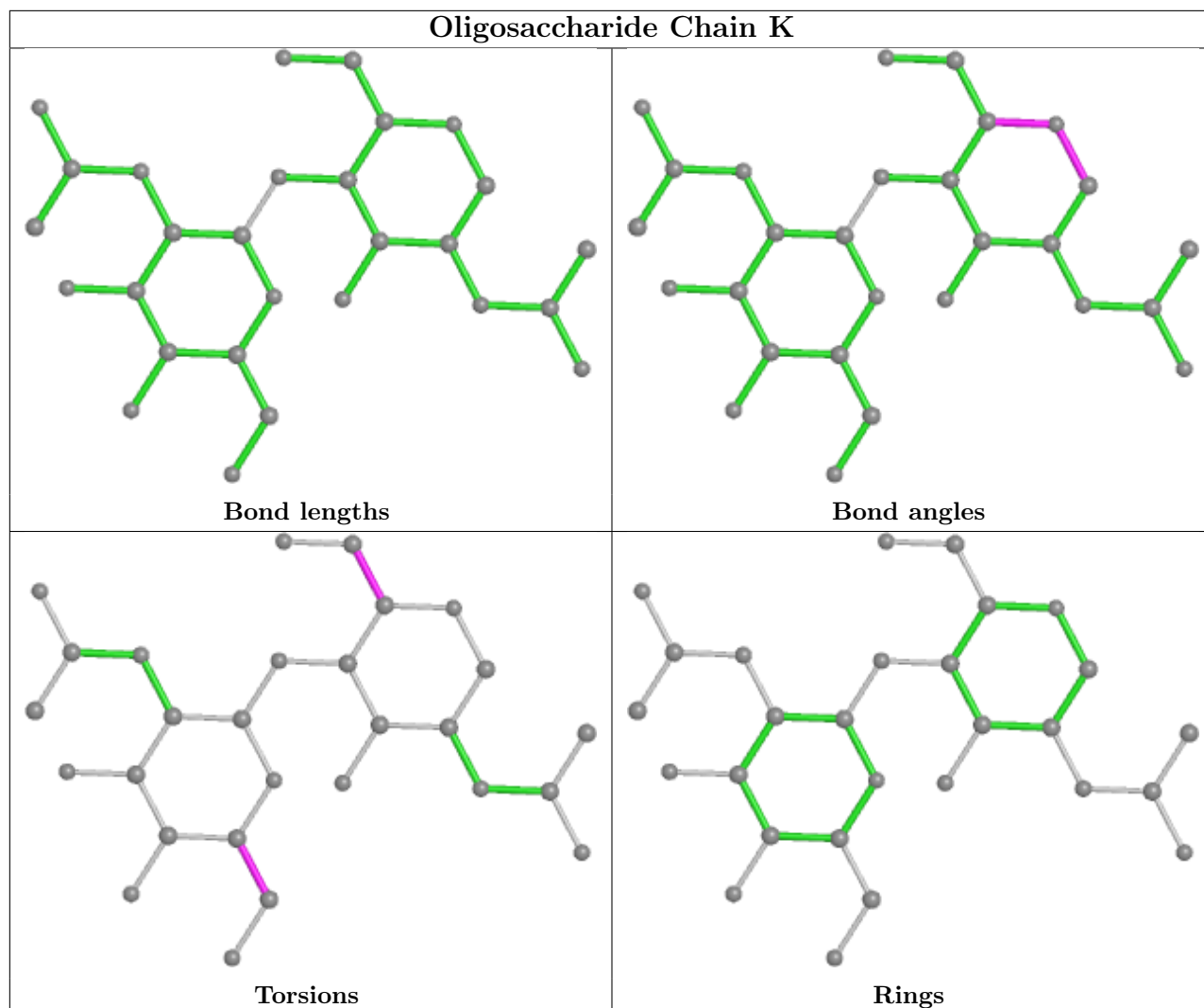
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	1	0
3	G	2	NAG	1	0
3	I	1	NAG	1	0
3	G	1	NAG	1	0
3	I	2	NAG	1	0

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 [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	701	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	B	706	1	14,14,15	0.41	0	17,19,21	0.60	1 (5%)
5	NAG	F	601	2	14,14,15	0.25	0	17,19,21	0.46	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	704	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	A	705	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	E	601	2	14,14,15	0.31	0	17,19,21	0.37	0
5	NAG	A	706	1	14,14,15	0.34	0	17,19,21	0.59	1 (5%)
8	EDO	B	704	-	3,3,3	0.46	0	2,2,2	0.30	0
8	EDO	B	705	-	3,3,3	0.45	0	2,2,2	0.33	0
8	EDO	B	707	-	3,3,3	0.46	0	2,2,2	0.29	0
5	NAG	A	701	-	14,14,15	0.30	0	17,19,21	0.56	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	701	1	-	2/6/23/26	0/1/1/1
5	NAG	B	706	1	-	2/6/23/26	0/1/1/1
5	NAG	F	601	2	-	0/6/23/26	0/1/1/1
5	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	2	-	1/6/23/26	0/1/1/1
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
8	EDO	B	704	-	-	0/1/1/1	-
8	EDO	B	705	-	-	0/1/1/1	-
8	EDO	B	707	-	-	1/1/1/1	-
5	NAG	A	701	-	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	NAG	C1-O5-C5	2.04	114.96	112.19
5	B	706	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	704	NAG	C4-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	704	NAG	O5-C5-C6-O6
5	A	705	NAG	O5-C5-C6-O6
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	A	701	NAG	C4-C5-C6-O6
5	A	705	NAG	C4-C5-C6-O6
5	A	701	NAG	C1-C2-N2-C7
5	E	601	NAG	O5-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
5	A	701	NAG	C3-C2-N2-C7
5	B	701	NAG	O5-C5-C6-O6
5	B	706	NAG	O5-C5-C6-O6
5	B	706	NAG	C4-C5-C6-O6
8	B	707	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	707	EDO	1	0
5	A	701	NAG	9	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	596/597 (99%)	0.42	31 (5%) 27 21	52, 87, 132, 179	0
1	B	596/597 (99%)	0.44	23 (3%) 39 33	45, 82, 141, 217	0
2	E	188/217 (86%)	0.54	16 (8%) 10 7	58, 87, 165, 205	0
2	F	190/217 (87%)	0.66	24 (12%) 3 2	70, 112, 170, 202	0
All	All	1570/1628 (96%)	0.47	94 (5%) 21 17	45, 88, 149, 217	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	387	LEU	8.3
2	F	456	PHE	6.9
2	E	515	PHE	5.6
2	F	368	LEU	5.6
2	F	455	LEU	5.5
2	F	338	PHE	5.0
2	F	434	LEU	4.7
1	A	424	LEU	4.3
2	F	495	TYR	4.2
1	A	525	PHE	4.1
2	F	395	VAL	4.1
1	B	464	PHE	4.1
2	E	368	LEU	4.0
1	B	202	TYR	4.0
2	E	508	TYR	3.9
1	B	97	LEU	3.9
2	E	365	TYR	3.8
2	F	508	TYR	3.8
1	A	333	LEU	3.7
1	A	488	VAL	3.7
1	A	357	ARG	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	418	ILE	3.5
1	A	550	ALA	3.3
1	B	100	LEU	3.3
1	A	52	THR	3.3
2	E	510	VAL	3.2
1	A	360	MET	3.2
1	A	140	GLU	3.2
2	F	365	TYR	3.2
1	A	551	GLY	3.2
2	F	358	ILE	3.1
2	F	356	LYS	3.1
1	A	48	TRP	3.0
1	A	332	MET	3.0
1	B	468	ILE	2.9
1	B	172	VAL	2.9
1	A	330	ASN	2.9
2	E	513	LEU	2.9
2	F	357	LYS	2.9
1	A	217	TYR	2.8
1	B	95	LEU	2.8
1	B	477	TRP	2.7
2	F	392	PHE	2.7
1	B	473	TRP	2.6
1	B	171	GLU	2.6
2	F	340	GLU	2.6
2	F	513	LEU	2.6
2	E	392	PHE	2.6
2	F	342	PHE	2.6
2	E	382	VAL	2.5
1	B	391	LEU	2.5
2	E	433	VAL	2.5
2	E	400	PHE	2.5
1	B	502	SER	2.5
1	A	359	LEU	2.5
1	B	233	ILE	2.5
1	B	404	VAL	2.4
1	A	412	ALA	2.4
2	F	387	LEU	2.4
1	A	85	LEU	2.3
1	A	248	LEU	2.3
1	A	529	LEU	2.3
2	F	410	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	455	LEU	2.3
2	E	350	VAL	2.3
1	A	409	SER	2.3
1	A	358	ILE	2.3
1	A	343	VAL	2.3
1	A	536	GLU	2.2
2	F	402	VAL	2.2
2	F	453	TYR	2.2
1	A	491	VAL	2.2
1	A	554	LEU	2.2
2	E	517	LEU	2.2
1	B	532	ALA	2.2
1	A	341	LYS	2.2
1	B	459	TRP	2.2
2	F	351	TYR	2.1
1	B	98	GLN	2.1
2	E	500	THR	2.1
1	A	172	VAL	2.1
2	E	338	PHE	2.1
2	F	433	VAL	2.1
1	B	256	ILE	2.1
1	A	25	ALA	2.1
1	B	525	PHE	2.1
1	B	91	LEU	2.0
1	B	226	VAL	2.0
2	F	461	LEU	2.0
1	A	345	HIS	2.0
1	A	49	ASN	2.0
1	A	581	VAL	2.0
1	B	463	VAL	2.0
1	B	520	LEU	2.0

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

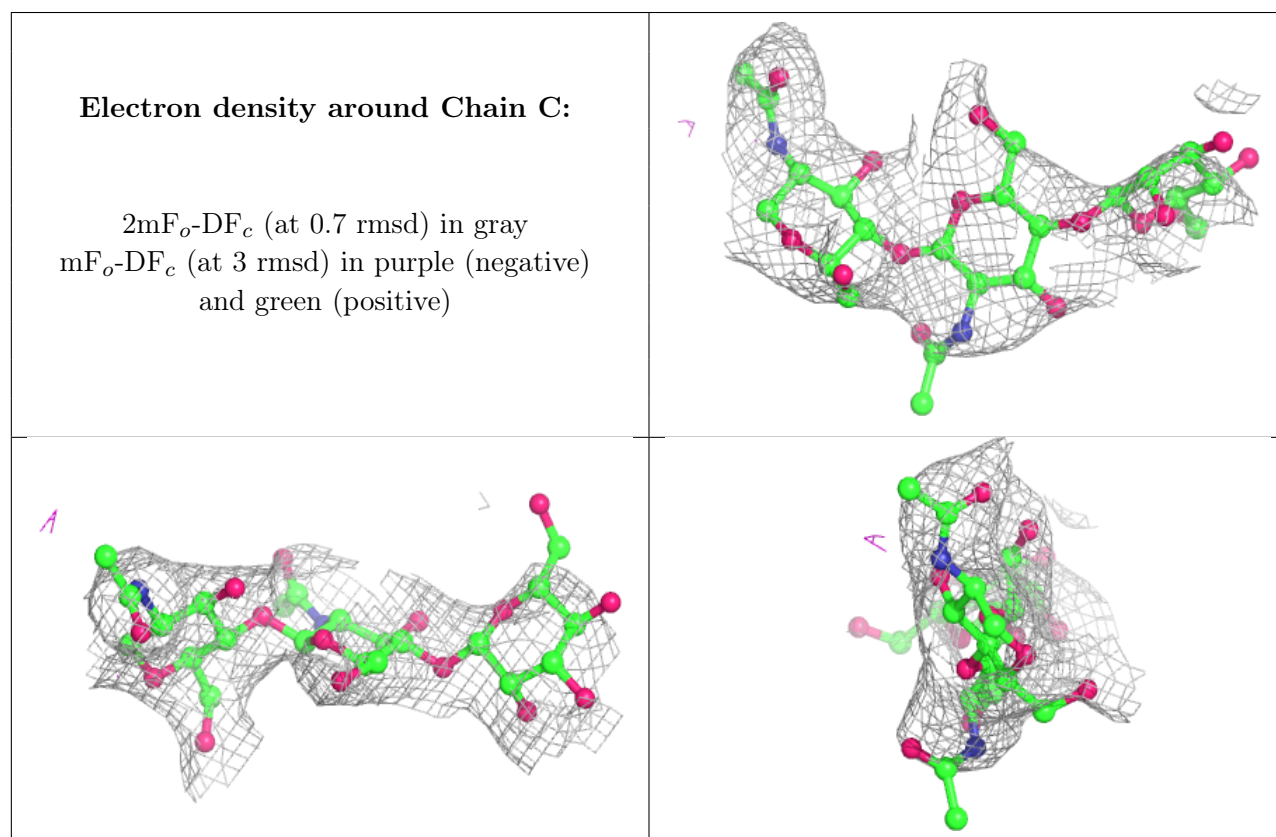
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

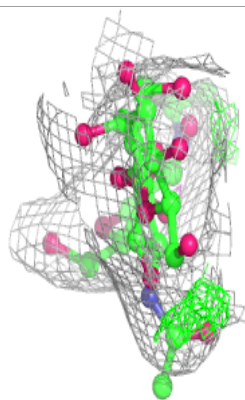
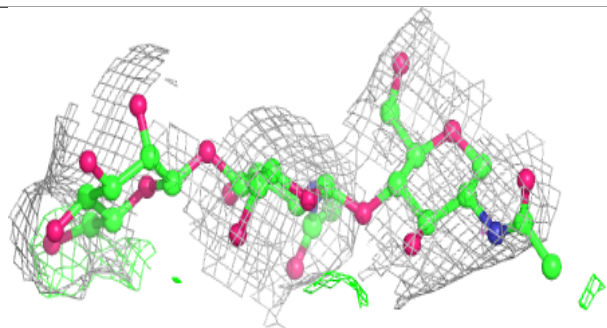
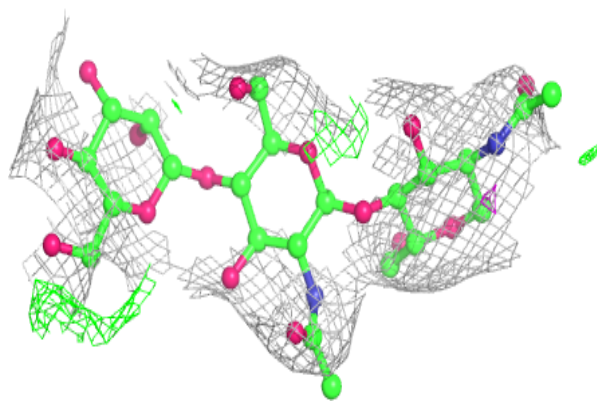
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	C	3	11/12	0.52	0.30	130,165,172,178	0
3	BMA	G	3	11/12	0.75	0.16	107,128,137,143	0
3	NAG	C	1	14/15	0.80	0.17	89,122,142,151	0
4	NAG	K	2	14/15	0.80	0.14	104,135,148,151	0
3	NAG	C	2	14/15	0.81	0.17	136,153,161,169	0
3	BMA	D	3	11/12	0.82	0.17	97,126,137,140	0
3	BMA	I	3	11/12	0.85	0.16	124,138,149,150	0
4	NAG	K	1	14/15	0.88	0.14	79,107,129,132	0
3	NAG	I	2	14/15	0.88	0.13	107,139,148,151	0
3	NAG	D	1	14/15	0.90	0.16	85,99,111,113	0
3	NAG	D	2	14/15	0.91	0.16	110,120,127,129	0
3	BMA	J	3	11/12	0.91	0.18	87,103,108,111	0
3	NAG	J	1	14/15	0.92	0.17	60,79,92,98	0
3	NAG	J	2	14/15	0.94	0.17	72,80,89,96	0
3	NAG	G	2	14/15	0.94	0.17	99,116,120,126	0
3	NAG	G	1	14/15	0.94	0.23	94,99,109,124	0
3	NAG	I	1	14/15	0.94	0.13	104,110,123,128	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.

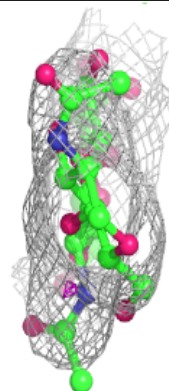
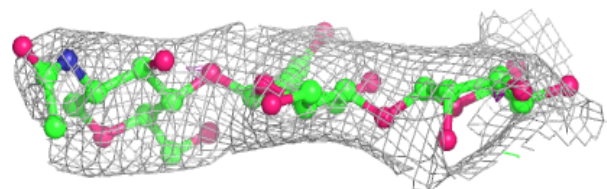
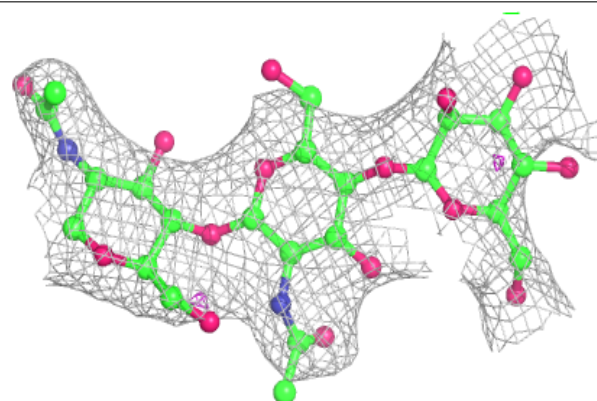


**Electron density around Chain D:**

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

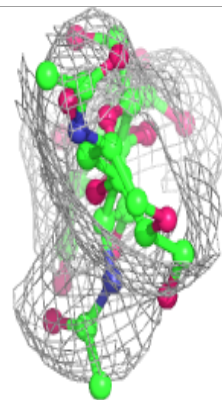
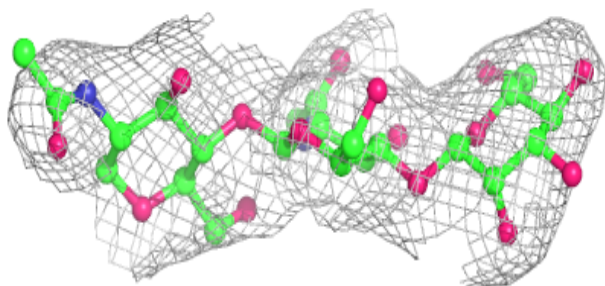
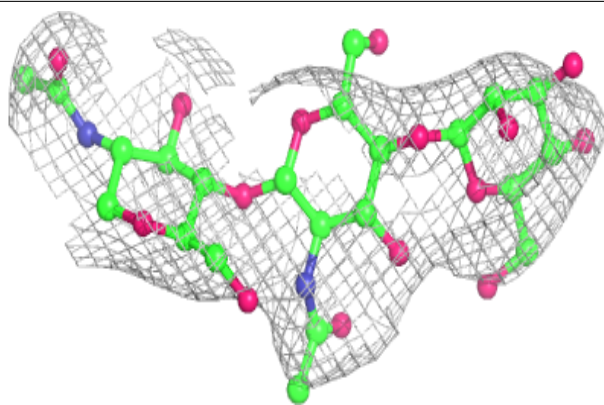
**Electron density around Chain G:**

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

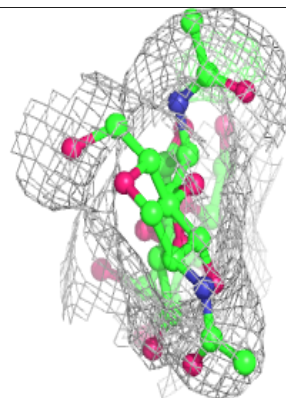
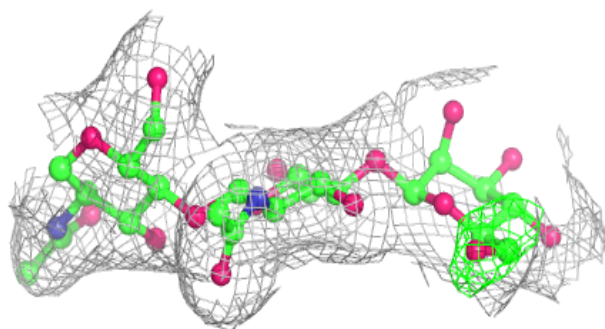
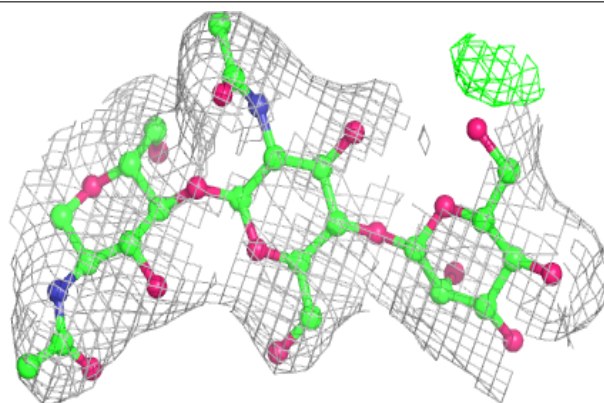


**Electron density around Chain I:**

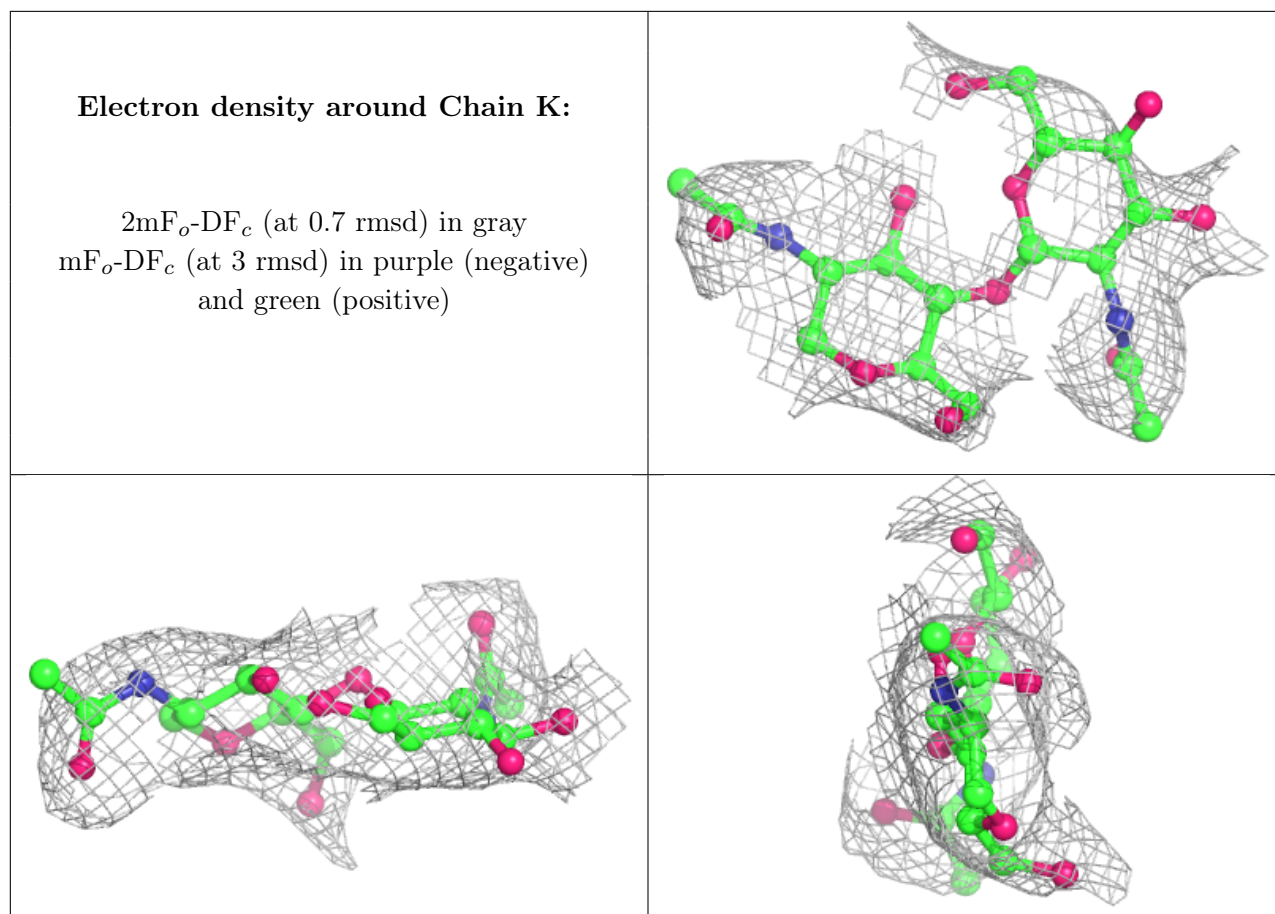
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain J:**

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







## 6.4 Ligands [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
7	CL	A	707	1/1	0.68	0.16	109,109,109,109	0
5	NAG	A	705	14/15	0.70	0.19	99,118,141,148	0
5	NAG	E	601	14/15	0.81	0.17	105,119,139,144	0
5	NAG	A	704	14/15	0.81	0.14	105,126,130,131	0
7	CL	B	708	1/1	0.81	0.10	88,88,88,88	0
5	NAG	F	601	14/15	0.82	0.18	118,139,148,151	0
5	NAG	A	706	14/15	0.86	0.12	95,118,127,138	0
7	CL	B	703	1/1	0.87	0.27	101,101,101,101	0
5	NAG	A	701	14/15	0.87	0.20	96,113,130,134	0
8	EDO	B	704	4/4	0.87	0.34	67,70,83,85	0
8	EDO	B	707	4/4	0.87	0.13	85,86,87,90	0
5	NAG	B	701	14/15	0.88	0.16	120,133,142,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	B	705	4/4	0.90	0.20	71,84,84,85	0
9	MG	B	709	1/1	0.90	0.21	78,78,78,78	0
5	NAG	B	706	14/15	0.93	0.24	83,121,124,124	0
7	CL	F	602	1/1	0.94	0.14	76,76,76,76	0
6	ZN	B	702	1/1	0.95	0.18	87,87,87,87	0
7	CL	A	703	1/1	0.97	0.09	63,63,63,63	0
6	ZN	A	702	1/1	0.98	0.19	100,100,100,100	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.