



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:32 PM EDT

PDB ID : 1DP4  
Title : DIMERIZED HORMONE BINDING DOMAIN OF THE ATRIAL NATRI-  
URETIC PEPTIDE RECEPTOR  
Authors : van den Akker, F.; Zhang, X.; Miyagi, M.; Huo, X.; Misono, K.S.; Yee, V.C.  
Deposited on : 1999-12-23  
Resolution : 2.00 Å(reported)

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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	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

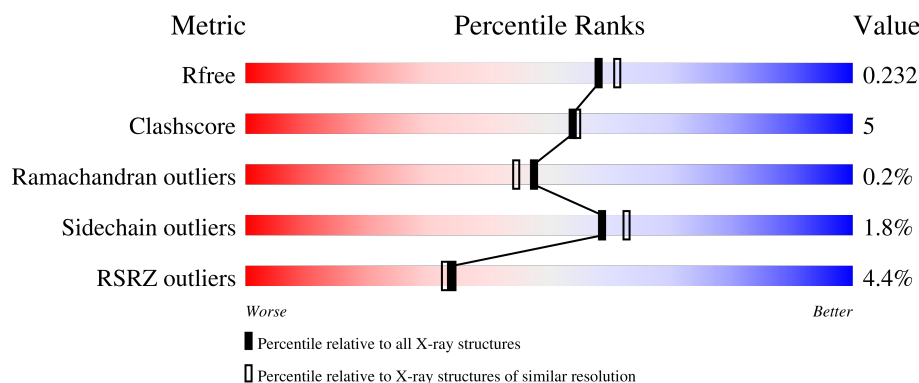
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



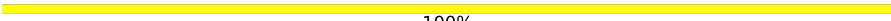
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	435	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	435	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

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	C	455	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7445 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 ATRIAL NATRIURETIC PEPTIDE RECEPTOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	3	0
			3360	2157	584	608	11			
1	C	429	Total	C	N	O	S	0	3	0
			3398	2174	590	622	12			

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



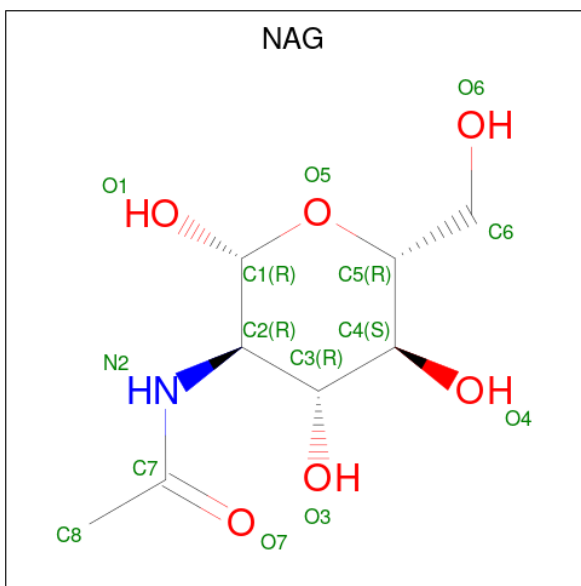
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

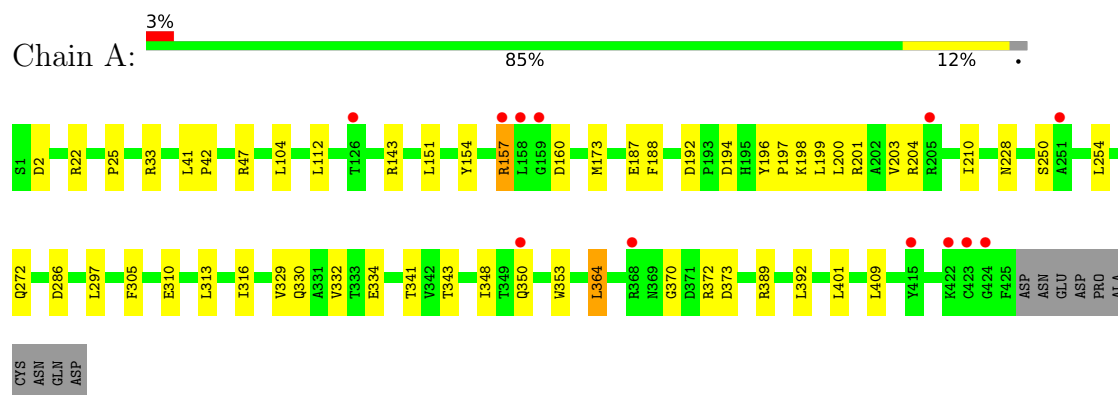
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	269	Total	O	0	0
			269	269		
6	C	245	Total	O	0	0
			245	245		

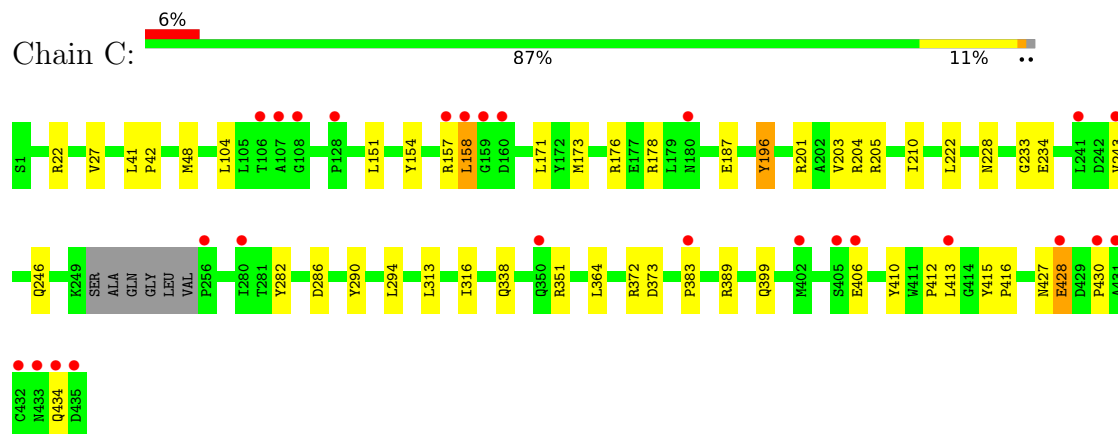
### 3 Residue-property plots

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: ATRIAL NATRIURETIC PEPTIDE RECEPTOR A



#### • Molecule 1: ATRIAL NATRIURETIC PEPTIDE RECEPTOR A



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




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

Chain D:  100%


MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.25Å 120.25Å 160.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.55 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.00) 98.2 (29.55-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.198 , 0.225 0.208 , 0.232	Depositor DCC
$R_{free}$ test set	4015 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% 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: NAG, CL, SO4

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	0.53	0/3464	0.69	0/4720
1	C	0.49	0/3502	0.68	0/4769
All	All	0.51	0/6966	0.69	0/9489

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	TYR	Sidechain

### 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	3360	0	3312	34	0
1	C	3398	0	3323	41	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
3	A	20	0	0	0	0
3	C	25	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	C	14	0	13	0	0
6	A	269	0	0	3	0
6	C	245	0	0	2	0
All	All	7445	0	6748	72	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 (72) 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:C:173:MET:HG2	6:C:834:HOH:O	1.69	0.90
1:C:158:LEU:HD12	1:C:158:LEU:H	1.34	0.88
1:C:338:GLN:NE2	1:C:351:ARG:HH21	1.83	0.76
1:A:157:ARG:HB2	1:A:160:ASP:OD2	1.85	0.75
1:C:338:GLN:HE21	1:C:351:ARG:HH21	1.34	0.75
1:A:228:ASN:ND2	1:C:204:ARG:HD3	2.04	0.73
1:A:25:PRO:HG3	1:A:305:PHE:CD1	2.24	0.72
1:C:178:ARG:HH22	1:C:399:GLN:HE22	1.41	0.67
1:C:234:GLU:HG2	1:C:413:LEU:HD12	1.77	0.66
1:A:2:ASP:HB3	1:A:47:ARG:HD3	1.77	0.66
1:C:415:TYR:HB2	1:C:416:PRO:HD2	1.77	0.65
1:C:158:LEU:H	1:C:158:LEU:CD1	2.09	0.62
1:C:383:PRO:HG3	1:C:410:TYR:CD1	2.35	0.62
1:C:203:VAL:HG13	1:C:210[A]:ILE:CD1	2.30	0.62
1:A:228:ASN:HD21	1:C:204:ARG:HD3	1.66	0.60
1:C:428:GLU:O	1:C:430:PRO:HD3	2.03	0.59
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.68	0.57
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.70	0.56
1:C:201:ARG:HD2	1:C:205:ARG:CZ	2.34	0.56
1:C:234:GLU:CG	1:C:413:LEU:HD12	2.34	0.56
1:C:158:LEU:HD12	1:C:158:LEU:N	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HB3	1:C:228:ASN:OD1	2.07	0.54
1:C:27:VAL:HG11	1:C:48:MET:CE	2.38	0.54
1:C:234:GLU:CD	1:C:413:LEU:HD12	2.28	0.54
1:C:151:LEU:HD23	1:C:210[B]:ILE:HD12	1.90	0.54
1:A:392:LEU:HG	1:A:409:LEU:HD21	1.90	0.54
1:C:157:ARG:HH11	2:E:2:NAG:H83	1.73	0.54
1:A:192:ASP:OD1	1:A:194:ASP:HB2	2.08	0.53
1:C:22:ARG:HG3	1:C:22:ARG:NH1	2.23	0.53
1:A:330:GLN:O	1:A:334:GLU:HG3	2.09	0.52
1:C:158:LEU:CD1	1:C:158:LEU:N	2.72	0.52
1:A:203:VAL:HG13	1:A:210[B]:ILE:CD1	2.41	0.51
1:C:233:GLY:HA3	1:C:412:PRO:HG2	1.91	0.51
1:A:272[B]:GLN:NE2	6:A:873:HOH:O	2.43	0.50
1:A:313:LEU:O	1:A:316:ILE:HG12	2.12	0.50
1:C:427:ASN:HD22	1:C:434:GLN:NE2	2.09	0.50
1:C:203:VAL:HG13	1:C:210[A]:ILE:HD11	1.93	0.49
1:A:204:ARG:HG2	1:A:204:ARG:NH1	2.28	0.48
1:C:313:LEU:O	1:C:316:ILE:HG12	2.14	0.47
1:A:364:LEU:C	1:A:364:LEU:HD12	2.35	0.47
1:C:27:VAL:HG11	1:C:48:MET:HE2	1.96	0.47
1:A:341:THR:HG23	1:A:343:THR:H	1.79	0.46
1:C:196:TYR:CD1	1:C:196:TYR:N	2.82	0.46
1:A:151:LEU:HD23	1:A:210[A]:ILE:HD12	1.97	0.45
1:C:104:LEU:C	1:C:104:LEU:HD23	2.37	0.45
1:A:41:LEU:N	1:A:42:PRO:HD3	2.31	0.45
1:A:2:ASP:CB	1:A:47:ARG:HD3	2.46	0.44
1:A:25:PRO:HB2	1:A:297:LEU:HD12	1.98	0.44
1:A:41:LEU:HG	1:A:329:VAL:HG13	1.99	0.44
1:A:143:ARG:HD2	1:A:401:LEU:HD13	2.00	0.44
1:A:196:TYR:HB2	1:A:197:PRO:HD3	1.99	0.44
1:A:353:TRP:CE2	1:A:370:GLY:HA3	2.52	0.44
1:A:154:TYR:CZ	1:A:187:GLU:HB2	2.53	0.43
1:A:198:LYS:HB3	6:A:798:HOH:O	2.19	0.43
1:A:286:ASP:OD1	1:A:286:ASP:N	2.51	0.43
1:A:201:ARG:HH11	1:A:201:ARG:HG3	1.84	0.43
1:C:41:LEU:N	1:C:42:PRO:HD3	2.33	0.43
1:C:243:VAL:HB	1:C:282:TYR:CE1	2.54	0.42
1:A:332:VAL:HG22	1:A:348:ILE:HD13	2.01	0.42
1:C:372:ARG:HG2	1:C:373:ASP:O	2.19	0.42
1:A:22:ARG:NH2	6:A:853:HOH:O	2.52	0.42
1:A:104:LEU:HD23	1:A:104:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:GLN:HE21	1:C:399:GLN:HB3	1.67	0.42
1:C:290:TYR:CE2	1:C:294:LEU:HD11	2.54	0.42
1:A:112:LEU:CD2	1:A:173:MET:HG3	2.49	0.42
1:A:188:PHE:CG	1:A:199:LEU:HD11	2.55	0.41
1:C:383:PRO:HG3	1:C:410:TYR:CE1	2.55	0.41
1:A:372:ARG:HG2	1:A:373:ASP:O	2.20	0.41
1:C:171:LEU:C	1:C:171:LEU:HD23	2.40	0.41
1:C:154:TYR:O	1:C:187:GLU:HA	2.20	0.41
1:C:286:ASP:HA	6:C:856:HOH:O	2.21	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.93	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	426/435 (98%)	418 (98%)	7 (2%)	1 (0%)	47	44
1	C	428/435 (98%)	414 (97%)	13 (3%)	1 (0%)	47	44
All	All	854/870 (98%)	832 (97%)	20 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	158	LEU
1	A	157	ARG

### 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	355/361 (98%)	348 (98%)	7 (2%)	55	58
1	C	360/361 (100%)	354 (98%)	6 (2%)	60	65
All	All	715/722 (99%)	702 (98%)	13 (2%)	59	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	250	SER
1	A	254	LEU
1	A	310	GLU
1	A	350	GLN
1	A	364	LEU
1	A	389	ARG
1	C	176	ARG
1	C	246	GLN
1	C	364	LEU
1	C	389	ARG
1	C	406	GLU
1	C	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	275	GLN
1	A	358	GLN
1	C	338	GLN
1	C	350	GLN
1	C	399	GLN
1	C	434	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 ⓘ

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	$\# Z  > 2$
2	NAG	B	1	2,1	14,14,15	0.71	0	17,19,21	0.59	0
2	NAG	B	2	2	14,14,15	0.62	0	17,19,21	0.78	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.42	0	17,19,21	0.63	0
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.61	0
2	NAG	E	1	2,1	14,14,15	0.58	0	17,19,21	1.05	1 (5%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	0.77	0
2	NAG	F	1	2,1	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
2	NAG	F	2	2	14,14,15	0.54	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	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(°)
2	E	1	NAG	C4-C3-C2	-3.42	106.00	111.02
2	F	2	NAG	C2-N2-C7	-2.13	119.87	122.90
2	F	1	NAG	C6-C5-C4	-2.02	108.27	113.00
2	B	2	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

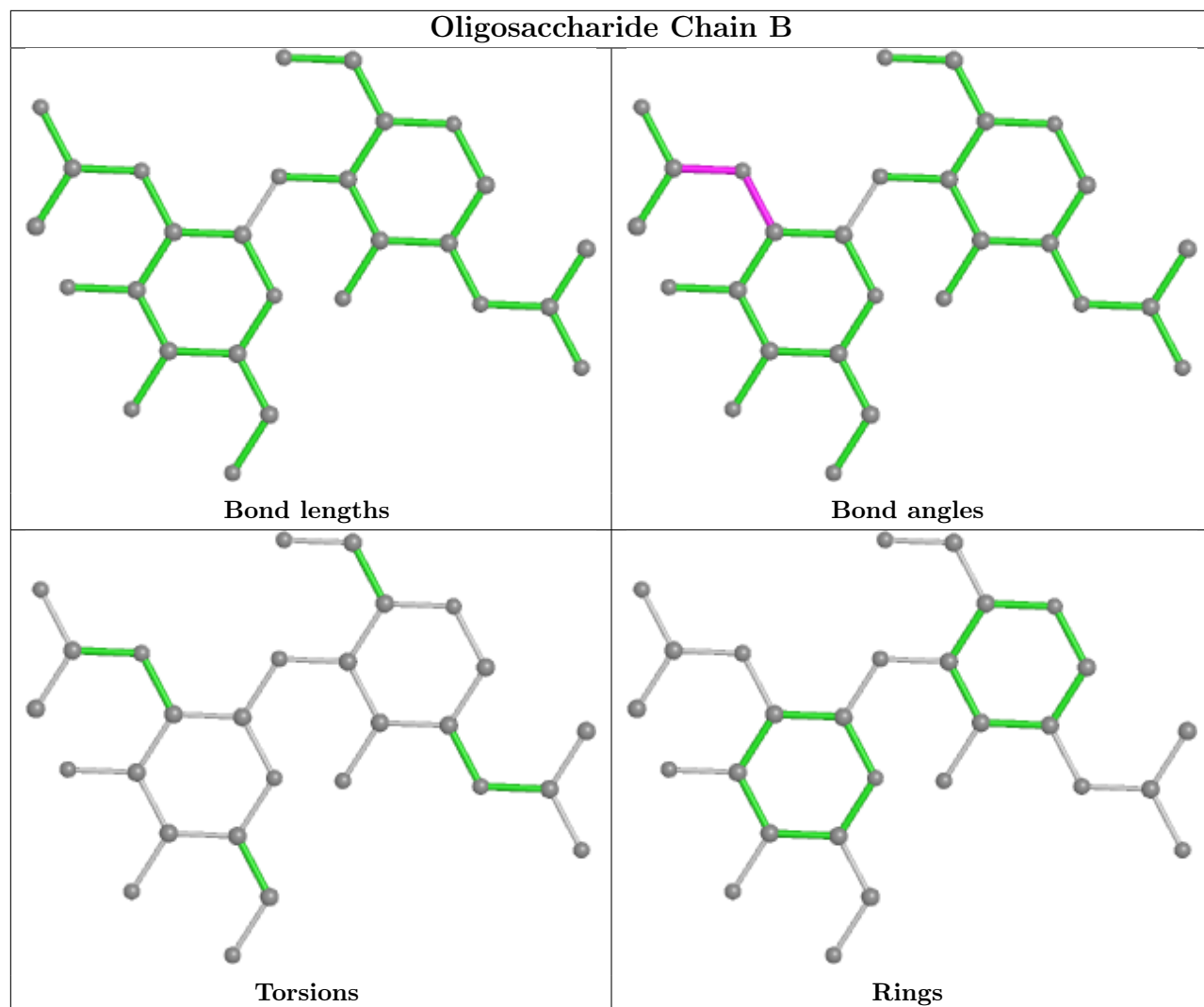
There are no ring outliers.

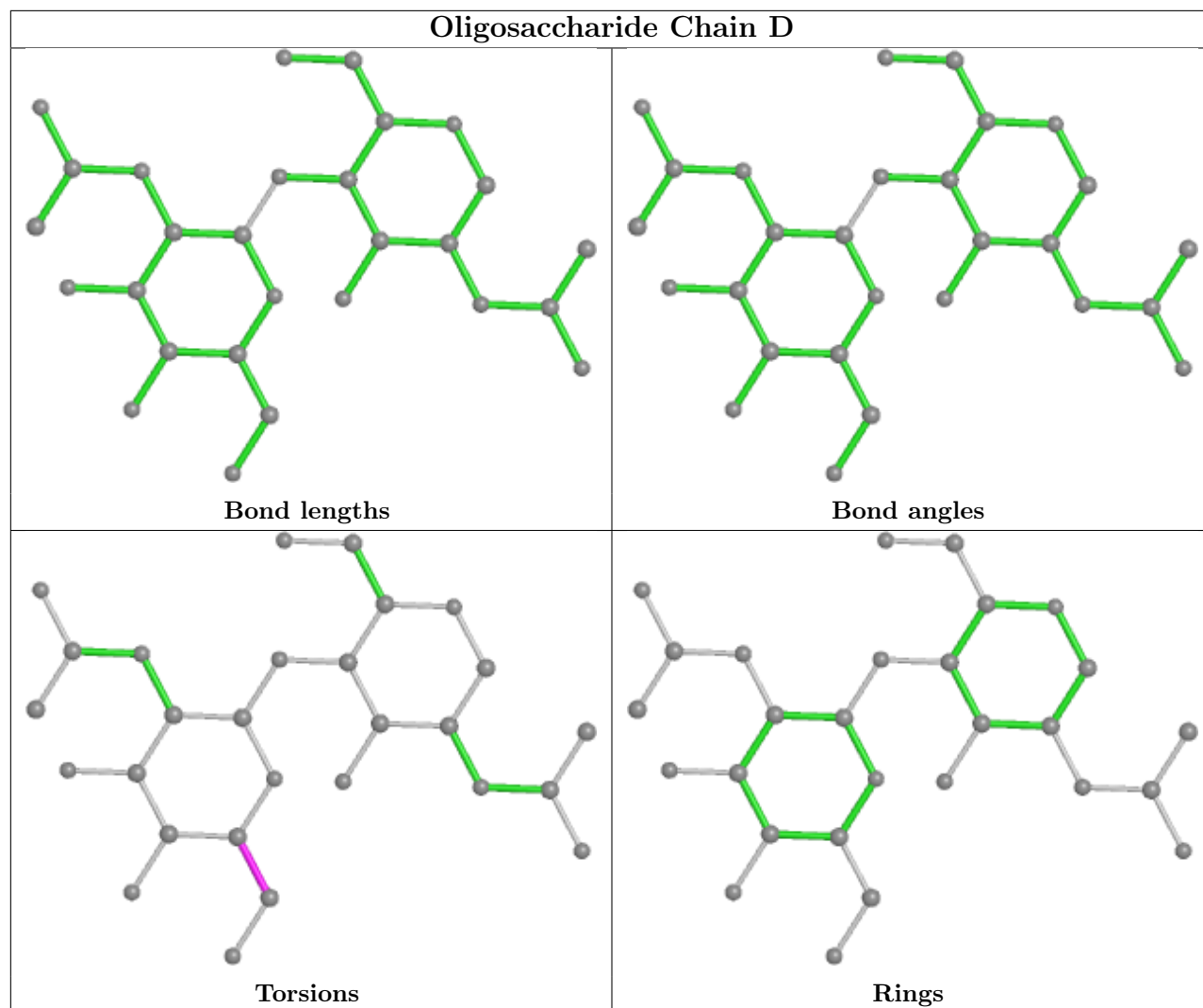
1 monomer is involved in 1 short contact:

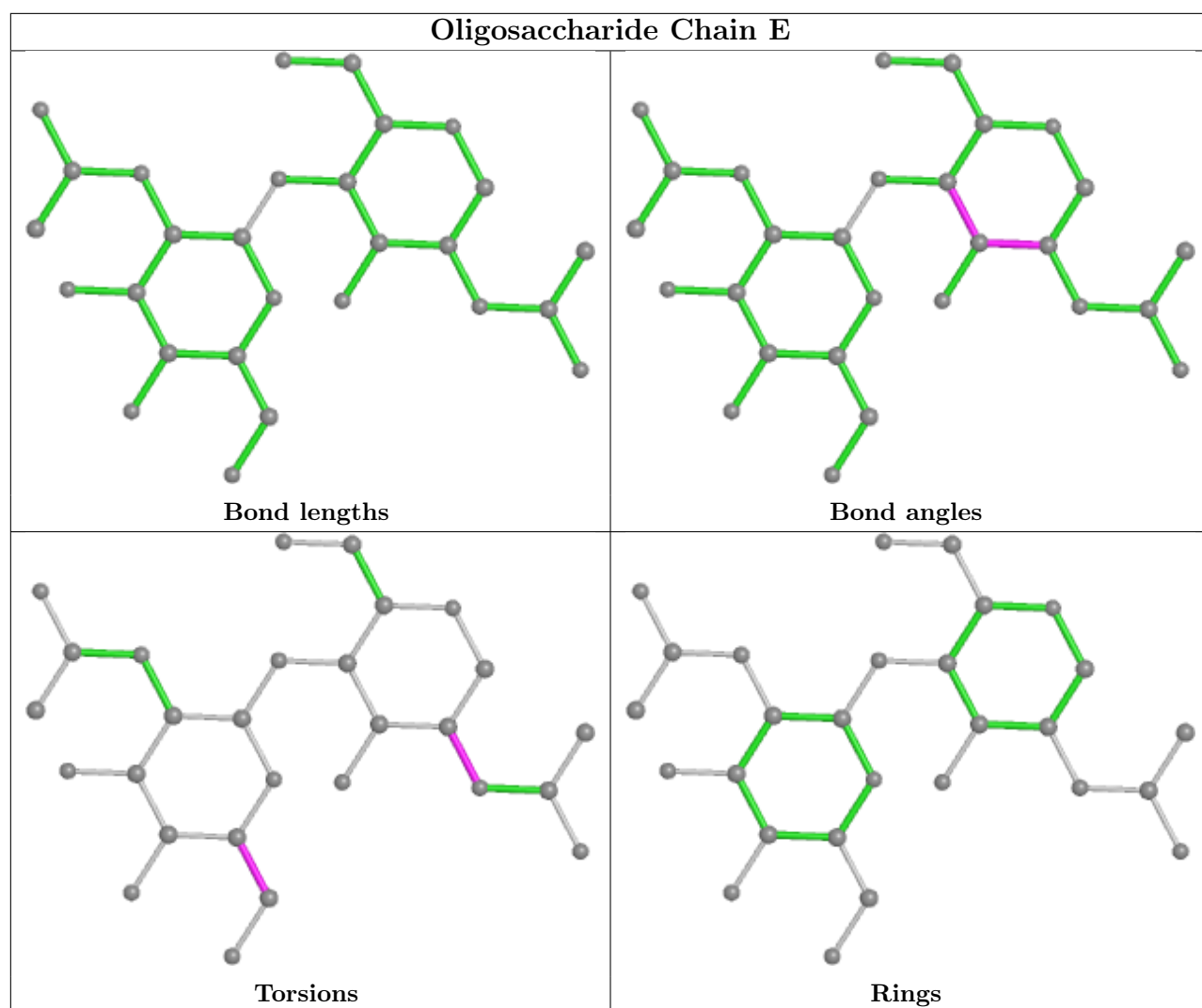
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0

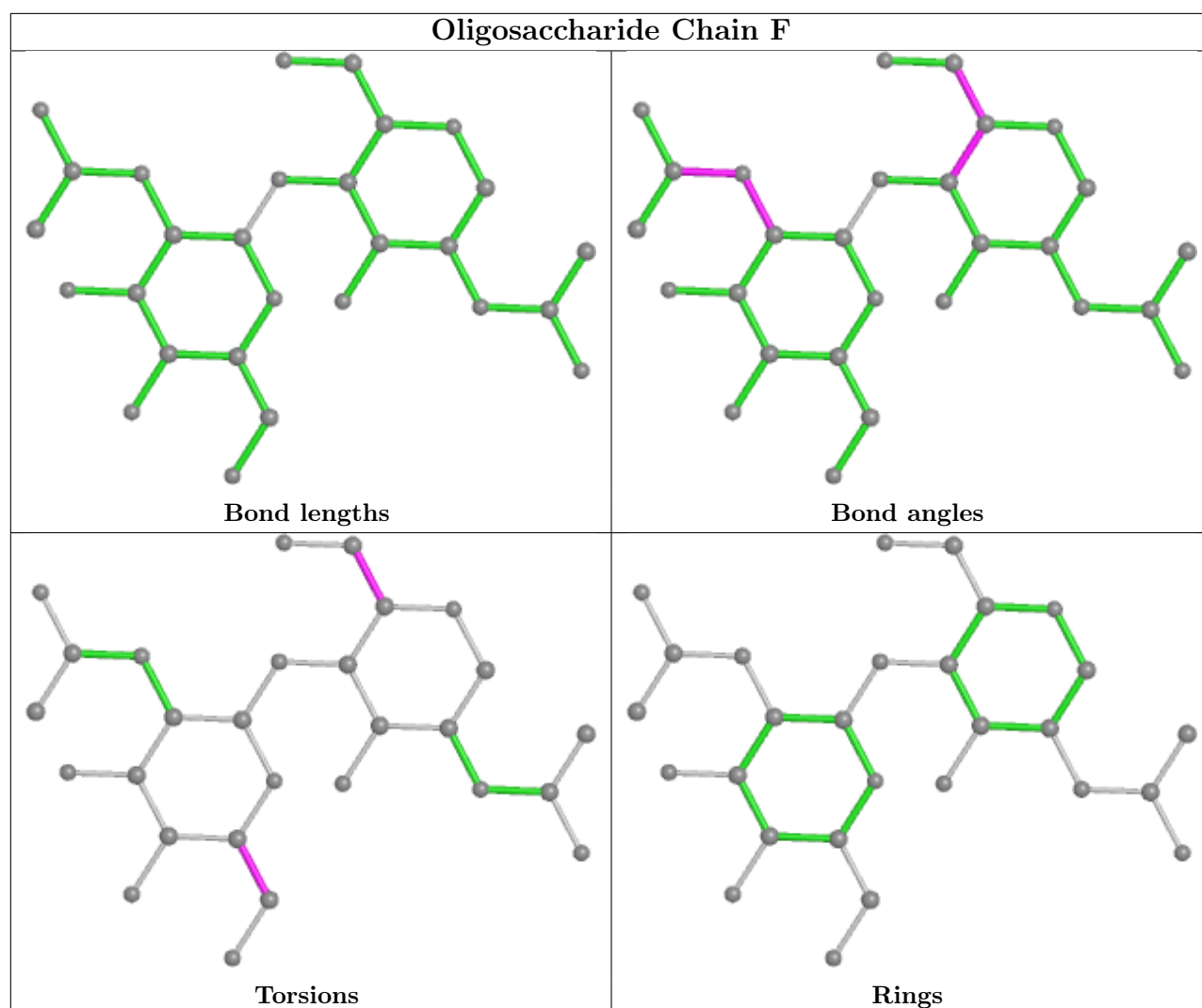
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z  > 2$
3	SO4	A	604	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	C	602	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	C	607	-	4,4,4	0.26	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	609	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.33	0
5	NAG	C	455	1	14,14,15	0.89	1 (7%)	17,19,21	0.61	0
3	SO4	C	608	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	C	606	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	605	-	4,4,4	0.32	0	6,6,6	0.09	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	C	455	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	455	NAG	C1-C2	2.28	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	455	NAG	C1-C2-N2-C7
5	C	455	NAG	O5-C5-C6-O6
5	C	455	NAG	C3-C2-N2-C7
5	C	455	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	425/435 (97%)	0.09	12 (2%) 53 51	15, 26, 48, 68	0
1	C	429/435 (98%)	0.14	26 (6%) 21 20	17, 28, 47, 71	0
All	All	854/870 (98%)	0.11	38 (4%) 34 33	15, 27, 48, 71	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	7.0
1	A	158	LEU	6.9
1	C	435	ASP	6.9
1	A	157	ARG	4.9
1	C	159	GLY	4.6
1	A	159	GLY	4.3
1	C	157	ARG	4.2
1	A	423	CYS	3.8
1	C	433	ASN	3.7
1	C	434	GLN	3.3
1	C	256	PRO	3.1
1	C	350	GLN	3.1
1	C	405	SER	3.1
1	C	430	PRO	3.0
1	C	243	VAL	2.8
1	C	383	PRO	2.7
1	C	428	GLU	2.7
1	A	422	LYS	2.7
1	C	406	GLU	2.6
1	A	205	ARG	2.5
1	C	107	ALA	2.5
1	C	128	PRO	2.5
1	C	432	CYS	2.4
1	C	431	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	402	MET	2.4
1	A	415	TYR	2.4
1	A	350	GLN	2.3
1	C	241	LEU	2.3
1	C	108	GLY	2.3
1	A	424	GLY	2.2
1	C	180	ASN	2.2
1	C	280	ILE	2.2
1	A	251	ALA	2.1
1	C	106	THR	2.1
1	C	413	LEU	2.1
1	A	368	ARG	2.1
1	C	160	ASP	2.1
1	A	126	THR	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.

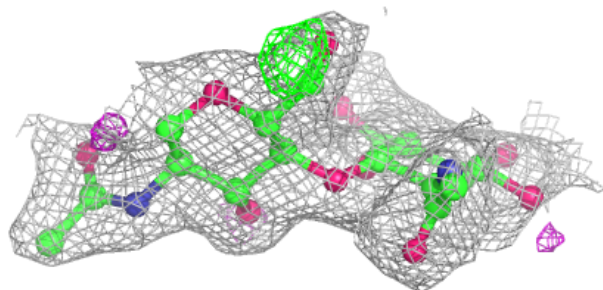
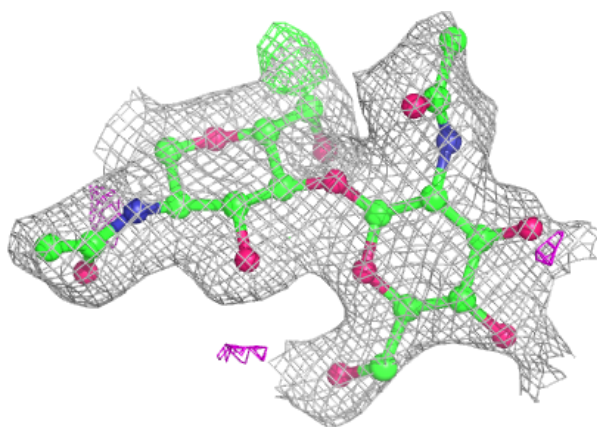
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	E	2	14/15	0.81	0.32	61,63,65,67	0
2	NAG	B	2	14/15	0.86	0.28	51,57,60,61	0
2	NAG	F	2	14/15	0.91	0.23	41,47,57,59	0
2	NAG	F	1	14/15	0.92	0.17	32,35,40,48	0
2	NAG	E	1	14/15	0.92	0.17	35,45,53,58	0
2	NAG	D	2	14/15	0.93	0.17	35,43,56,58	0
2	NAG	D	1	14/15	0.94	0.11	29,33,35,38	0
2	NAG	B	1	14/15	0.96	0.16	27,35,44,45	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.



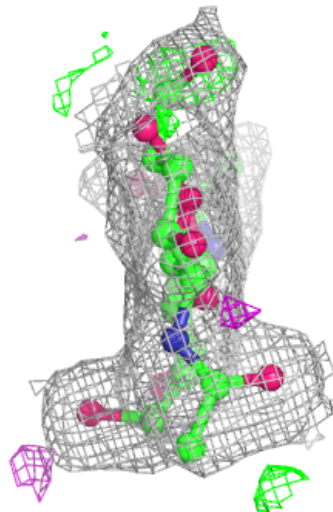
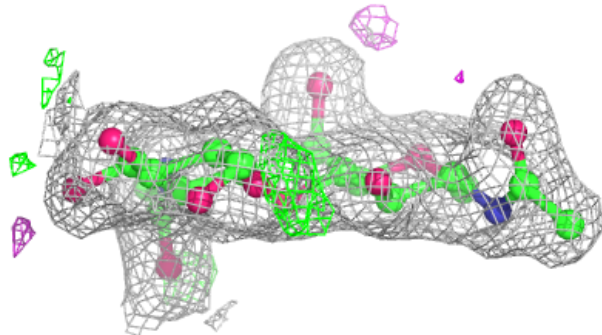
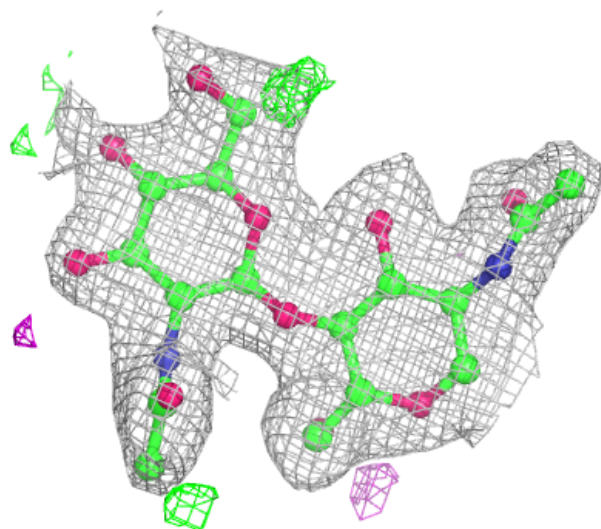
**Electron density around Chain B:**

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



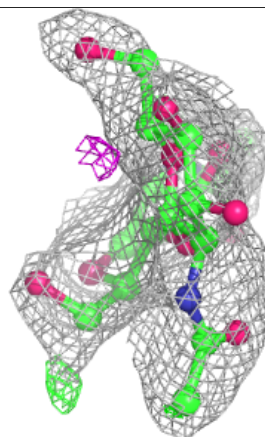
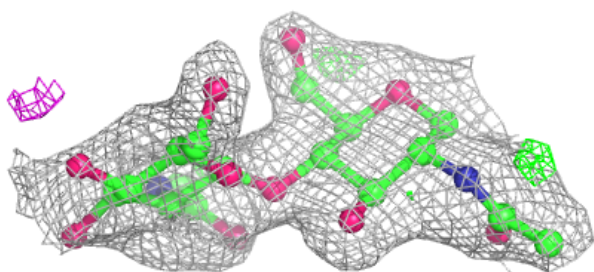
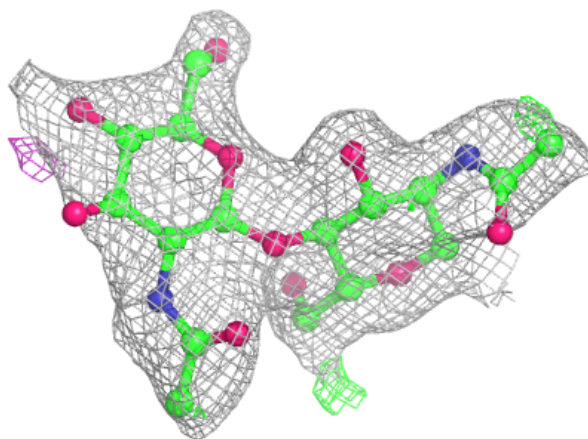
**Electron density around Chain D:**

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

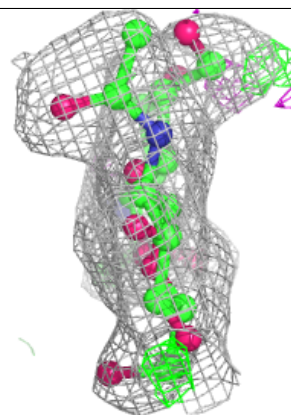
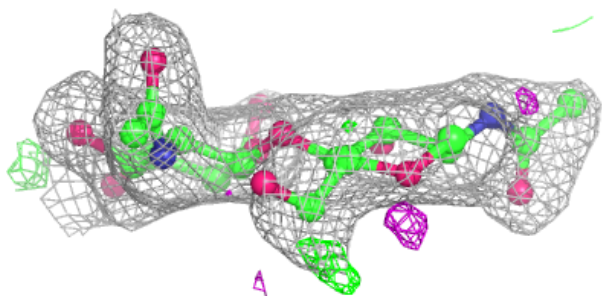
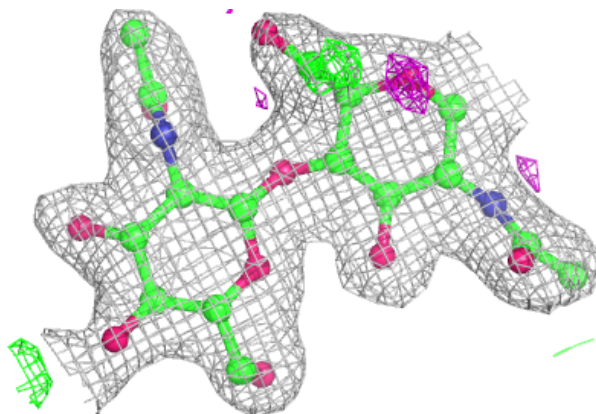


**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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
5	NAG	C	455	14/15	0.60	0.52	63,68,73,75	0
3	SO4	C	609	5/5	0.84	0.30	73,73,76,76	0
3	SO4	A	604	5/5	0.96	0.17	57,58,61,61	0
3	SO4	C	608	5/5	0.97	0.22	48,49,53,55	0
3	SO4	C	607	5/5	0.98	0.16	52,54,58,59	0
3	SO4	A	601	5/5	0.98	0.09	25,29,33,34	0
3	SO4	A	605	5/5	0.98	0.17	39,39,42,43	0
3	SO4	C	606	5/5	0.98	0.11	48,49,50,55	0
3	SO4	C	602	5/5	0.99	0.11	30,31,32,34	5
4	CL	C	611	1/1	0.99	0.10	21,21,21,21	0
3	SO4	A	603	5/5	0.99	0.10	31,32,36,41	0
4	CL	A	610	1/1	1.00	0.14	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.