



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:21 PM BST

PDB ID : 2AJC  
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with 4-(2-Aminoethyl)-b  
enzyme sulphonyl fluoride (AEBSF)  
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.;  
Demuth, H.U.; Bode, W.  
Deposited on : 2005-08-01  
Resolution : 1.95 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

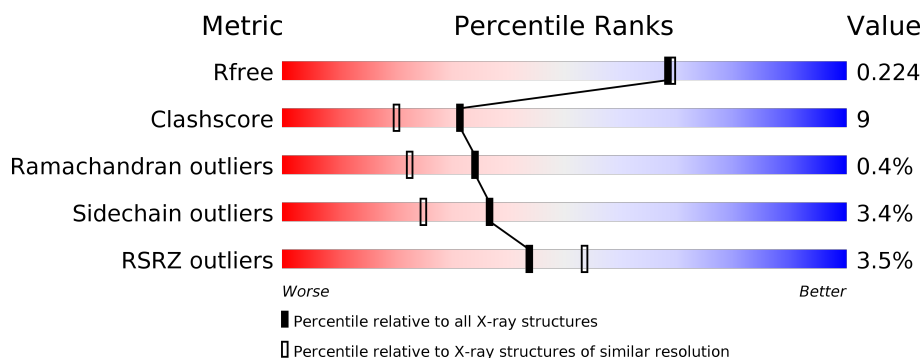
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	728	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	728	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	728	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	I	2	 100%
2	K	2	 50% 50%
2	L	2	 100%
2	M	2	 50% 50%
3	G	3	 67% 33%
3	J	3	 33% 33% 33%

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
4	NAG	D	767(A)	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 25912 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	80	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	79	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

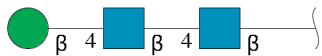
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	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			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

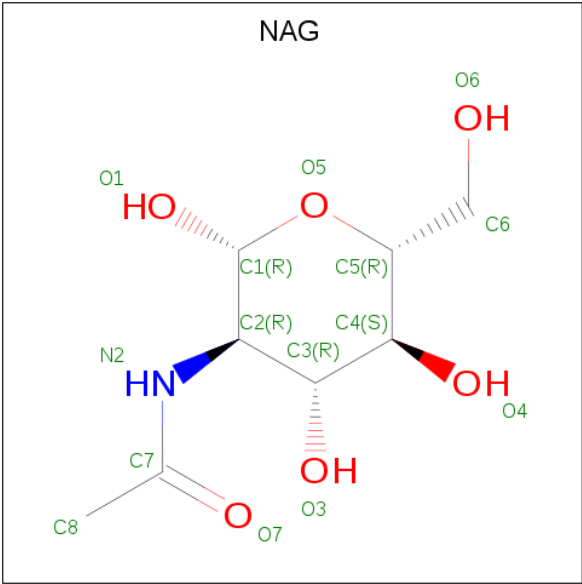
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 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>).



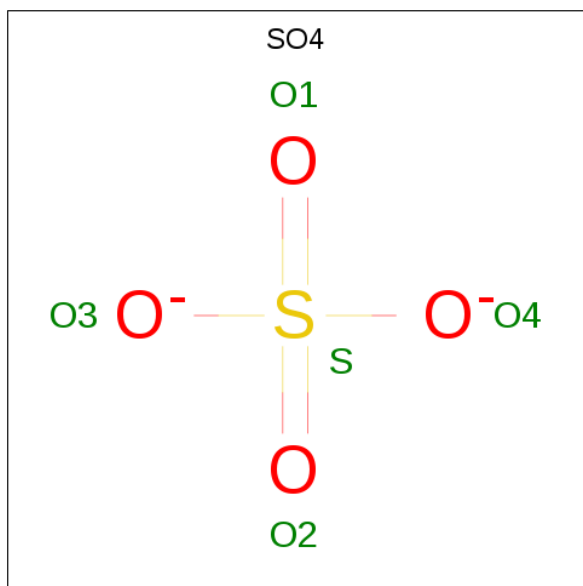
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	3	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



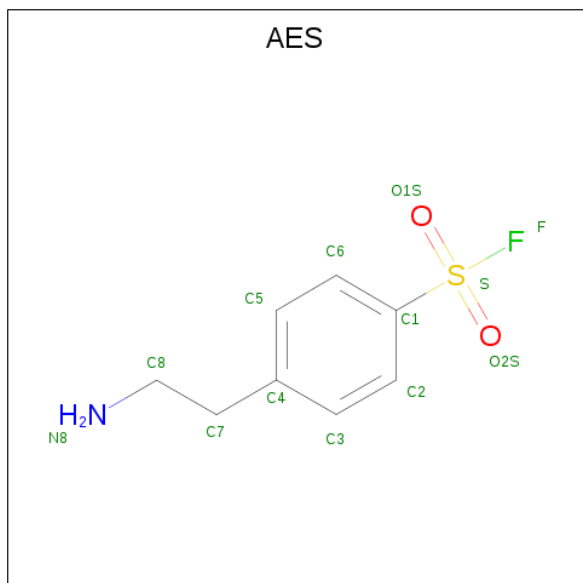
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula:  $C_8H_{10}FNO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	B	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	C	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
6	D	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	354	Total	O	0	0
			354	354		
7	B	433	Total	O	0	0
			433	433		
7	C	385	Total	O	0	0
			385	385		

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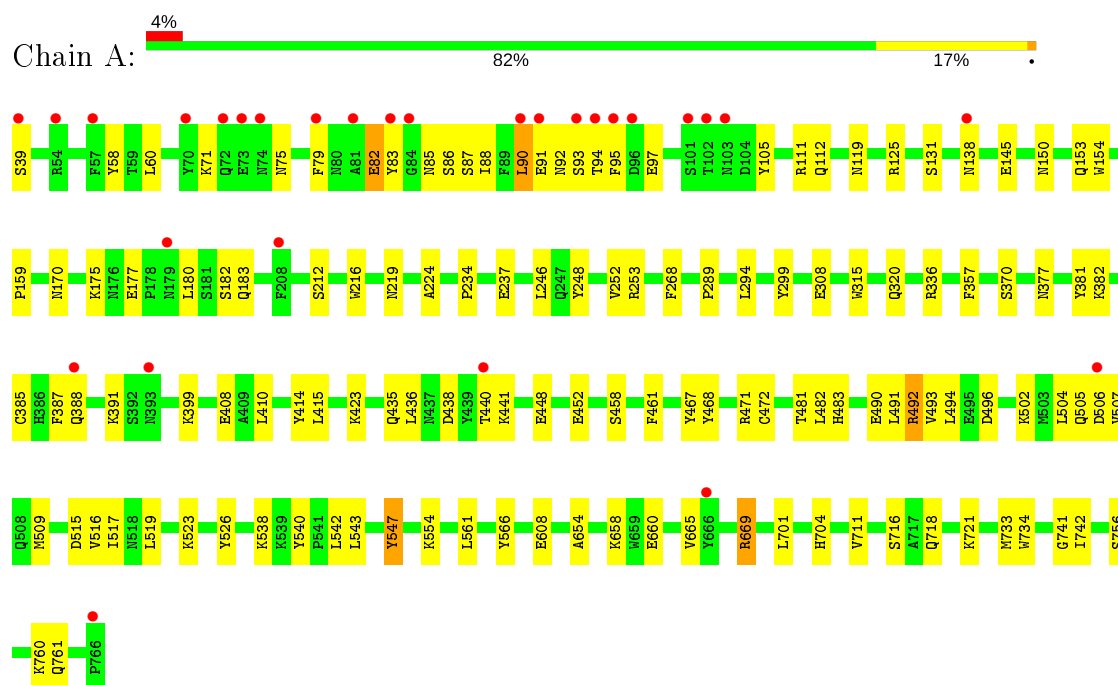
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	324	Total 324	O 324	0	0



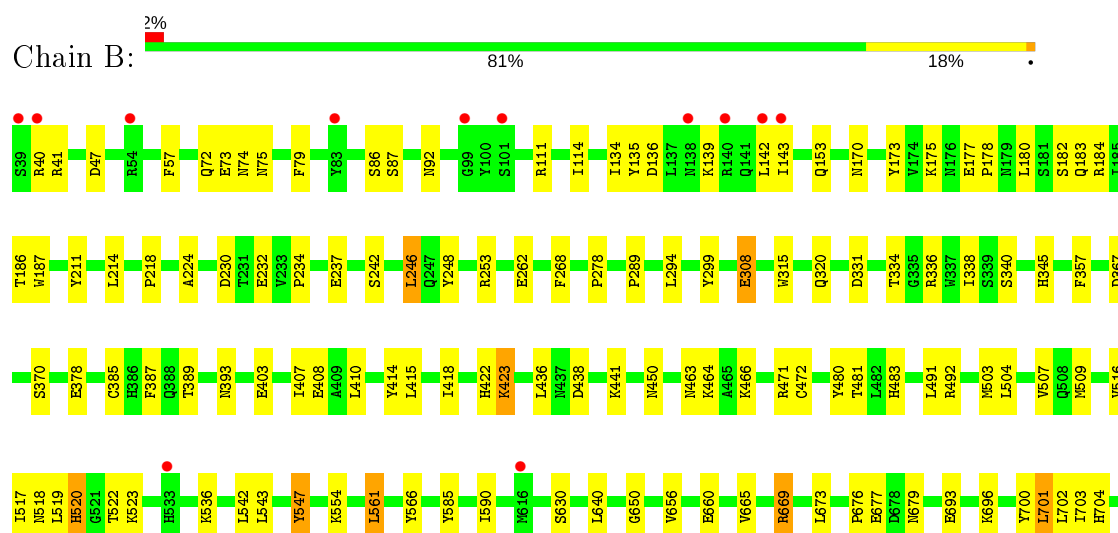
### 3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4

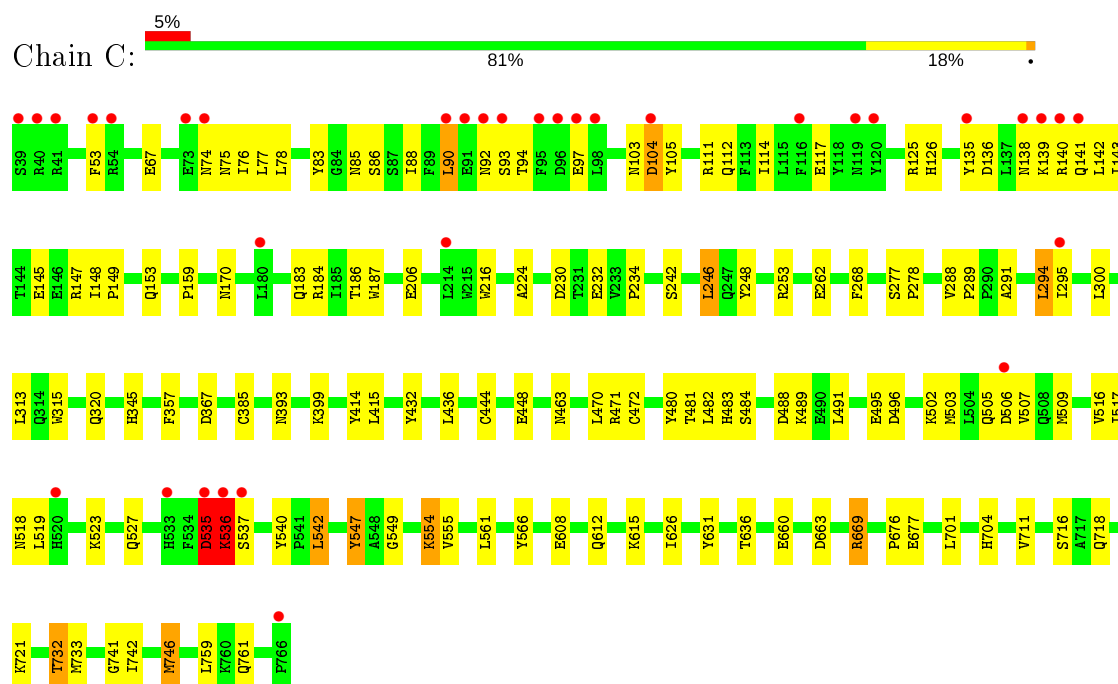


#### • Molecule 1: Dipeptidyl peptidase 4

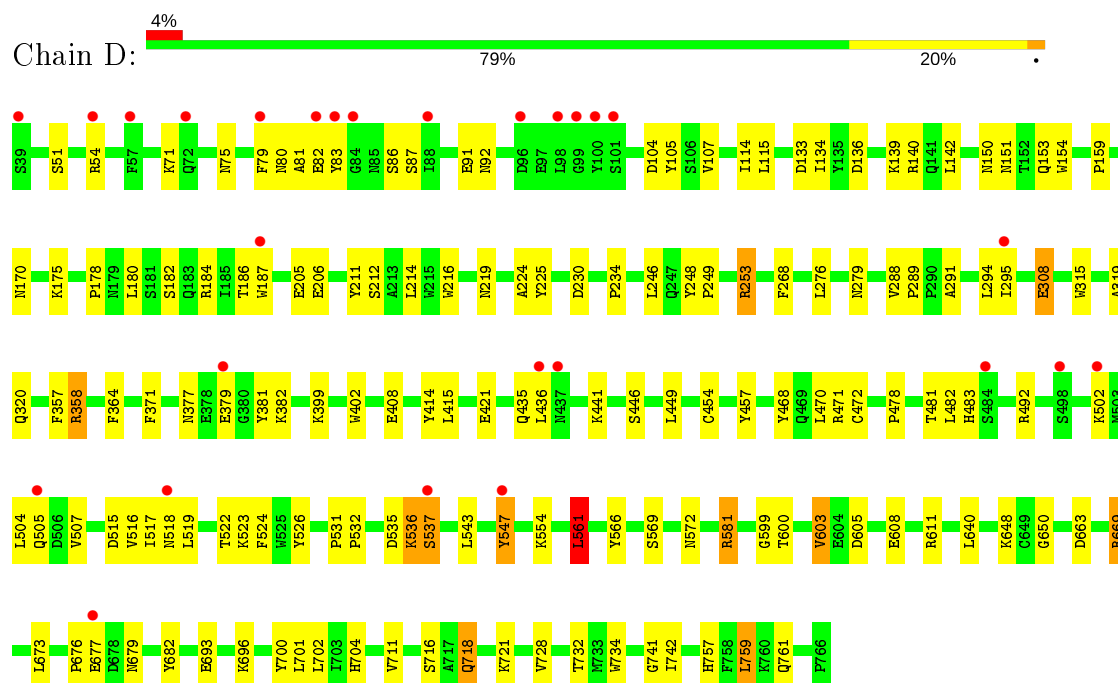




- Molecule 1: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



- 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:  50% 50%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2

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

Chain I:  100%

MAG1  
MAG2

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

Chain K:  50% 50%

MAG1  
MAG2

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

Chain L:  100%

MAG1  
MAG2

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

Chain M:  50% 50%

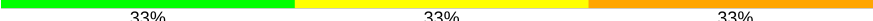
MAG1  
MAG2

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

Chain G:  67% 33%

MAC1  
MAC2  
EMJ3

- 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:  33% 33% 33%

MAC1  
MAC2  
EMJ3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.35Å 118.68Å 133.68Å 112.76° 95.16° 90.95°	Depositor
Resolution (Å)	39.90 – 1.95 39.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.90-1.95) 96.7 (39.90-1.95)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.234 0.193 , 0.224	Depositor DCC
$R_{free}$ test set	12343 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AES, BMA, NAG, 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	0.58	0/6141	0.73	1/8353 (0.0%)
1	B	0.62	0/6141	0.77	3/8353 (0.0%)
1	C	0.60	0/6141	0.76	4/8353 (0.0%)
1	D	0.55	0/6141	0.72	4/8353 (0.0%)
All	All	0.59	0/24564	0.75	12/33412 (0.0%)

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	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	669	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	B	669	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	C	669	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	669	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	669	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	669	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	669	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	542	LEU	CA-CB-CG	5.65	128.29	115.30
1	D	319	ALA	N-CA-C	-5.49	96.17	111.00
1	D	561	LEU	N-CA-C	-5.14	97.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	LEU	N-CA-C	-5.11	97.21	111.00
1	B	656	VAL	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	B	700	TYR	Sidechain
1	D	211	TYR	Sidechain
1	D	700	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5662	90	0
1	B	5966	0	5662	103	0
1	C	5966	0	5661	128	0
1	D	5966	0	5662	114	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
3	G	39	0	34	0	0
3	J	39	0	34	1	0
4	A	56	0	52	1	0
4	B	56	0	52	1	0
4	C	70	0	65	3	0
4	D	28	0	26	2	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	10	1	0
6	B	12	0	10	1	0
6	C	12	0	10	2	0
6	D	12	0	10	2	0
7	A	354	0	0	4	0
7	B	433	0	0	7	0
7	C	385	0	0	7	0
7	D	324	0	0	5	0
All	All	25912	0	23125	421	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 9.

All (421) 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:536:LYS:HG2	1:C:537:SER:H	1.19	1.00
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.42	0.98
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.71	0.89
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.72	0.88
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.37	0.88
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.75	0.87
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.72	0.86
1:D:536:LYS:O	1:D:537:SER:HB2	1.74	0.86
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.08	0.83
1:D:291:ALA:O	1:D:295:ILE:HG13	1.77	0.83
1:C:612:GLN:O	1:C:615:LYS:HG2	1.79	0.83
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.60	0.82
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.78	0.80
1:C:676:PRO:HG2	1:C:677:GLU:OE2	1.82	0.80
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.25	0.80
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.66	0.78
1:B:184:ARG:HD3	1:B:186:THR:O	1.84	0.77
1:D:75:ASN:ND2	1:D:92:ASN:H	1.82	0.77
1:C:704:HIS:HD2	1:C:716:SER:OG	1.69	0.76
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.82	0.76
1:A:547:TYR:HB3	1:A:554:LYS:HG2	1.66	0.76
1:B:378:GLU:H	1:B:378:GLU:CD	1.88	0.75
1:A:492:ARG:NH2	1:A:492:ARG:HB3	2.01	0.74
1:A:408:GLU:HG2	7:A:1767:HOH:O	1.86	0.74
1:C:536:LYS:HG2	1:C:537:SER:N	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:HB3	1:A:92:ASN:N	2.03	0.74
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.70	0.74
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.68	0.73
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.71	0.73
1:A:438:ASP:HB3	1:A:441:LYS:HD2	1.71	0.73
1:C:184:ARG:HD3	1:C:186:THR:O	1.89	0.72
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.71	0.72
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.71	0.72
1:C:291:ALA:O	1:C:295:ILE:HG13	1.89	0.72
1:C:111:ARG:HD2	7:C:1843:HOH:O	1.91	0.71
1:D:693:GLU:HG3	7:D:1662:HOH:O	1.92	0.69
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.90	0.69
1:C:313:LEU:HD12	1:C:313:LEU:N	2.07	0.69
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.74	0.69
1:B:693:GLU:OE1	1:B:696:LYS:HE3	1.92	0.68
1:B:111:ARG:HD2	7:B:1783:HOH:O	1.94	0.68
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.09	0.68
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.92	0.67
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.95	0.67
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.29	0.67
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.95	0.67
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.95	0.66
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.79	0.66
1:D:704:HIS:HD2	1:D:716:SER:OG	1.79	0.66
1:B:334:THR:OG1	1:B:336:ARG:HG2	1.96	0.66
1:C:535:ASP:C	1:C:536:LYS:HD3	2.17	0.66
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.94	0.65
1:C:746:MET:CE	1:C:746:MET:H	2.10	0.65
1:D:414:TYR:HA	1:D:436:LEU:HD13	1.79	0.65
1:C:502:LYS:O	1:C:505:GLN:HG2	1.96	0.65
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.24	0.65
1:D:547:TYR:HB3	1:D:554:LYS:HG2	1.77	0.65
1:A:111:ARG:HD2	7:A:1819:HOH:O	1.97	0.64
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.79	0.64
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.42	0.64
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.96	0.63
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.14	0.63
1:D:184:ARG:HD3	1:D:186:THR:O	1.98	0.63
1:C:76:ILE:HB	1:C:90:LEU:HD13	1.80	0.63
1:B:704:HIS:HD2	1:B:716:SER:OG	1.81	0.63
1:B:75:ASN:ND2	1:B:92:ASN:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:CG	1:C:537:SER:H	1.99	0.62
1:D:175:LYS:CG	1:D:182:SER:HB3	2.30	0.62
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.62
1:C:232:GLU:HB3	1:C:262:GLU:HG2	1.82	0.62
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.81	0.62
1:D:75:ASN:HD22	1:D:91:GLU:HA	1.65	0.62
1:B:177:GLU:CB	1:B:180:LEU:HD23	2.29	0.62
1:C:536:LYS:N	1:C:536:LYS:HD3	2.15	0.61
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.82	0.61
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.21	0.61
1:C:535:ASP:O	1:C:536:LYS:HB3	1.99	0.61
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.29	0.61
1:C:733:MET:HA	1:D:732:THR:HG22	1.81	0.61
1:C:733:MET:HA	1:D:732:THR:CG2	2.31	0.60
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.65	0.60
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.32	0.60
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.84	0.60
1:B:438:ASP:OD2	1:B:441:LYS:HE3	2.01	0.60
1:C:153:GLN:HE22	1:C:170:ASN:HD22	1.49	0.59
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.22	0.59
1:D:377:ASN:HB3	1:D:379:GLU:H	1.67	0.59
1:B:218:PRO:HD2	1:B:308:GLU:OE2	2.02	0.59
1:A:88:ILE:HG21	1:A:91:GLU:HG2	1.85	0.59
1:D:543:LEU:HD22	1:D:759:LEU:HD11	1.84	0.59
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.85	0.59
1:C:53:PHE:CD1	1:C:503:MET:HG2	2.37	0.59
1:C:104:ASP:HB3	1:C:117:GLU:HB3	1.85	0.59
1:C:253:ARG:NH2	1:D:253:ARG:HH22	2.00	0.59
1:D:357:PHE:CE1	6:D:801:AES:H2	2.38	0.58
1:A:87:SER:OG	4:A:767(A):NAG:H81	2.04	0.58
1:C:547:TYR:HB3	1:C:554:LYS:HG2	1.85	0.58
1:C:718:GLN:HE22	1:C:721:LYS:NZ	2.02	0.58
1:D:676:PRO:HG2	1:D:677:GLU:OE1	2.03	0.58
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.85	0.58
1:D:536:LYS:HB3	1:D:536:LYS:NZ	2.19	0.58
1:B:408:GLU:HG2	7:B:1639:HOH:O	2.02	0.58
1:B:718:GLN:HE21	1:B:718:GLN:HA	1.67	0.58
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.85	0.58
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.39	0.58
1:A:377:ASN:HB2	1:A:381:TYR:O	2.04	0.58
1:C:519:LEU:HD22	1:C:608:GLU:CD	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.86	0.57
1:A:704:HIS:HD2	1:A:716:SER:OG	1.87	0.57
1:A:175:LYS:CG	1:A:182:SER:HB3	2.35	0.57
1:B:357:PHE:CE1	6:B:801:AES:H2	2.40	0.57
1:D:408:GLU:HG2	7:D:1571:HOH:O	2.04	0.57
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.03	0.57
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.40	0.57
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.87	0.56
1:B:422:HIS:NE2	1:B:423:LYS:HD3	2.20	0.56
1:C:535:ASP:C	1:C:536:LYS:CD	2.73	0.56
1:D:718:GLN:HE22	1:D:721:LYS:NZ	2.03	0.56
1:D:536:LYS:O	1:D:537:SER:CB	2.48	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.87	0.56
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.35	0.56
3:J:1:NAG:H62	3:J:2:NAG:HN2	1.70	0.56
1:A:502:LYS:O	1:A:505:GLN:HG2	2.06	0.56
1:B:73:GLU:OE2	1:B:73:GLU:HA	2.05	0.56
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.40	0.56
1:A:458:SER:OG	1:A:471:ARG:HD3	2.05	0.56
1:D:133:ASP:HB3	1:D:142:LEU:HD21	1.87	0.56
1:D:600:THR:O	1:D:603:VAL:HG13	2.06	0.55
1:B:175:LYS:CG	1:B:182:SER:HB3	2.36	0.55
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.41	0.55
1:C:53:PHE:CE1	1:C:503:MET:HG2	2.42	0.55
1:C:718:GLN:HE22	1:C:721:LYS:HZ1	1.52	0.55
1:B:41:ARG:NH1	1:B:47:ASP:OD1	2.40	0.55
1:A:39:SER:HA	1:A:506:ASP:OD2	2.06	0.55
1:D:599:GLY:O	1:D:603:VAL:HG11	2.07	0.55
1:B:232:GLU:HB3	1:B:262:GLU:HG2	1.89	0.55
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.89	0.55
1:A:112:GLN:HG2	1:A:138:ASN:HD21	1.71	0.54
1:A:131:SER:OG	1:A:150:ASN:ND2	2.40	0.54
1:A:92:ASN:C	1:A:94:THR:H	2.10	0.54
1:D:518:ASN:O	1:D:519:LEU:HD23	2.07	0.54
1:B:418:ILE:HD11	7:B:1506:HOH:O	2.06	0.54
1:C:139:LYS:O	1:C:141:GLN:HG3	2.07	0.54
1:D:175:LYS:HG3	1:D:182:SER:HB3	1.89	0.54
1:B:516:VAL:HG11	1:B:523:LYS:HB2	1.90	0.54
1:B:414:TYR:HA	1:B:436:LEU:HD13	1.89	0.54
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.90	0.54
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:LEU:HD13	1:C:608:GLU:OE1	2.07	0.54
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.90	0.53
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.09	0.53
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.43	0.53
1:C:114:ILE:HG22	1:C:135:TYR:HB3	1.91	0.53
1:D:516:VAL:HG12	1:D:517:ILE:N	2.24	0.53
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.44	0.52
1:C:75:ASN:ND2	1:C:92:ASN:H	2.07	0.52
1:A:482:LEU:O	1:A:490:GLU:O	2.27	0.52
1:C:139:LYS:HD3	1:C:141:GLN:CD	2.30	0.52
1:D:472:CYS:O	1:D:478:PRO:HA	2.10	0.52
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.09	0.52
1:C:357:PHE:CE1	6:C:801:AES:H2	2.44	0.52
1:B:464:LYS:HE2	1:B:466:LYS:HE2	1.92	0.52
1:D:677:GLU:OE1	1:D:677:GLU:N	2.41	0.52
1:D:71:LYS:HA	1:D:75:ASN:O	2.10	0.52
1:B:660:GLU:OE2	7:B:1543:HOH:O	2.19	0.52
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.40	0.52
1:B:741:GLY:O	1:B:742:ILE:C	2.48	0.51
1:B:214:LEU:HD12	1:B:214:LEU:O	2.11	0.51
1:D:105:TYR:HB2	1:D:114:ILE:HD11	1.92	0.51
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.57	0.51
1:B:175:LYS:NZ	1:B:178:PRO:HA	2.26	0.51
1:B:758:PHE:O	1:B:761:GLN:HG2	2.10	0.51
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.45	0.51
1:D:536:LYS:HZ3	1:D:536:LYS:HB3	1.74	0.51
1:D:757:HIS:O	1:D:761:GLN:HG2	2.11	0.51
1:C:90:LEU:HD13	1:C:90:LEU:O	2.11	0.51
1:A:435:GLN:HE22	1:A:441:LYS:HD3	1.76	0.50
1:C:527:GLN:HB3	1:C:555:VAL:HG13	1.94	0.50
1:D:516:VAL:HG13	1:D:524:PHE:O	2.12	0.50
1:A:125:ARG:HB3	7:A:1596:HOH:O	2.11	0.50
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.92	0.50
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.46	0.50
1:A:507:VAL:HG13	1:A:509:MET:HG2	1.93	0.50
1:B:704:HIS:HE1	1:B:711:VAL:O	1.95	0.50
1:C:67:GLU:HB3	1:C:78:LEU:HD11	1.94	0.50
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.94	0.50
1:C:491:LEU:HD22	1:C:491:LEU:N	2.27	0.50
1:C:612:GLN:HA	1:C:615:LYS:HD3	1.94	0.49
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.94	0.49
1:B:79:PHE:CD1	1:B:86:SER:HB3	2.48	0.49
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.47	0.49
1:B:677:GLU:CD	1:B:677:GLU:H	2.16	0.49
1:C:547:TYR:CB	1:C:554:LYS:HG2	2.43	0.49
1:D:504:LEU:HD23	1:D:507:VAL:HG11	1.94	0.49
1:C:704:HIS:CD2	1:C:716:SER:OG	2.57	0.49
1:A:75:ASN:HB3	1:A:92:ASN:H	1.75	0.49
1:A:71:LYS:HE3	1:A:105:TYR:CD2	2.48	0.49
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.61	0.49
1:B:345:HIS:HD2	7:B:1522:HOH:O	1.96	0.49
1:C:746:MET:H	1:C:746:MET:HE3	1.75	0.49
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.43	0.49
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.19	0.49
1:D:547:TYR:CB	1:D:554:LYS:HG2	2.43	0.49
1:B:693:GLU:OE1	1:B:696:LYS:CE	2.61	0.48
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.95	0.48
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.48	0.48
1:D:581:ARG:HB2	1:D:605:ASP:OD2	2.12	0.48
1:C:518:ASN:O	1:C:519:LEU:HD23	2.13	0.48
1:D:535:ASP:C	1:D:536:LYS:O	2.48	0.48
1:B:370:SER:HB2	1:B:387:PHE:O	2.14	0.48
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.34	0.48
1:C:86:SER:HA	4:C:767(A):NAG:H81	1.95	0.48
1:C:357:PHE:CZ	6:C:801:AES:H2	2.48	0.48
1:D:502:LYS:O	1:D:505:GLN:HG2	2.13	0.48
1:A:83:TYR:HB2	1:A:85:ASN:OD1	2.13	0.48
1:A:538:LYS:HD3	1:A:540:TYR:CZ	2.49	0.48
1:C:535:ASP:O	1:C:536:LYS:CB	2.62	0.48
1:D:206:GLU:OE2	1:D:663:ASP:OD2	2.32	0.48
1:A:92:ASN:O	1:A:94:THR:N	2.43	0.48
1:A:93:SER:C	1:A:95:PHE:N	2.65	0.47
1:A:253:ARG:CZ	1:B:253:ARG:HH21	2.27	0.47
1:A:734:TRP:H	1:B:732:THR:HG21	1.79	0.47
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.48	0.47
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.49	0.47
1:D:107:VAL:HG23	7:D:1806:HOH:O	2.15	0.47
1:D:279:ASN:OD1	4:D:773(A):NAG:N2	2.47	0.47
1:D:414:TYR:CA	1:D:436:LEU:HD13	2.44	0.47
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.49	0.47
1:C:484:SER:O	1:C:488:ASP:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.79	0.47
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.50	0.47
1:D:611:ARG:HH11	1:D:611:ARG:HG3	1.79	0.47
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.49	0.47
1:A:733:MET:HA	1:B:732:THR:CG2	2.45	0.47
1:B:289:PRO:HB3	1:B:315:TRP:CD2	2.50	0.47
4:C:770(A):NAG:O3	4:C:770(A):NAG:H83	2.14	0.47
1:A:92:ASN:O	1:A:93:SER:OG	2.29	0.47
1:C:660:GLU:CG	7:C:1787:HOH:O	2.62	0.47
1:C:97:GLU:O	1:C:97:GLU:HG2	2.15	0.47
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.96	0.47
1:B:393:ASN:H	1:B:393:ASN:HD22	1.63	0.47
1:C:516:VAL:HG12	1:C:517:ILE:N	2.30	0.47
1:A:175:LYS:HG3	1:A:182:SER:CB	2.44	0.47
1:D:741:GLY:O	1:D:742:ILE:C	2.53	0.47
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.50	0.46
1:A:493:VAL:HG11	1:A:496:ASP:HB3	1.96	0.46
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.80	0.46
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.49	0.46
1:C:142:LEU:HD23	1:C:143:ILE:N	2.31	0.46
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.50	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.54	0.46
1:C:507:VAL:HG23	1:C:509:MET:HG2	1.98	0.46
1:C:90:LEU:O	1:C:90:LEU:HD22	2.15	0.46
1:D:175:LYS:HE3	1:D:180:LEU:O	2.15	0.46
1:A:414:TYR:CA	1:A:436:LEU:HD13	2.45	0.46
1:D:682:TYR:OH	2:M:2:NAG:H83	2.16	0.46
1:B:378:GLU:N	1:B:378:GLU:CD	2.65	0.46
1:B:673:LEU:N	1:B:673:LEU:HD12	2.31	0.46
1:C:549:GLY:HA2	1:C:631:TYR:CE1	2.51	0.46
1:D:516:VAL:CG1	1:D:517:ILE:N	2.79	0.46
1:D:87:SER:HB3	4:D:767(A):NAG:O6	2.16	0.46
1:D:600:THR:O	1:D:603:VAL:CG1	2.63	0.46
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.50	0.46
1:C:313:LEU:CD1	1:C:313:LEU:N	2.78	0.46
1:A:93:SER:C	1:A:95:PHE:H	2.20	0.45
1:B:491:LEU:O	1:B:492:ARG:HB3	2.15	0.45
1:B:519:LEU:HB3	1:B:520:HIS:CE1	2.51	0.45
1:C:489:LYS:O	1:C:491:LEU:HD22	2.16	0.45
1:D:502:LYS:HD2	1:D:505:GLN:OE1	2.15	0.45
1:C:112:GLN:HB3	1:C:138:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.98	0.45
1:B:718:GLN:NE2	1:B:718:GLN:HA	2.31	0.45
1:D:718:GLN:HE22	1:D:721:LYS:HZ1	1.65	0.45
1:D:81:ALA:O	1:D:82:GLU:HB3	2.17	0.45
1:A:438:ASP:OD1	1:A:440:THR:HB	2.17	0.45
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.37	0.45
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.52	0.45
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.63	0.45
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.82	0.45
1:C:496:ASP:HB2	7:C:1694:HOH:O	2.17	0.45
1:D:532:PRO:HD3	1:D:569:SER:HA	1.98	0.45
1:A:547:TYR:HB2	1:A:554:LYS:HD3	1.98	0.45
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.52	0.45
1:C:183:GLN:HE22	1:C:278:PRO:N	2.15	0.45
1:D:446:SER:HA	1:D:449:LEU:HG	1.99	0.45
1:C:484:SER:CB	1:C:491:LEU:HD21	2.46	0.45
1:A:336:ARG:HD3	1:C:277:SER:OG	2.17	0.44
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.52	0.44
1:B:547:TYR:HB3	1:B:554:LYS:HG2	1.98	0.44
1:B:471:ARG:NH2	7:B:1882:HOH:O	2.50	0.44
1:C:432:TYR:CE2	1:C:444:CYS:HB2	2.53	0.44
1:C:535:ASP:N	1:C:540:TYR:OH	2.40	0.44
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.44
1:D:379:GLU:HG2	1:D:381:TYR:CD1	2.53	0.44
1:C:345:HIS:HD2	7:C:1601:HOH:O	2.01	0.44
1:D:51:SER:O	1:D:54:ARG:HD2	2.17	0.44
1:D:648:LYS:HE3	7:D:1701:HOH:O	2.17	0.44
1:A:490:GLU:HG3	1:A:490:GLU:O	2.17	0.44
1:B:415:LEU:C	1:B:415:LEU:HD13	2.38	0.44
1:B:75:ASN:HD22	1:B:92:ASN:H	1.66	0.44
1:B:73:GLU:O	1:B:74:ASN:HB2	2.18	0.44
1:D:104:ASP:OD1	1:D:105:TYR:N	2.49	0.44
1:C:105:TYR:HB2	1:C:114:ILE:HD11	1.99	0.44
1:C:704:HIS:HE1	1:C:711:VAL:O	2.00	0.44
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.15	0.44
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.83	0.44
1:C:732:THR:HG21	1:D:734:TRP:H	1.82	0.44
1:C:97:GLU:N	1:C:97:GLU:OE1	2.50	0.44
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.83	0.44
1:D:105:TYR:HA	1:D:115:LEU:O	2.18	0.44
1:A:90:LEU:HD21	1:A:94:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLN:HE22	1:B:721:LYS:HZ1	1.64	0.44
1:C:393:ASN:ND2	1:C:393:ASN:H	2.16	0.43
1:A:357:PHE:CE1	6:A:801:AES:H2	2.53	0.43
1:A:704:HIS:HE1	1:A:711:VAL:O	2.00	0.43
1:A:88:ILE:HG21	1:A:91:GLU:CG	2.47	0.43
1:C:83:TYR:HB2	1:C:85:ASN:OD1	2.18	0.43
1:D:468:TYR:CE2	1:D:483:HIS:HB2	2.53	0.43
1:A:382:LYS:HE2	7:A:1774:HOH:O	2.18	0.43
1:A:515:ASP:HB3	1:A:526:TYR:CE2	2.53	0.43
1:C:660:GLU:HG3	7:C:1787:HOH:O	2.18	0.43
1:D:205:GLU:OE2	6:D:801:AES:N8	2.51	0.43
1:D:535:ASP:OD1	1:D:536:LYS:O	2.36	0.43
1:D:561:LEU:HD12	1:D:561:LEU:HA	1.89	0.43
1:D:80:ASN:OD1	1:D:83:TYR:HD2	2.01	0.43
1:A:415:LEU:C	1:A:415:LEU:HD13	2.39	0.43
1:A:490:GLU:O	1:A:492:ARG:N	2.51	0.43
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.54	0.43
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.49	0.43
1:C:536:LYS:CG	1:C:537:SER:N	2.68	0.43
1:D:150:ASN:O	1:D:151:ASN:HB2	2.19	0.43
1:A:219:ASN:HD22	1:A:308:GLU:CG	2.32	0.43
1:B:507:VAL:HG13	1:B:509:MET:HG2	2.01	0.43
1:B:72:GLN:HG2	1:B:73:GLU:HG2	2.00	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HB2	2.00	0.43
1:B:704:HIS:CD2	1:B:716:SER:OG	2.67	0.43
7:C:1840:HOH:O	1:D:249:PRO:HB2	2.19	0.43
1:A:219:ASN:HB2	1:A:308:GLU:CD	2.38	0.43
1:B:414:TYR:CA	1:B:436:LEU:HD13	2.49	0.43
1:B:463:ASN:HD22	1:B:463:ASN:N	2.16	0.43
1:C:495:GLU:HA	7:C:1719:HOH:O	2.19	0.43
1:C:288:VAL:HG11	1:C:294:LEU:HD11	2.01	0.42
1:D:382:LYS:HE2	7:D:1788:HOH:O	2.19	0.42
1:D:704:HIS:HE1	1:D:711:VAL:O	2.01	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.53	0.42
1:B:134:ILE:HG21	1:B:178:PRO:HB3	2.00	0.42
1:B:331:ASP:HB2	1:B:338:ILE:HD12	2.01	0.42
1:B:87:SER:OG	4:B:767(A):NAG:H81	2.19	0.42
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.33	0.42
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.40	0.42
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.54	0.42
1:C:626:ILE:HG23	1:C:636:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:CD2	1:C:88:ILE:HG12	2.50	0.42
1:B:142:LEU:HD23	1:B:143:ILE:N	2.34	0.42
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.84	0.42
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.55	0.42
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.85	0.42
1:C:148:ILE:HA	1:C:149:PRO:HD3	1.86	0.42
1:B:516:VAL:CG1	1:B:523:LYS:HB2	2.48	0.42
1:C:484:SER:N	1:C:491:LEU:HD21	2.34	0.42
4:C:771(A):NAG:H83	4:C:771(A):NAG:H2	1.94	0.42
1:A:370:SER:HB2	1:A:387:PHE:O	2.19	0.42
1:B:184:ARG:CD	1:B:186:THR:O	2.61	0.42
1:C:206:GLU:OE2	1:C:663:ASP:OD2	2.38	0.42
1:D:415:LEU:C	1:D:415:LEU:HD23	2.40	0.42
1:D:457:TYR:HA	1:D:471:ARG:O	2.20	0.42
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.19	0.42
1:C:484:SER:N	1:C:491:LEU:CD2	2.83	0.42
1:B:134:ILE:O	1:B:143:ILE:HD13	2.19	0.41
1:A:253:ARG:HH22	1:B:253:ARG:HH21	1.62	0.41
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.55	0.41
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.03	0.41
1:B:143:ILE:N	1:B:143:ILE:HD12	2.35	0.41
1:B:516:VAL:CG1	1:B:517:ILE:N	2.83	0.41
1:C:75:ASN:HD21	1:C:92:ASN:HB2	1.84	0.41
1:D:358:ARG:HB3	1:D:358:ARG:HE	1.61	0.41
1:D:435:GLN:HE22	1:D:441:LYS:HD2	1.85	0.41
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.01	0.41
1:C:77:LEU:HD23	1:C:88:ILE:HA	2.03	0.41
1:A:658:LYS:HE2	1:A:660:GLU:HB2	2.02	0.41
1:B:180:LEU:N	1:B:180:LEU:HD22	2.36	0.41
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.35	0.41
1:B:516:VAL:HG12	1:B:517:ILE:N	2.36	0.41
1:C:463:ASN:N	1:C:463:ASN:HD22	2.18	0.41
1:B:393:ASN:ND2	1:B:393:ASN:H	2.19	0.41
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.35	0.41
1:C:94:THR:O	1:C:94:THR:HG22	2.20	0.41
1:D:515:ASP:HB3	1:D:526:TYR:CZ	2.56	0.41
1:D:718:GLN:NE2	1:D:718:GLN:HA	2.34	0.41
1:B:136:ASP:HB2	1:B:143:ILE:HD11	2.03	0.41
1:C:516:VAL:CG1	1:C:517:ILE:N	2.84	0.41
1:B:561:LEU:HD12	1:B:561:LEU:HA	1.99	0.41
1:B:701:LEU:HD13	1:B:703:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:HD23	1:C:143:ILE:O	2.21	0.41
1:C:506:ASP:OD1	1:C:506:ASP:O	2.38	0.41
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.41
1:A:60:LEU:C	1:A:60:LEU:HD12	2.41	0.41
1:B:503:MET:HE1	7:B:1743:HOH:O	2.20	0.41
1:D:522:THR:HB	1:D:524:PHE:CE1	2.56	0.41
1:A:452:GLU:OE1	1:A:452:GLU:HA	2.21	0.41
1:D:214:LEU:HD23	1:D:225:TYR:HB3	2.03	0.41
1:D:481:THR:OG1	1:D:483:HIS:CE1	2.71	0.41
1:D:492:ARG:HG2	1:D:492:ARG:HH11	1.85	0.41
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.56	0.40
1:C:183:GLN:NE2	1:C:277:SER:C	2.74	0.40
1:C:414:TYR:HA	1:C:436:LEU:HD13	2.01	0.40
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.57	0.40
1:B:242:SER:HB3	1:B:246:LEU:HD12	2.04	0.40
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.56	0.40
1:C:125:ARG:HG2	1:C:126:HIS:CD2	2.57	0.40
1:C:148:ILE:HG23	1:C:149:PRO:HD2	2.03	0.40
1:C:288:VAL:CG1	1:C:289:PRO:HD2	2.48	0.40
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.56	0.40
1:A:756:SER:O	1:A:760:LYS:HG3	2.21	0.40
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.96	0.40
1:C:536:LYS:N	1:C:536:LYS:CD	2.84	0.40
1:D:470:LEU:HA	1:D:470:LEU:HD23	1.87	0.40
1:B:345:HIS:HE1	1:B:389:THR:O	2.04	0.40
1:C:142:LEU:C	1:C:142:LEU:HD23	2.42	0.40
1:C:463:ASN:N	1:C:463:ASN:ND2	2.69	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	726/728 (100%)	690 (95%)	33 (4%)	3 (0%)	34	22
1	B	726/728 (100%)	703 (97%)	22 (3%)	1 (0%)	51	43
1	C	726/728 (100%)	692 (95%)	28 (4%)	6 (1%)	19	9
1	D	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	51	43
All	All	2904/2912 (100%)	2778 (96%)	115 (4%)	11 (0%)	34	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ARG
1	C	74	ASN
1	C	103	ASN
1	C	104	ASP
1	C	535	ASP
1	C	536	LYS
1	C	93	SER
1	A	97	GLU
1	A	491	LEU
1	A	82	GLU
1	D	537	SER

### 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	652/652 (100%)	633 (97%)	19 (3%)	42	31
1	B	652/652 (100%)	629 (96%)	23 (4%)	36	24
1	C	652/652 (100%)	628 (96%)	24 (4%)	34	22
1	D	652/652 (100%)	630 (97%)	22 (3%)	37	25
All	All	2608/2608 (100%)	2520 (97%)	88 (3%)	37	25

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	119	ASN
1	A	145	GLU
1	A	183	GLN
1	A	246	LEU
1	A	294	LEU
1	A	385	CYS
1	A	399	LYS
1	A	423	LYS
1	A	448	GLU
1	A	472	CYS
1	A	492	ARG
1	A	542	LEU
1	A	543	LEU
1	A	547	TYR
1	A	561	LEU
1	A	566	TYR
1	A	701	LEU
1	A	761	GLN
1	B	230	ASP
1	B	246	LEU
1	B	294	LEU
1	B	308	GLU
1	B	340	SER
1	B	367	ASP
1	B	385	CYS
1	B	423	LYS
1	B	450	ASN
1	B	472	CYS
1	B	518	ASN
1	B	520	HIS
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	547	TYR
1	B	561	LEU
1	B	566	TYR
1	B	630	SER
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	732	THR
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	145	GLU
1	C	147	ARG
1	C	230	ASP
1	C	246	LEU
1	C	294	LEU
1	C	367	ASP
1	C	385	CYS
1	C	399	LYS
1	C	448	GLU
1	C	472	CYS
1	C	482	LEU
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	547	TYR
1	C	554	LYS
1	C	561	LEU
1	C	566	TYR
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	C	761	GLN
1	D	230	ASP
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	294	LEU
1	D	308	GLU
1	D	358	ARG
1	D	399	LYS
1	D	482	LEU
1	D	536	LYS
1	D	547	TYR
1	D	561	LEU
1	D	566	TYR
1	D	581	ARG
1	D	603	VAL
1	D	608	GLU
1	D	673	LEU
1	D	679	ASN
1	D	701	LEU

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Mol	Chain	Res	Type
1	D	702	LEU
1	D	718	GLN
1	D	759	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN
1	A	123	GLN
1	A	138	ASN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	183	GLN
1	A	192	ASN
1	A	219	ASN
1	A	247	GLN
1	A	345	HIS
1	A	430	ASN
1	A	435	GLN
1	A	463	ASN
1	A	483	HIS
1	A	518	ASN
1	A	572	ASN
1	A	586	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	B	61	GLN
1	B	75	ASN
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	247	GLN
1	B	345	HIS
1	B	369	ASN
1	B	393	ASN
1	B	430	ASN
1	B	435	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	533	HIS
1	B	572	ASN
1	B	586	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	761	GLN
1	C	72	GLN
1	C	74	ASN
1	C	75	ASN
1	C	119	ASN
1	C	138	ASN
1	C	141	GLN
1	C	150	ASN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	183	GLN
1	C	192	ASN
1	C	247	GLN
1	C	345	HIS
1	C	393	ASN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN

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Mol	Chain	Res	Type
1	C	761	GLN
1	D	61	GLN
1	D	72	GLN
1	D	75	ASN
1	D	103	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	247	GLN
1	D	435	GLN
1	D	463	ASN
1	D	483	HIS
1	D	572	ASN
1	D	586	GLN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	745	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 ⓘ

20 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	E	1	1,2	14,14,15	0.74	0	17,19,21	0.80	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.75	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.76	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.58	0	17,19,21	0.74	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.55	0	17,19,21	0.80	0
3	NAG	G	2	3	14,14,15	0.48	0	17,19,21	0.75	0
3	BMA	G	3	3	11,11,12	0.64	0	15,15,17	1.23	2 (13%)
2	NAG	H	1	1,2	14,14,15	0.68	0	17,19,21	0.73	0
2	NAG	H	2	2	14,14,15	0.64	0	17,19,21	0.75	0
2	NAG	I	1	1,2	14,14,15	0.78	0	17,19,21	0.65	0
2	NAG	I	2	2	14,14,15	0.67	0	17,19,21	0.78	0
3	NAG	J	1	1,3	14,14,15	0.60	0	17,19,21	0.76	1 (5%)
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	0.58	0
3	BMA	J	3	3	11,11,12	0.63	0	15,15,17	0.39	0
2	NAG	K	1	1,2	14,14,15	0.63	0	17,19,21	0.66	0
2	NAG	K	2	2	14,14,15	0.52	0	17,19,21	0.68	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
2	NAG	L	2	2	14,14,15	0.64	0	17,19,21	0.81	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.78	0	17,19,21	0.61	0
2	NAG	M	2	2	14,14,15	0.58	0	17,19,21	0.86	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	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	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-O5-C5	3.03	116.29	112.19
2	E	1	NAG	C2-N2-C7	-2.51	119.33	122.90
2	E	2	NAG	C2-N2-C7	-2.41	119.47	122.90
2	L	1	NAG	C2-N2-C7	-2.22	119.75	122.90
3	G	3	BMA	C3-C4-C5	2.19	114.14	110.24
2	K	2	NAG	C2-N2-C7	-2.17	119.82	122.90
2	L	2	NAG	C2-N2-C7	-2.13	119.86	122.90
2	F	2	NAG	C2-N2-C7	-2.13	119.87	122.90
3	J	1	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2

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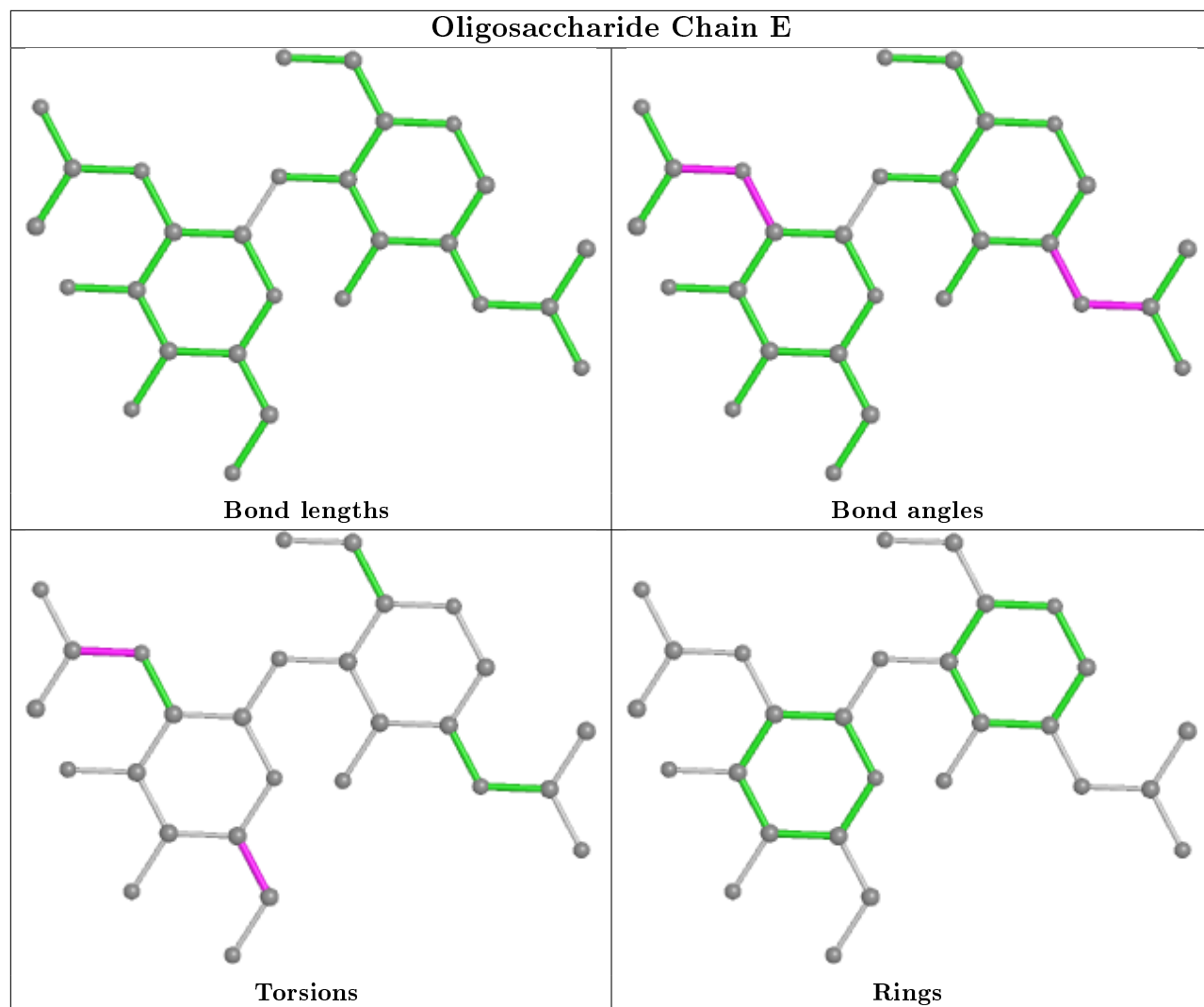
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
2	M	2	NAG	C1-C2-N2-C7
3	G	2	NAG	O7-C7-N2-C2
3	G	3	BMA	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

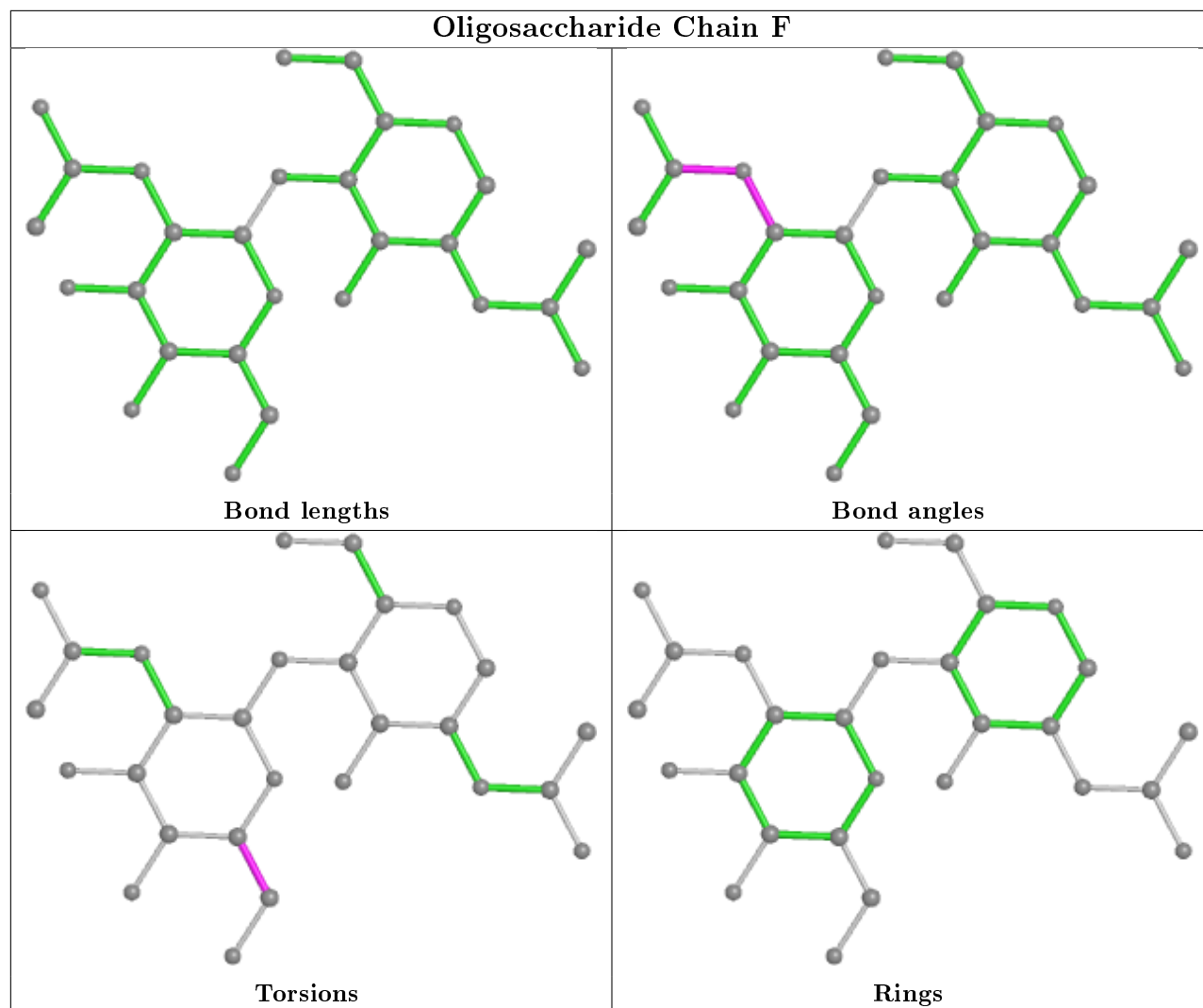
There are no ring outliers.

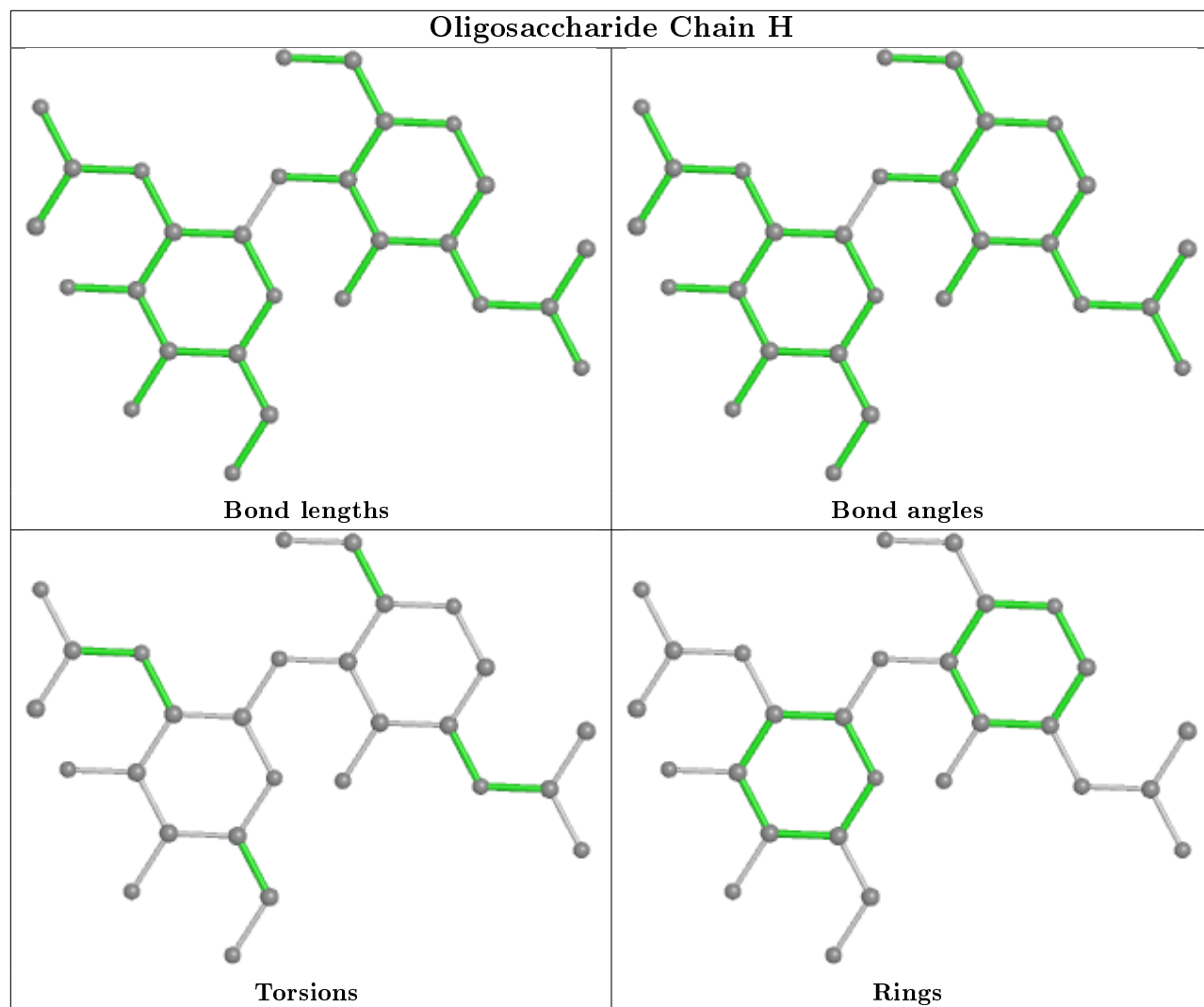
3 monomers are involved in 2 short contacts:

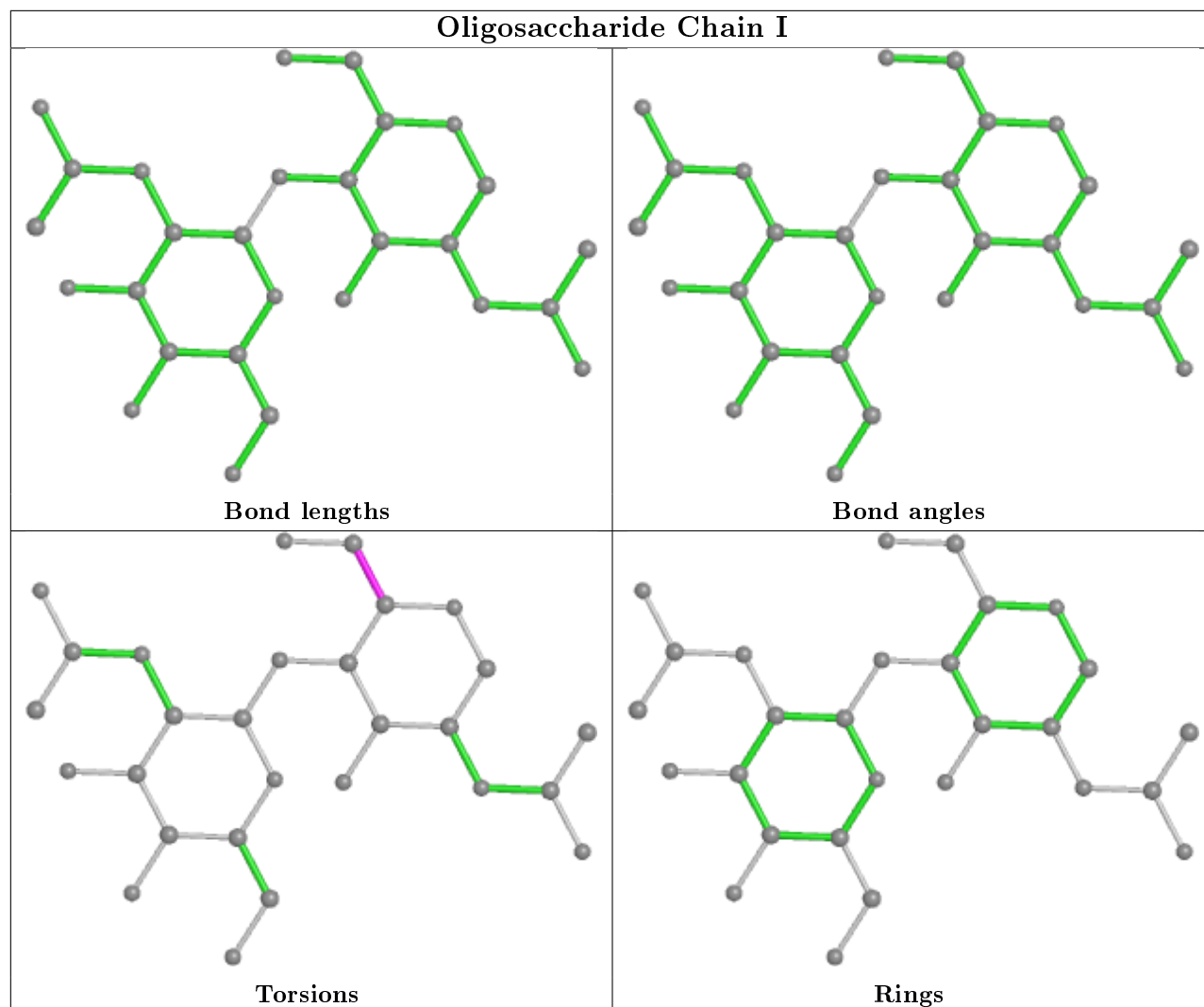
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
2	M	2	NAG	1	0
3	J	2	NAG	1	0

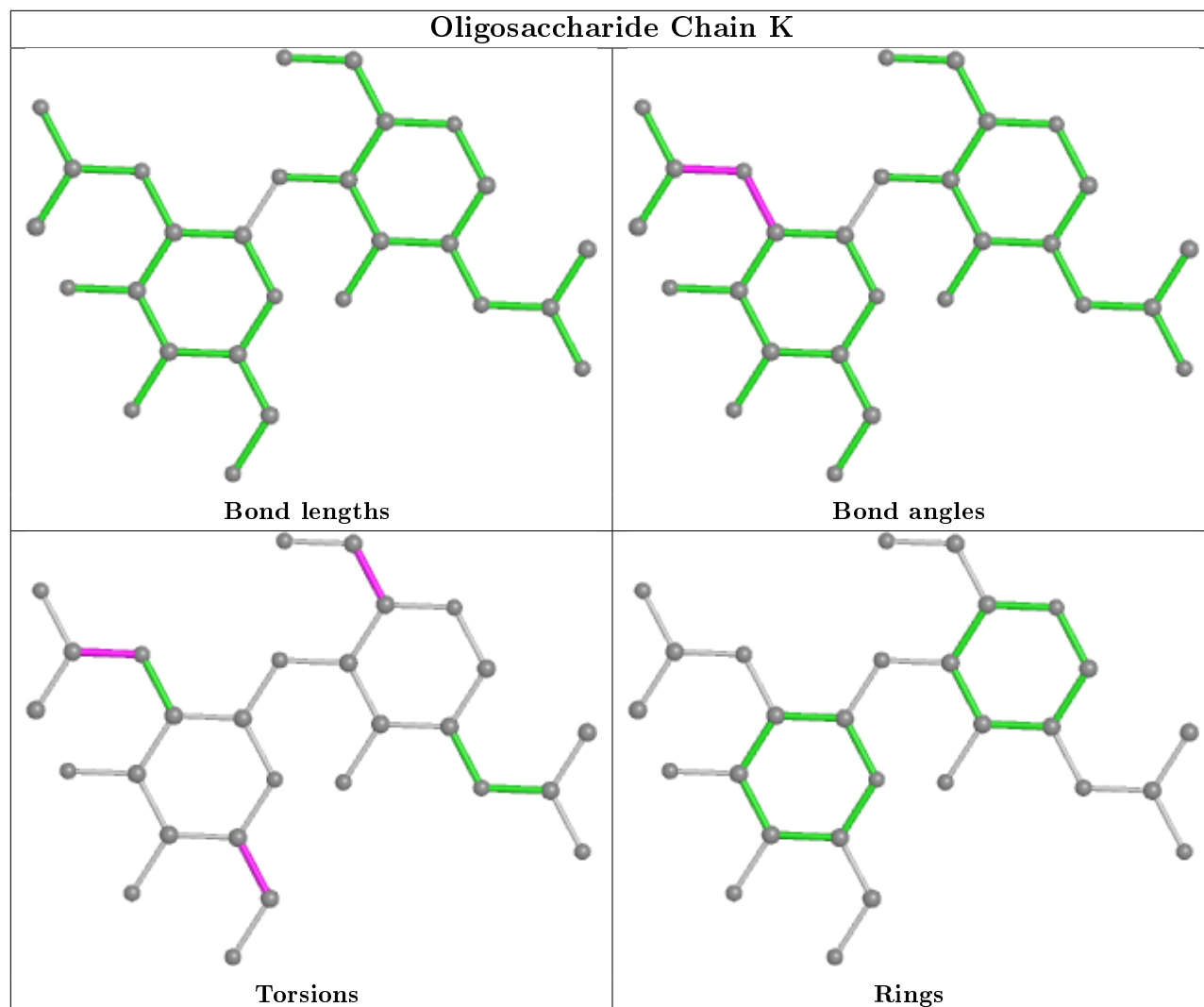
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



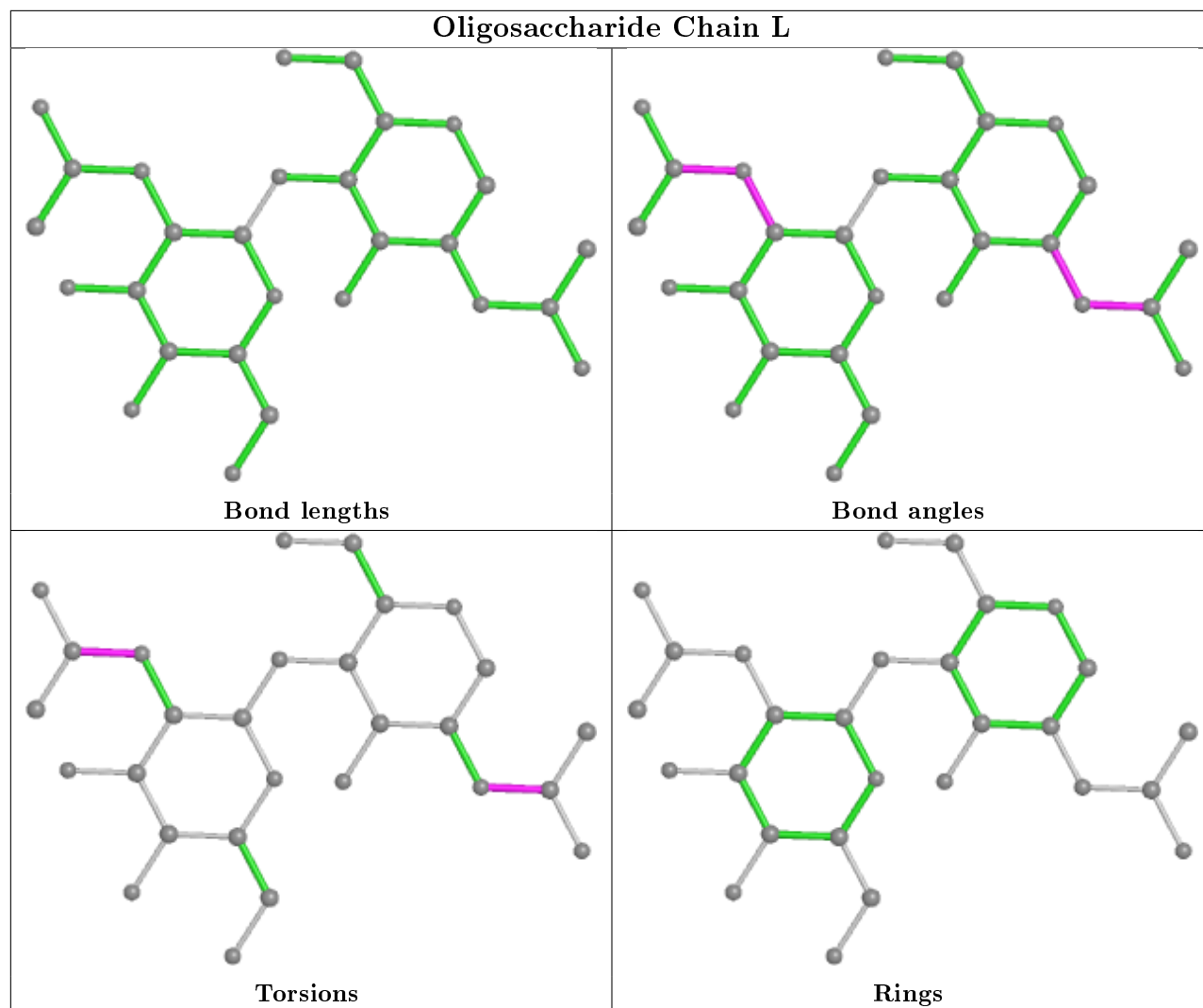


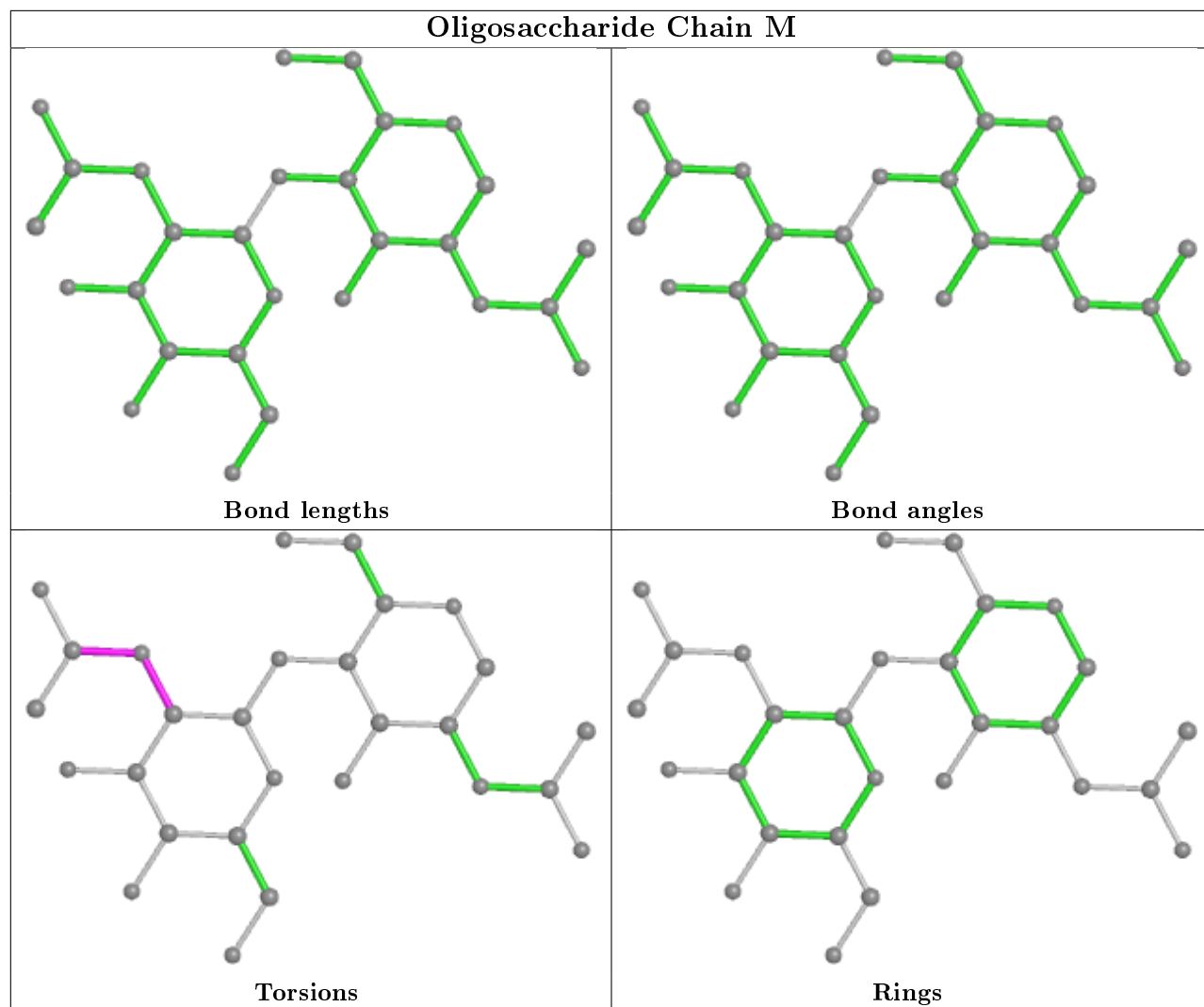


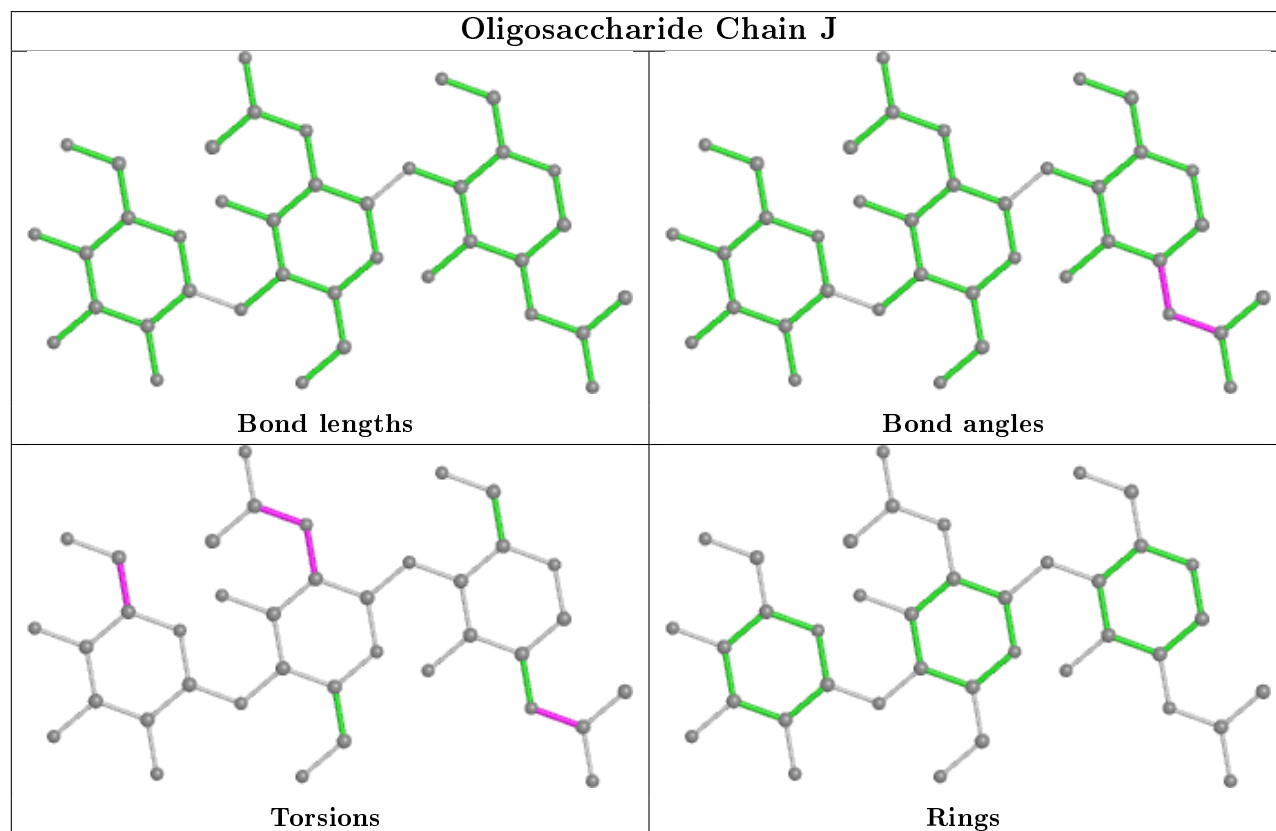
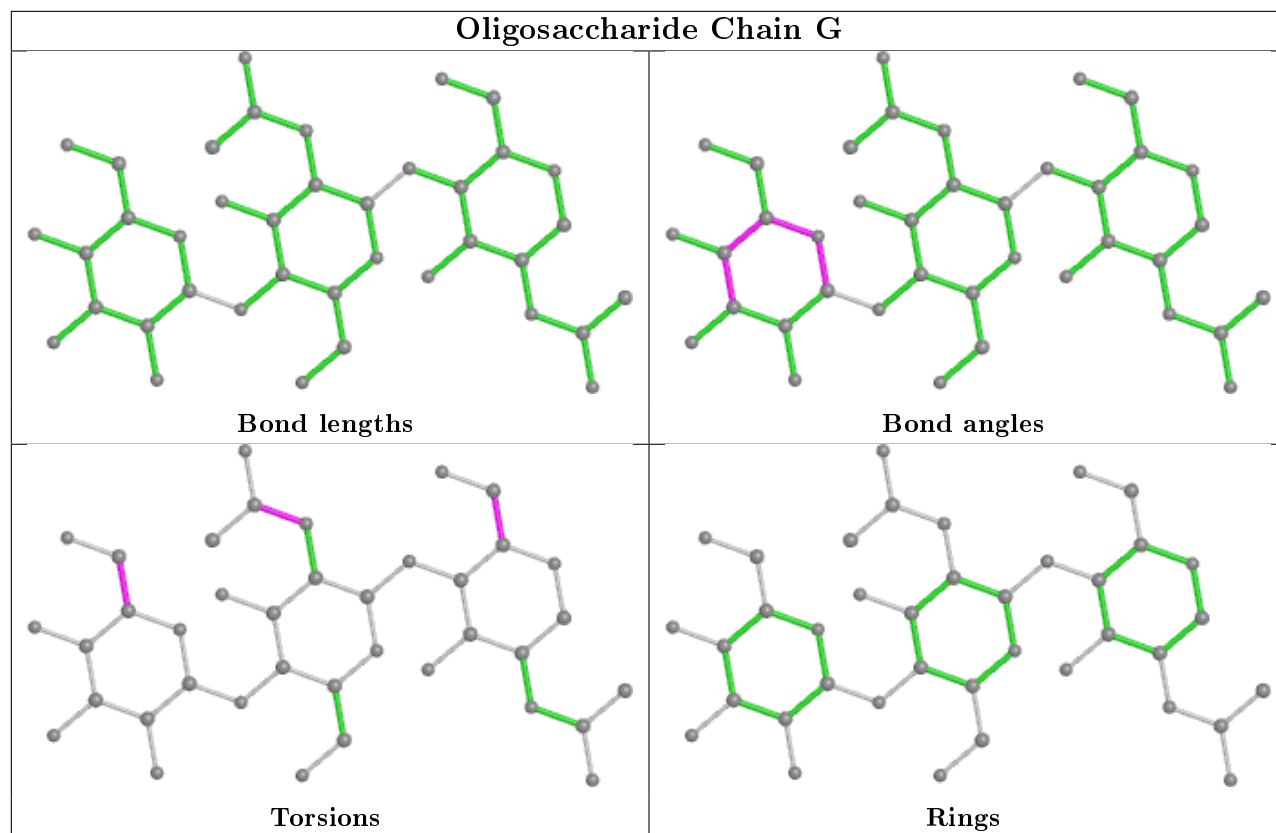












## 5.6 Ligand geometry

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	771(A)	1	14,14,15	0.58	0	17,19,21	0.62	0
4	NAG	B	772(A)	1	14,14,15	0.60	0	17,19,21	1.02	1 (5%)
4	NAG	C	768(A)	1	14,14,15	0.51	0	17,19,21	0.72	0
4	NAG	D	773(A)	1	14,14,15	0.57	0	17,19,21	0.84	1 (5%)
4	NAG	A	767(A)	1	14,14,15	0.58	0	17,19,21	0.56	0
4	NAG	A	768(A)	1	14,14,15	0.59	0	17,19,21	0.71	0
6	AES	C	801	1	8,12,13	2.02	4 (50%)	13,15,18	1.36	2 (15%)
5	SO4	C	1502	-	4,4,4	0.42	0	6,6,6	0.66	0
4	NAG	C	771(A)	1	14,14,15	0.48	0	17,19,21	0.89	0
4	NAG	C	770(A)	1	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
4	NAG	B	767(A)	1	14,14,15	0.59	0	17,19,21	0.68	0
4	NAG	D	767(A)	1	14,14,15	0.61	0	17,19,21	0.66	0
6	AES	B	801	1	8,12,13	2.15	4 (50%)	13,15,18	1.35	2 (15%)
4	NAG	A	772(A)	1	14,14,15	0.51	0	17,19,21	0.93	0
6	AES	D	801	1	8,12,13	2.21	4 (50%)	13,15,18	1.51	3 (23%)
4	NAG	C	769(A)	1	14,14,15	0.48	0	17,19,21	0.76	0
4	NAG	A	771(A)	1	14,14,15	0.53	0	17,19,21	0.70	0
5	SO4	D	1503	-	4,4,4	0.42	0	6,6,6	0.61	0
5	SO4	A	1500	-	4,4,4	0.49	0	6,6,6	0.67	0
5	SO4	B	1501	-	4,4,4	0.43	0	6,6,6	0.66	0
4	NAG	B	773(A)	1	14,14,15	0.55	0	17,19,21	0.65	0
4	NAG	C	767(A)	1	14,14,15	0.59	0	17,19,21	0.70	0
6	AES	A	801	1	8,12,13	2.25	4 (50%)	13,15,18	1.43	2 (15%)

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
4	NAG	A	768(A)	1	-	2/6/23/26	0/1/1/1
6	AES	C	801	1	-	0/7/7/9	0/1/1/1
6	AES	D	801	1	-	2/7/7/9	0/1/1/1
4	NAG	C	771(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	768(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	772(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	A	771(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	770(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	772(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	767(A)	1	-	3/6/23/26	0/1/1/1
4	NAG	D	773(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	D	767(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	767(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	767(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	B	773(A)	1	-	0/6/23/26	0/1/1/1
6	AES	A	801	1	-	2/7/7/9	0/1/1/1
6	AES	B	801	1	-	3/7/7/9	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	801	AES	C6-C1	4.05	1.44	1.38
6	B	801	AES	C6-C1	3.85	1.44	1.38
6	A	801	AES	C6-C1	3.71	1.44	1.38
6	C	801	AES	C6-C1	3.37	1.43	1.38
6	A	801	AES	C5-C6	3.13	1.44	1.38
6	D	801	AES	C5-C6	2.71	1.43	1.38
6	B	801	AES	C5-C6	2.56	1.43	1.38
6	A	801	AES	C5-C4	2.55	1.44	1.38
6	C	801	AES	C5-C6	2.48	1.43	1.38
6	A	801	AES	C2-C1	2.44	1.42	1.38
6	C	801	AES	C5-C4	2.40	1.44	1.38
6	C	801	AES	C2-C1	2.31	1.41	1.38
6	D	801	AES	C2-C1	2.30	1.41	1.38
6	B	801	AES	C5-C4	2.27	1.43	1.38
6	B	801	AES	C2-C1	2.18	1.41	1.38
6	D	801	AES	C5-C4	2.16	1.43	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	801	AES	O2S-S-C1	3.26	112.00	104.58
6	B	801	AES	O2S-S-C1	2.72	110.78	104.58
6	C	801	AES	C8-C7-C4	-2.59	106.90	112.85
6	A	801	AES	O2S-S-C1	2.58	110.46	104.58
6	C	801	AES	O2S-S-C1	2.57	110.44	104.58
4	C	770(A)	NAG	C2-N2-C7	-2.44	119.43	122.90
6	B	801	AES	C8-C7-C4	-2.35	107.46	112.85
4	D	773(A)	NAG	C2-N2-C7	-2.33	119.58	122.90
4	B	772(A)	NAG	C3-C4-C5	2.31	114.36	110.24
6	D	801	AES	C8-C7-C4	-2.16	107.89	112.85
6	D	801	AES	C6-C1-C2	-2.05	119.30	121.59
6	A	801	AES	C8-C7-C4	-2.02	108.22	112.85

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	768(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O7-C7-N2-C2
4	A	767(A)	NAG	C8-C7-N2-C2
4	A	767(A)	NAG	O7-C7-N2-C2
4	A	768(A)	NAG	C8-C7-N2-C2
4	A	768(A)	NAG	O7-C7-N2-C2
4	C	771(A)	NAG	C8-C7-N2-C2
4	C	771(A)	NAG	O7-C7-N2-C2
4	C	770(A)	NAG	C8-C7-N2-C2
4	C	770(A)	NAG	O7-C7-N2-C2
4	B	767(A)	NAG	C8-C7-N2-C2
4	B	767(A)	NAG	O7-C7-N2-C2
4	D	767(A)	NAG	C8-C7-N2-C2
4	D	767(A)	NAG	O7-C7-N2-C2
6	B	801	AES	C4-C7-C8-N8
4	A	771(A)	NAG	C8-C7-N2-C2
4	A	771(A)	NAG	O7-C7-N2-C2
4	B	772(A)	NAG	C8-C7-N2-C2
4	B	772(A)	NAG	O7-C7-N2-C2
4	C	767(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O5-C5-C6-O6
4	C	767(A)	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	768(A)	NAG	C4-C5-C6-O6
4	D	773(A)	NAG	C4-C5-C6-O6
4	A	771(A)	NAG	O5-C5-C6-O6
4	C	767(A)	NAG	O5-C5-C6-O6
4	D	767(A)	NAG	O5-C5-C6-O6
4	C	768(A)	NAG	O5-C5-C6-O6
4	A	771(A)	NAG	C4-C5-C6-O6
4	C	767(A)	NAG	C4-C5-C6-O6
4	B	767(A)	NAG	O5-C5-C6-O6
4	D	767(A)	NAG	C4-C5-C6-O6
6	B	801	AES	C2-C1-S-O2S
6	B	801	AES	C6-C1-S-O2S
6	D	801	AES	C2-C1-S-O2S
6	D	801	AES	C6-C1-S-O2S
6	A	801	AES	C2-C1-S-O2S
6	A	801	AES	C6-C1-S-O2S

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	773(A)	NAG	1	0
4	A	767(A)	NAG	1	0
6	C	801	AES	2	0
4	C	771(A)	NAG	1	0
4	C	770(A)	NAG	1	0
4	B	767(A)	NAG	1	0
4	D	767(A)	NAG	1	0
6	B	801	AES	1	0
6	D	801	AES	2	0
4	C	767(A)	NAG	1	0
6	A	801	AES	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	724/728 (99%)	0.08	29 (4%)	38	48	16, 30, 56, 99	13 (1%)
1	B	728/728 (100%)	-0.10	13 (1%)	68	76	16, 27, 50, 72	12 (1%)
1	C	723/728 (99%)	0.01	34 (4%)	31	41	16, 29, 56, 104	11 (1%)
1	D	728/728 (100%)	0.14	27 (3%)	41	51	18, 33, 61, 87	10 (1%)
All	All	2903/2912 (99%)	0.03	103 (3%)	44	53	16, 30, 56, 104	46 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	13.2
1	C	98	LEU	12.7
1	C	97	GLU	8.5
1	A	101	SER	8.4
1	D	83	TYR	8.3
1	B	39	SER	8.0
1	D	99	GLY	6.1
1	D	82	GLU	5.8
1	A	96	ASP	5.7
1	C	90	LEU	5.6
1	D	84	GLY	5.0
1	A	83	TYR	4.9
1	A	95	PHE	4.8
1	C	39	SER	4.6
1	B	83	TYR	4.5
1	C	73	GLU	4.5
1	A	93	SER	4.4
1	A	103	ASN	4.2
1	C	141	GLN	4.2
1	A	81	ALA	4.1
1	B	99	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	GLY	4.1
1	B	54	ARG	4.0
1	B	40	ARG	4.0
1	C	40	ARG	4.0
1	C	537	SER	3.9
1	A	39	SER	3.8
1	A	138	ASN	3.8
1	C	295	ILE	3.7
1	C	120	TYR	3.6
1	B	101	SER	3.6
1	C	766	PRO	3.6
1	A	74	ASN	3.5
1	A	102	THR	3.5
1	A	506	ASP	3.4
1	A	766	PRO	3.3
1	C	104	ASP	3.3
1	C	116	PHE	3.2
1	D	98	LEU	3.2
1	D	79	PHE	3.2
1	C	54	ARG	3.2
1	B	766	PRO	3.1
1	C	506	ASP	3.1
1	C	180	LEU	3.1
1	C	91	GLU	3.1
1	C	93	SER	3.1
1	A	72	GLN	3.1
1	B	142	LEU	3.1
1	B	616	MET	3.0
1	C	138	ASN	3.0
1	A	57	PHE	2.9
1	A	70	TYR	2.9
1	A	94	THR	2.9
1	C	74	ASN	2.9
1	A	90	LEU	2.7
1	D	88	ILE	2.7
1	C	140	ARG	2.7
1	D	436	LEU	2.7
1	D	295	ILE	2.7
1	D	484	SER	2.7
1	D	72	GLN	2.6
1	A	393	ASN	2.6
1	A	440	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	536	LYS	2.6
1	B	138	ASN	2.6
1	D	518	ASN	2.6
1	B	533	HIS	2.6
1	D	379	GLU	2.6
1	B	140	ARG	2.6
1	A	73	GLU	2.5
1	D	101	SER	2.5
1	C	92	ASN	2.4
1	D	537	SER	2.4
1	C	135	TYR	2.4
1	D	100	TYR	2.4
1	C	41	ARG	2.4
1	C	96	ASP	2.4
1	C	119	ASN	2.4
1	D	54	ARG	2.4
1	D	39	SER	2.3
1	A	79	PHE	2.3
1	D	677	GLU	2.3
1	D	502	LYS	2.3
1	A	179	ASN	2.2
1	C	139	LYS	2.2
1	D	437	ASN	2.2
1	B	143	ILE	2.2
1	A	54	ARG	2.2
1	D	187	TRP	2.2
1	C	535	ASP	2.2
1	C	53	PHE	2.2
1	C	520	HIS	2.1
1	D	505	GLN	2.1
1	A	208	PHE	2.1
1	D	57	PHE	2.1
1	A	666	TYR	2.1
1	C	214	LEU	2.1
1	A	91	GLU	2.0
1	D	547	TYR	2.0
1	C	533	HIS	2.0
1	A	388	GLN	2.0
1	D	96	ASP	2.0
1	D	498	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

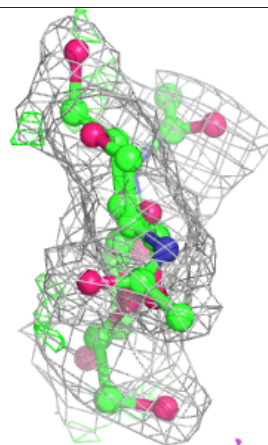
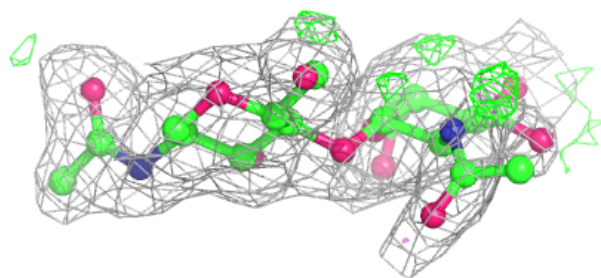
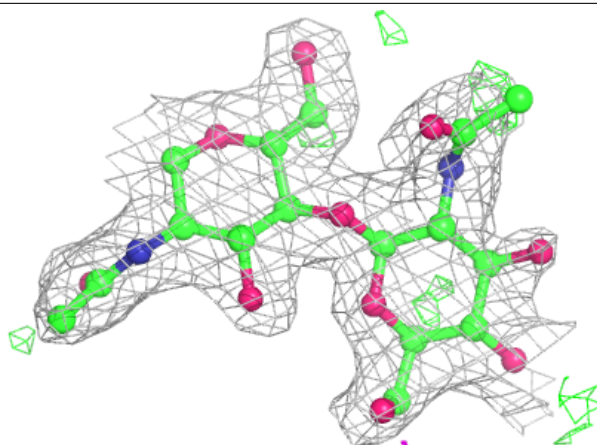
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	J	3	11/12	0.51	0.38	83,84,84,84	0
2	NAG	L	2	14/15	0.73	0.31	69,70,72,72	0
2	NAG	K	2	14/15	0.73	0.32	53,57,61,61	0
3	NAG	J	1	14/15	0.74	0.15	74,76,79,79	0
2	NAG	E	2	14/15	0.77	0.24	54,60,61,62	0
2	NAG	L	1	14/15	0.81	0.18	55,62,65,66	0
2	NAG	M	2	14/15	0.82	0.21	51,55,58,59	0
3	NAG	J	2	14/15	0.83	0.24	80,81,82,83	0
3	BMA	G	3	11/12	0.83	0.14	48,50,51,56	0
2	NAG	H	2	14/15	0.84	0.24	44,51,55,58	0
2	NAG	F	2	14/15	0.87	0.20	47,50,54,56	0
2	NAG	M	1	14/15	0.88	0.11	28,34,40,45	0
2	NAG	F	1	14/15	0.90	0.11	29,36,43,43	0
2	NAG	I	2	14/15	0.91	0.17	40,44,50,50	0
3	NAG	G	1	14/15	0.92	0.10	37,40,42,47	0
2	NAG	K	1	14/15	0.92	0.11	35,37,44,46	0
2	NAG	I	1	14/15	0.94	0.09	25,32,38,38	0
3	NAG	G	2	14/15	0.94	0.11	43,45,48,48	0
2	NAG	E	1	14/15	0.95	0.09	32,37,42,46	0
2	NAG	H	1	14/15	0.96	0.07	26,33,42,42	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.

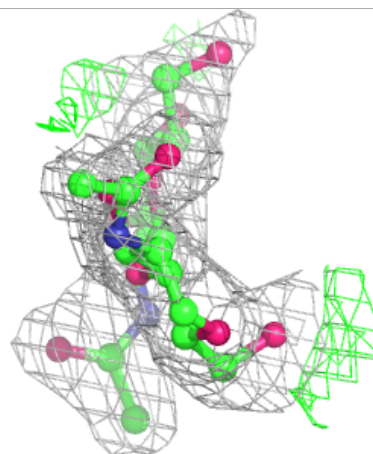
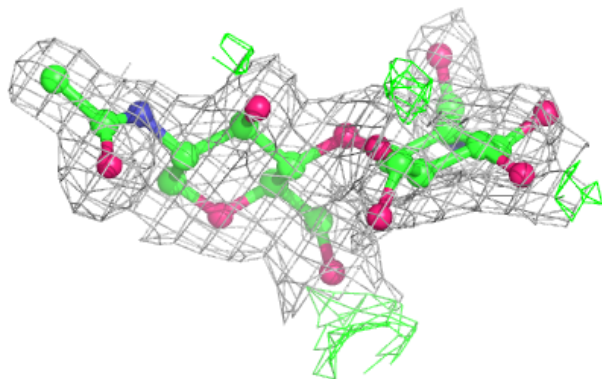
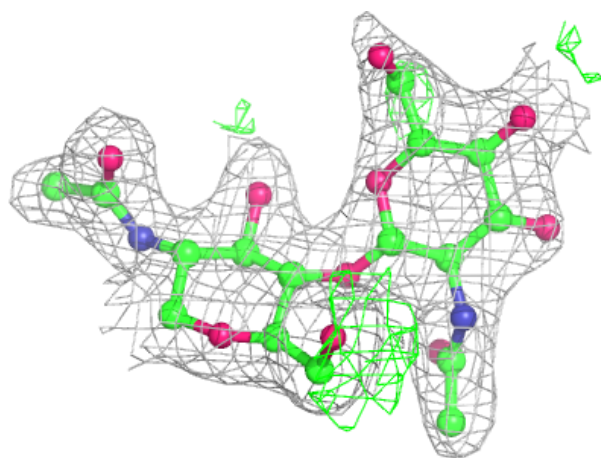
**Electron density around Chain E:**

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



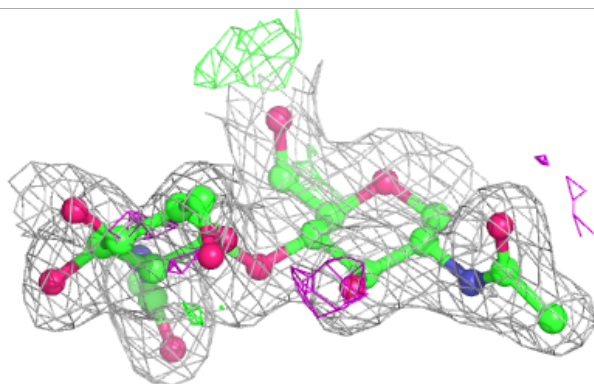
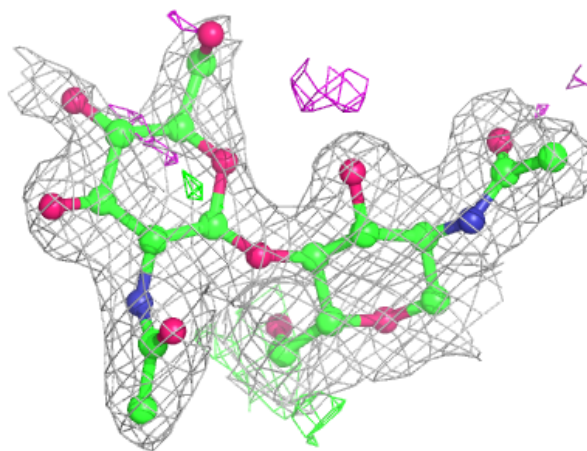
**Electron density around Chain F:**

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



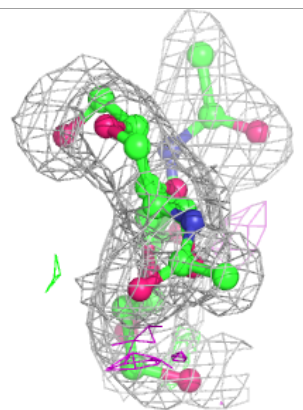
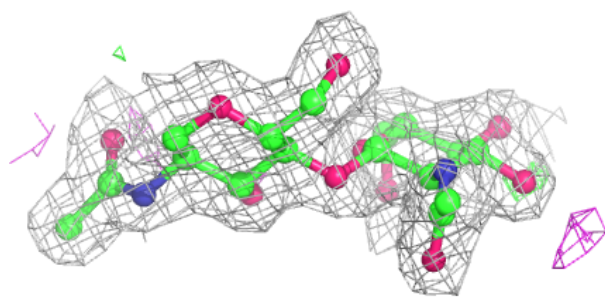
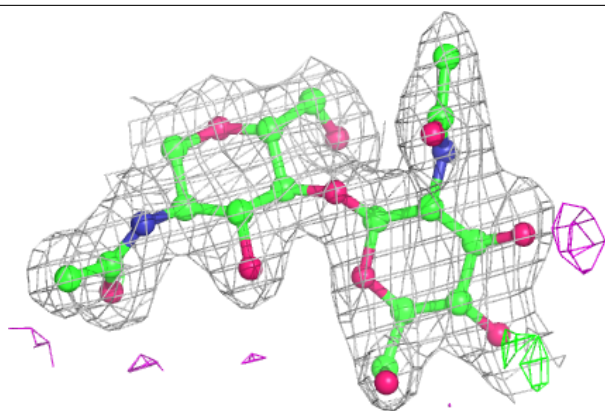
**Electron density around Chain H:**

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



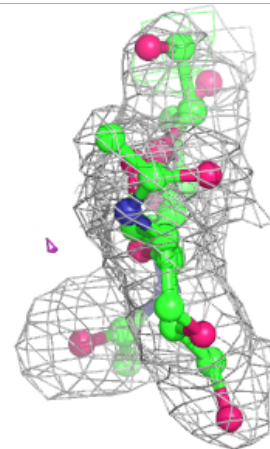
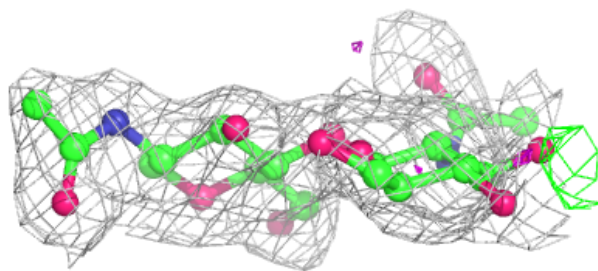
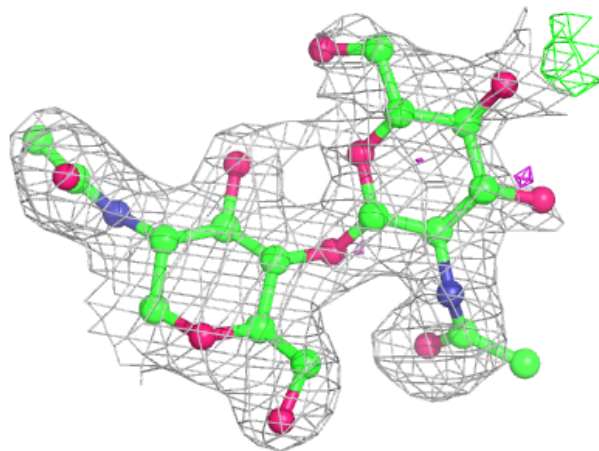
**Electron density around Chain I:**

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



**Electron density around Chain K:**

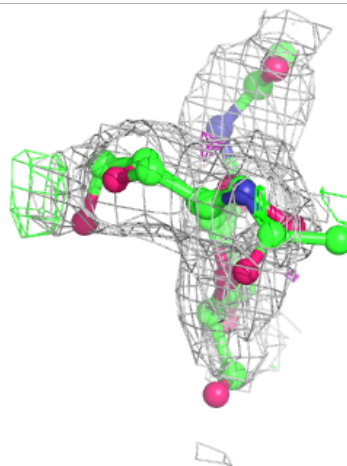
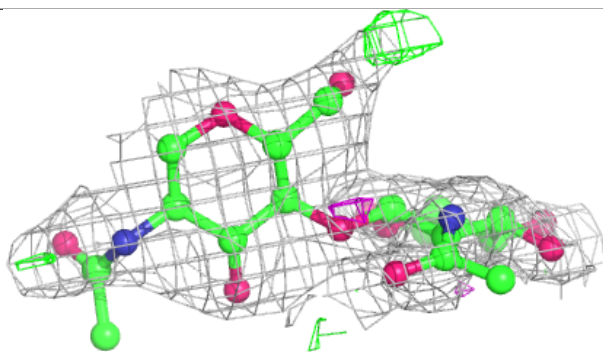
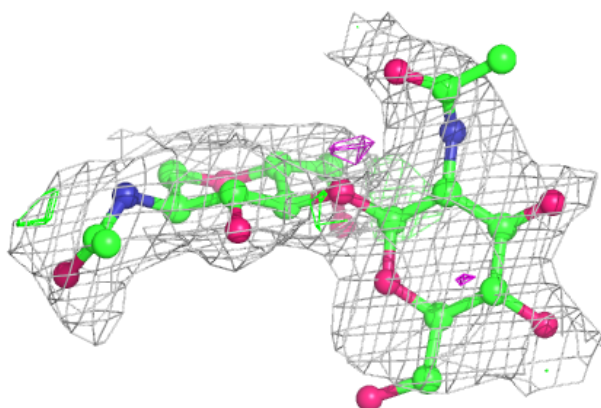
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





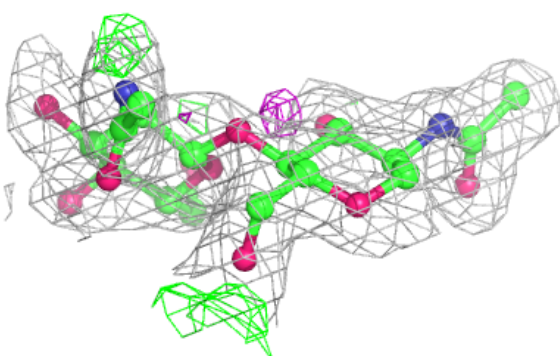
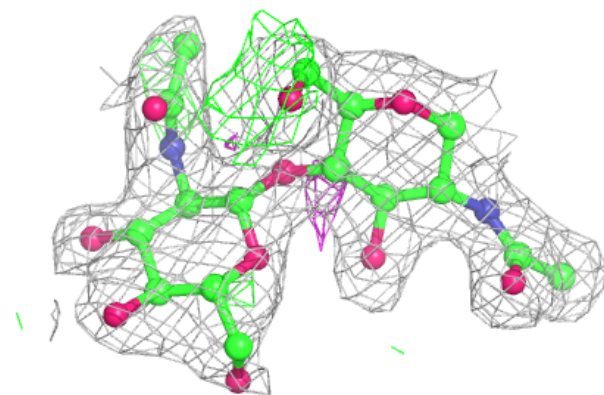
**Electron density around Chain L:**

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

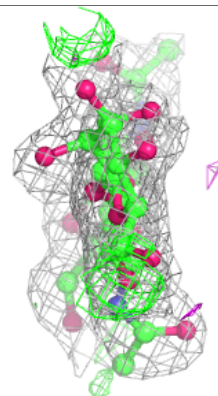
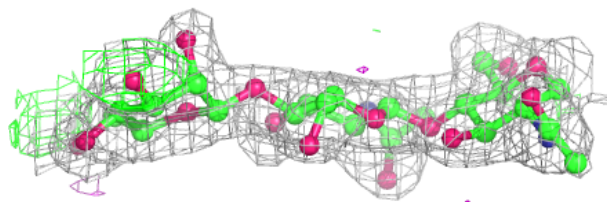
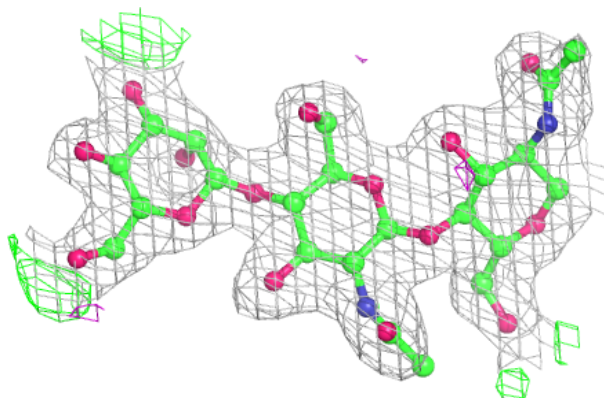


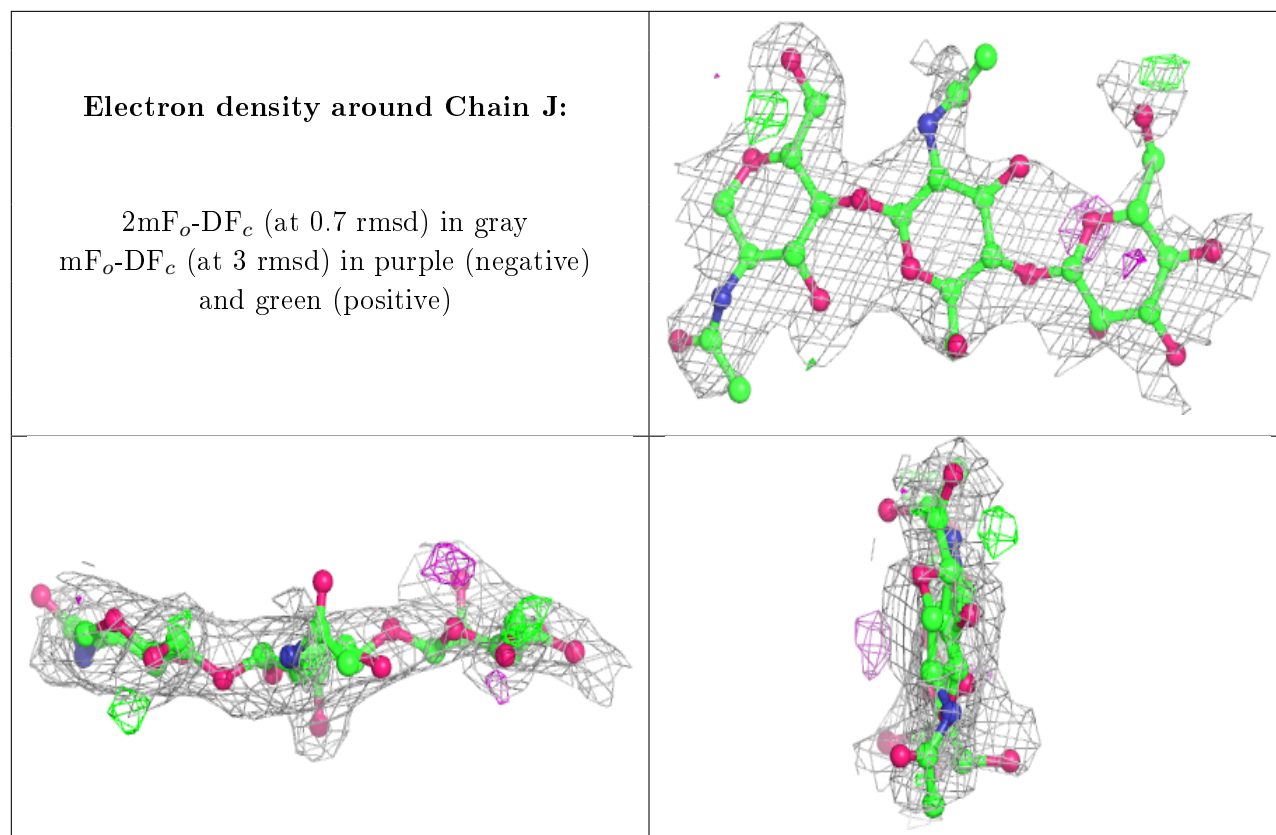
**Electron density around Chain M:**

$2mF_o-DF_c$  (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
4	NAG	D	767(A)	14/15	0.44	0.50	89,90,91,92	0
6	AES	D	801	12/13	0.51	0.35	63,67,69,69	0
4	NAG	C	768(A)	14/15	0.62	0.23	88,89,90,91	0
6	AES	B	801	12/13	0.65	0.26	48,55,59,61	0
6	AES	A	801	12/13	0.68	0.26	30,53,59,62	0
4	NAG	B	767(A)	14/15	0.69	0.28	68,70,73,73	0
6	AES	C	801	12/13	0.70	0.26	33,53,60,61	0
4	NAG	A	767(A)	14/15	0.70	0.33	81,83,84,84	0
4	NAG	D	773(A)	14/15	0.76	0.17	56,60,62,64	0
4	NAG	C	767(A)	14/15	0.78	0.16	60,63,65,65	0
4	NAG	A	768(A)	14/15	0.79	0.17	77,79,80,80	0
4	NAG	A	771(A)	14/15	0.81	0.14	49,52,54,54	3
4	NAG	C	770(A)	14/15	0.82	0.18	44,47,53,55	0
4	NAG	C	771(A)	14/15	0.82	0.14	43,48,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	772(A)	14/15	0.88	0.12	46,48,53,54	0
4	NAG	A	772(A)	14/15	0.89	0.12	41,44,51,53	0
4	NAG	B	771(A)	14/15	0.92	0.10	28,33,37,40	0
4	NAG	B	773(A)	14/15	0.93	0.11	36,40,45,48	0
4	NAG	C	769(A)	14/15	0.94	0.09	31,35,37,42	0
5	SO4	B	1501	5/5	0.97	0.08	29,30,32,32	0
5	SO4	D	1503	5/5	0.99	0.06	41,43,45,45	0
5	SO4	A	1500	5/5	0.99	0.08	33,35,35,36	0
5	SO4	C	1502	5/5	0.99	0.07	32,32,34,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.