



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:22 am GMT

PDB ID : 5NNJ  
Title : Dimer structure of Sortilin ectodomain crystal form 3, 4.0 Angstrom  
Authors : Leloup, N.O.L.; Janssen, B.J.C.  
Deposited on : 2017-04-09  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

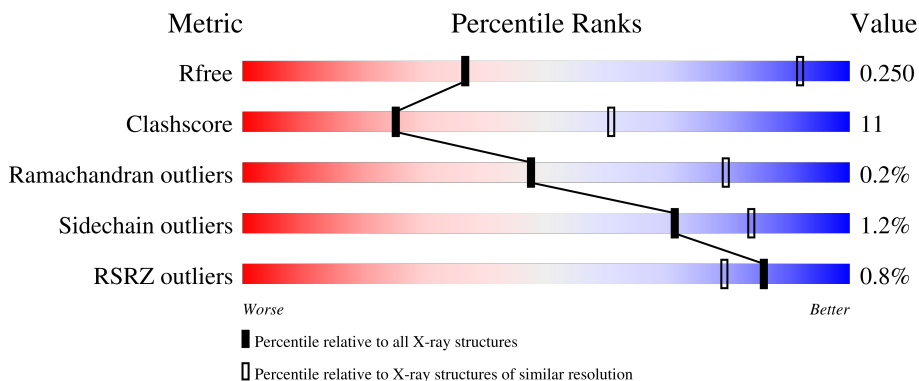
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.




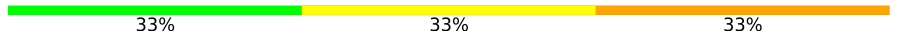
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	732	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 64%; height: 10px; background-color: green;"></div> <div style="width: 24%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
1	B	732	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 65%; height: 10px; background-color: green;"></div> <div style="width: 23%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
1	C	732	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 68%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	D	732	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 65%; height: 10px; background-color: green;"></div> <div style="width: 23%; height: 10px; background-color: yellow;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
2	E	3	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 33%; height: 10px; background-color: yellow;"></div> <div style="width: 67%; height: 10px; background-color: orange;"></div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	3	 33% 67%
2	G	3	 33% 33% 33%
2	H	3	 33% 67%
2	I	3	 33% 33% 33%
2	J	3	 67% 33%
2	K	3	 33% 67%
2	L	3	 67% 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
2	BMA	G	3	-	-	-	X
2	BMA	I	3	-	-	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20730 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	648	5094	3220	855	990	29	0	0	0
1	B	648	5094	3220	855	990	29	0	0	0
1	D	648	5094	3220	855	990	29	0	0	0
1	C	646	5080	3213	853	986	28	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

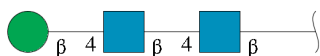
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	ALA	-	expression tag	UNP Q6PHU5
A	724	ALA	-	expression tag	UNP Q6PHU5
A	725	ALA	-	expression tag	UNP Q6PHU5
A	726	HIS	-	expression tag	UNP Q6PHU5
A	727	HIS	-	expression tag	UNP Q6PHU5
A	728	HIS	-	expression tag	UNP Q6PHU5
A	729	HIS	-	expression tag	UNP Q6PHU5
A	730	HIS	-	expression tag	UNP Q6PHU5
A	731	HIS	-	expression tag	UNP Q6PHU5
B	723	ALA	-	expression tag	UNP Q6PHU5
B	724	ALA	-	expression tag	UNP Q6PHU5
B	725	ALA	-	expression tag	UNP Q6PHU5
B	726	HIS	-	expression tag	UNP Q6PHU5
B	727	HIS	-	expression tag	UNP Q6PHU5
B	728	HIS	-	expression tag	UNP Q6PHU5
B	729	HIS	-	expression tag	UNP Q6PHU5
B	730	HIS	-	expression tag	UNP Q6PHU5
B	731	HIS	-	expression tag	UNP Q6PHU5
D	723	ALA	-	expression tag	UNP Q6PHU5
D	724	ALA	-	expression tag	UNP Q6PHU5
D	725	ALA	-	expression tag	UNP Q6PHU5

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	726	HIS	-	expression tag	UNP Q6PHU5
D	727	HIS	-	expression tag	UNP Q6PHU5
D	728	HIS	-	expression tag	UNP Q6PHU5
D	729	HIS	-	expression tag	UNP Q6PHU5
D	730	HIS	-	expression tag	UNP Q6PHU5
D	731	HIS	-	expression tag	UNP Q6PHU5
C	723	ALA	-	expression tag	UNP Q6PHU5
C	724	ALA	-	expression tag	UNP Q6PHU5
C	725	ALA	-	expression tag	UNP Q6PHU5
C	726	HIS	-	expression tag	UNP Q6PHU5
C	727	HIS	-	expression tag	UNP Q6PHU5
C	728	HIS	-	expression tag	UNP Q6PHU5
C	729	HIS	-	expression tag	UNP Q6PHU5
C	730	HIS	-	expression tag	UNP Q6PHU5
C	731	HIS	-	expression tag	UNP Q6PHU5

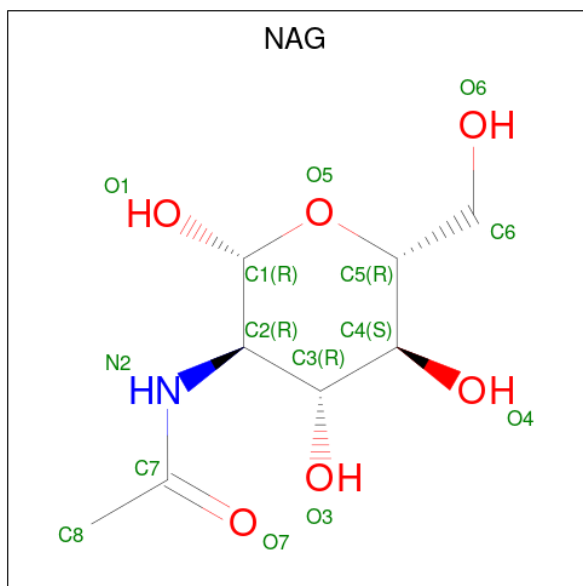
- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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>).

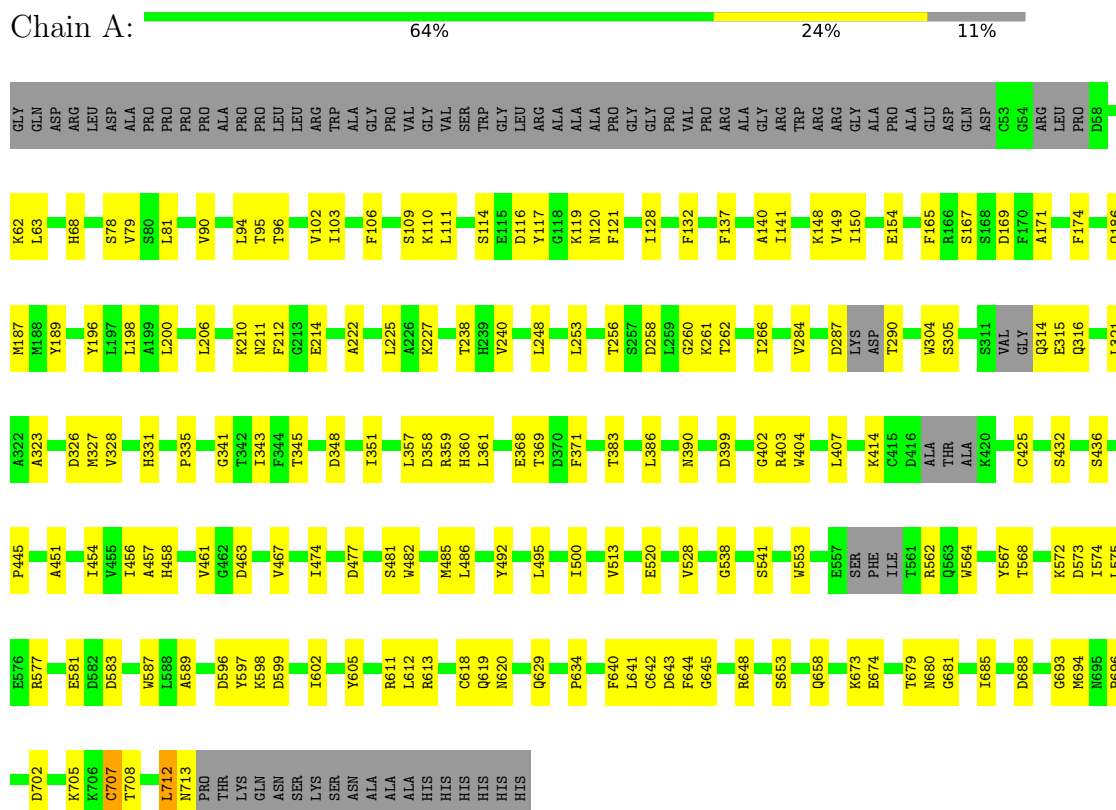


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	8	1	5	0	0
3	B	1	Total 14	8	1	5	0	0
3	D	1	Total 14	8	1	5	0	0
3	C	1	Total 14	8	1	5	0	0

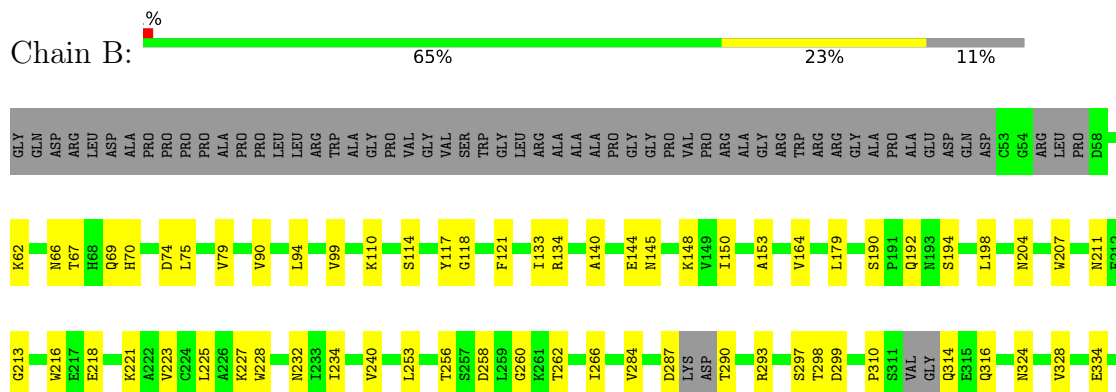
### 3 Residue-property plots

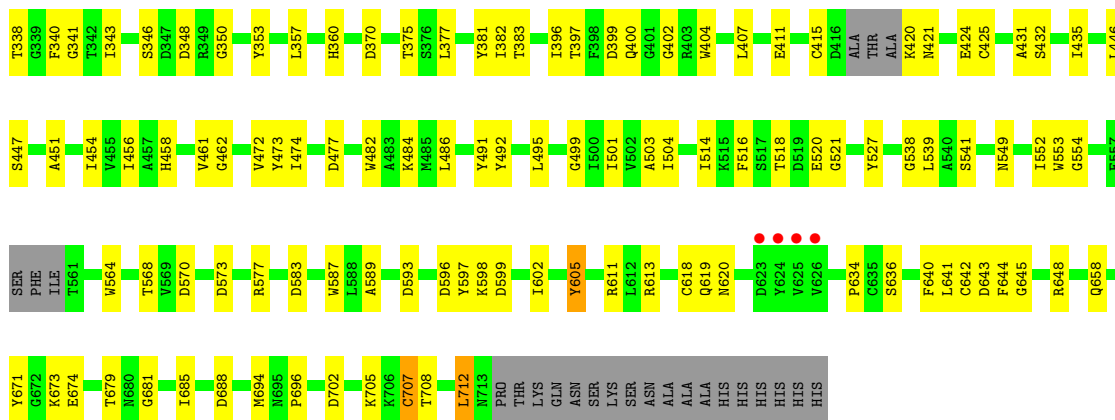
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Sortilin

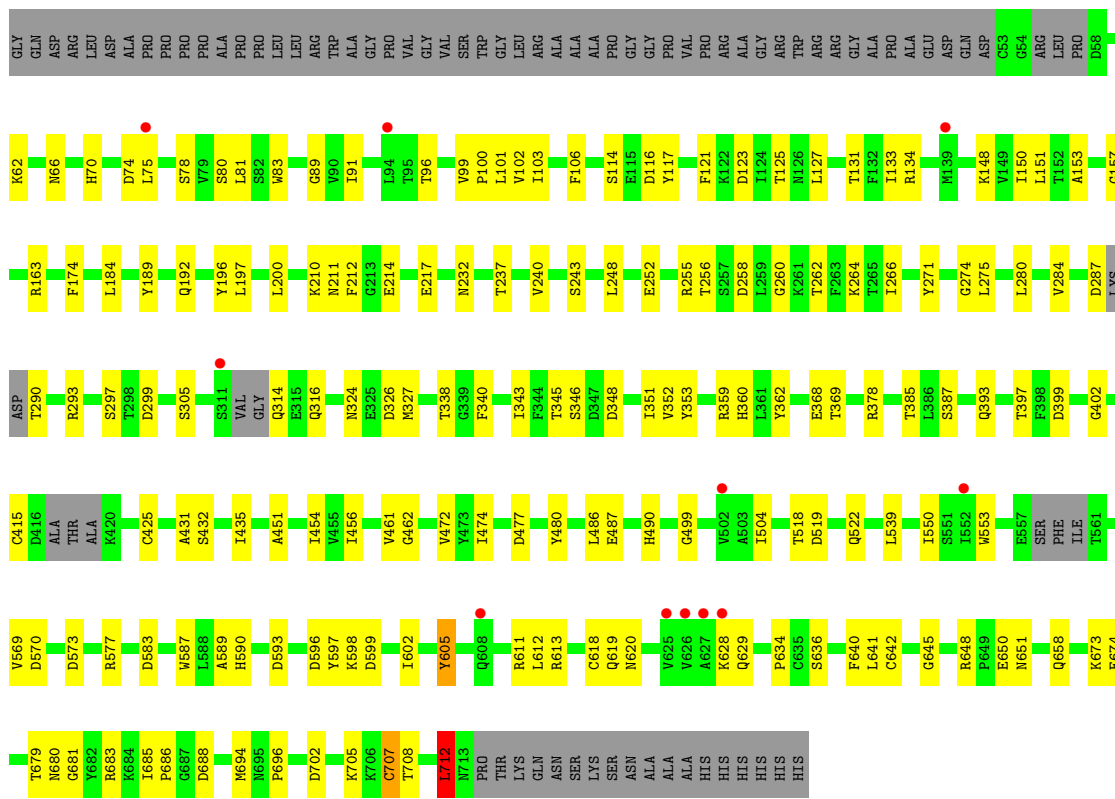


#### • Molecule 1: Sortilin

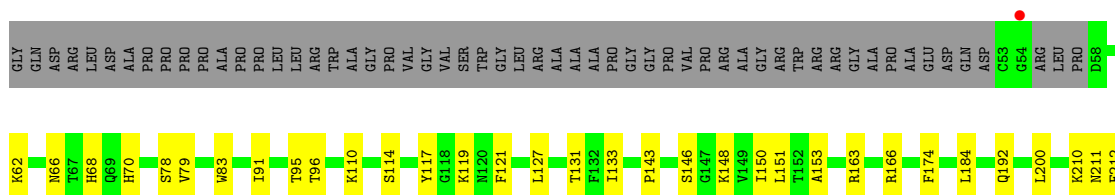




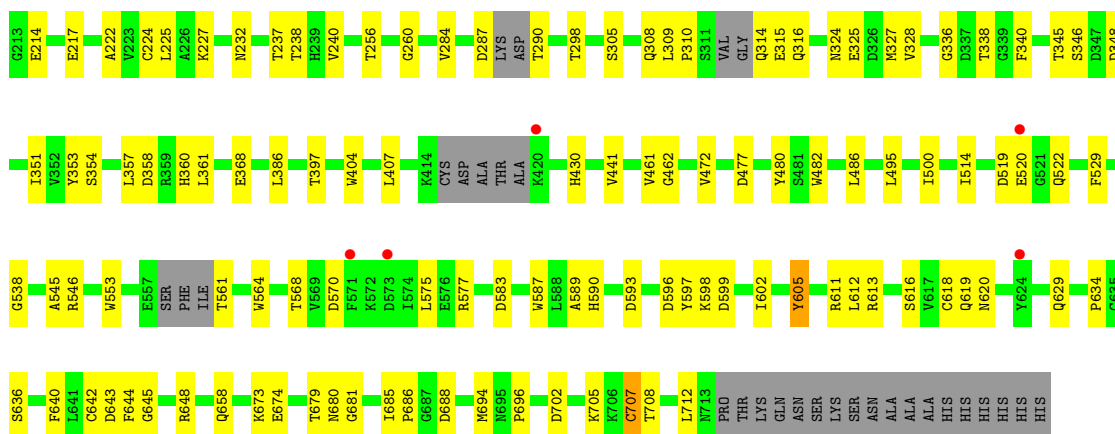
● Molecule 1: Sortilin



● Molecule 1: Sortilin







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



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



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



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

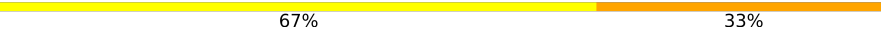


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain J:  67% 33%




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

Chain K:  33% 67%



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

Chain L:  67% 33%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.32Å 151.82Å 162.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.72 – 4.00 71.72 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.72-4.00) 99.8 (71.72-4.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 4.01Å)	Xtrriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, $R_{free}$	0.186 , 0.250 0.186 , 0.250	Depositor DCC
$R_{free}$ test set	1433 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	155.7	Xtrriage
Anisotropy	0.477	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 139.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.029 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	202.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.50	0/5212	0.66	0/7055
1	B	0.47	0/5212	0.63	0/7055
1	C	0.47	1/5198 (0.0%)	0.61	0/7036
1	D	0.47	1/5212 (0.0%)	0.60	0/7055
All	All	0.48	2/20834 (0.0%)	0.63	0/28201

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	712	LEU	C-N	11.16	1.59	1.34
1	C	561	THR	C-N	8.39	1.53	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5094	0	4871	123	3
1	B	5094	0	4871	115	0
1	C	5080	0	4864	89	2
1	D	5094	0	4871	107	0
2	E	39	0	34	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	39	0	34	5	0
2	G	39	0	34	6	0
2	H	39	0	34	4	0
2	I	39	0	34	1	0
2	J	39	0	34	3	0
2	K	39	0	33	4	1
2	L	39	0	34	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	4	0
All	All	20730	0	19800	434	3

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 11.

All (434) 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:D:651:ASN:ND2	3:D:807:NAG:C1	1.70	1.50
1:B:298:THR:OG1	1:D:629:GLN:NE2	1.90	1.04
1:D:570:ASP:HB2	2:J:1:NAG:H82	1.47	0.96
2:H:1:NAG:H62	2:H:2:NAG:HN2	1.35	0.90
1:B:298:THR:HG1	1:D:629:GLN:NE2	1.71	0.89
1:C:472:VAL:HB	1:C:486:LEU:HB2	1.54	0.88
1:D:570:ASP:HB2	2:J:1:NAG:C8	2.06	0.85
1:A:513:VAL:HG22	1:A:528:VAL:HG22	1.60	0.84
1:B:375:THR:HA	2:G:1:NAG:O6	1.79	0.83
1:D:192:GLN:HB3	1:D:232:ASN:OD1	1.81	0.79
1:B:598:LYS:NZ	1:B:634:PRO:O	2.18	0.76
1:D:651:ASN:CG	3:D:807:NAG:C1	2.54	0.75
1:C:325:GLU:HG2	2:K:2:NAG:H81	1.69	0.75
1:A:598:LYS:NZ	1:A:634:PRO:O	2.18	0.74
1:D:598:LYS:NZ	1:D:634:PRO:O	2.18	0.74
1:C:598:LYS:NZ	1:C:634:PRO:O	2.18	0.74
1:A:225:LEU:HD21	1:A:227:LYS:HE3	1.69	0.74
1:A:707:CYS:SG	1:A:708:THR:N	2.62	0.73
2:H:1:NAG:H62	2:H:2:NAG:N2	2.04	0.72
1:B:707:CYS:SG	1:B:708:THR:N	2.62	0.72
1:A:572:LYS:NZ	2:F:2:NAG:H81	2.05	0.72
1:D:148:LYS:HD2	1:D:212:PHE:CE1	2.25	0.72

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:HB2	1:C:290:THR:HG22	1.70	0.72
1:D:707:CYS:SG	1:D:708:THR:N	2.62	0.71
1:C:707:CYS:SG	1:C:708:THR:N	2.62	0.71
1:D:210:LYS:HE2	1:D:217:GLU:OE1	1.90	0.71
1:C:324:ASN:HB2	2:K:2:NAG:H82	1.71	0.71
1:B:504:ILE:HD12	1:B:539:LEU:HD22	1.73	0.71
1:D:184:LEU:HD23	1:D:200:LEU:HD23	1.73	0.71
1:D:287:ASP:HB2	1:D:290:THR:HG22	1.72	0.70
1:C:310:PRO:HD3	1:C:644:PHE:CE1	2.26	0.70
1:C:127:LEU:HD21	1:C:174:PHE:HB2	1.74	0.70
1:C:225:LEU:HD21	1:C:227:LYS:HE3	1.72	0.70
1:A:321:LEU:HD11	1:A:331:HIS:HB2	1.74	0.70
1:D:451:ALA:HB1	1:D:454:ILE:HD12	1.74	0.69
1:A:425:CYS:HA	1:A:461:VAL:HG13	1.75	0.68
1:D:651:ASN:ND2	3:D:807:NAG:C2	2.55	0.68
1:D:66:ASN:HB3	1:D:570:ASP:HB3	1.77	0.67
1:C:712:LEU:HD12	1:C:712:LEU:O	1.96	0.66
1:A:304:TRP:CG	1:A:712:LEU:HD11	2.31	0.66
1:B:287:ASP:HB2	1:B:290:THR:HA	1.78	0.66
1:B:456:ILE:HD12	1:B:474:ILE:HD11	1.77	0.65
1:A:316:GLN:HE21	1:A:335:PRO:HD3	1.63	0.64
1:A:327:MET:HE3	1:A:345:THR:HB	1.81	0.63
1:B:324:ASN:HD22	2:G:1:NAG:H81	1.63	0.63
1:B:297:SER:OG	1:B:299:ASP:OD1	2.18	0.62
1:C:192:GLN:HB3	1:C:232:ASN:OD1	1.99	0.62
1:D:258:ASP:OD2	1:D:262:THR:OG1	2.12	0.62
1:D:324:ASN:HB3	2:I:1:NAG:O7	2.00	0.62
1:A:148:LYS:HB3	1:A:212:PHE:CE1	2.35	0.62
1:B:570:ASP:OD2	2:H:1:NAG:O6	2.17	0.61
1:C:287:ASP:HB2	1:C:290:THR:HA	1.82	0.61
1:D:345:THR:O	1:D:353:TYR:HA	2.00	0.61
1:D:297:SER:OG	1:D:299:ASP:OD1	2.19	0.61
1:A:258:ASP:OD2	1:A:262:THR:OG1	2.15	0.61
1:A:287:ASP:HB2	1:A:290:THR:HG22	1.81	0.60
1:B:407:LEU:HD11	1:B:482:TRP:HE1	1.67	0.60
1:D:369:THR:O	1:D:432:SER:HB2	2.01	0.60
1:D:402:GLY:O	1:D:648:ARG:NH1	2.35	0.60
1:C:361:LEU:HD21	1:C:386:LEU:HB2	1.84	0.59
1:D:62:LYS:O	1:D:66:ASN:ND2	2.35	0.59
1:A:137:PHE:O	1:A:186:GLN:NE2	2.32	0.59
1:D:674:GLU:HG3	1:D:705:LYS:HB2	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:TYR:CD2	1:D:628:LYS:HE2	2.38	0.59
1:B:287:ASP:HB2	1:B:290:THR:HG22	1.83	0.59
1:A:674:GLU:HG3	1:A:705:LYS:HB2	1.85	0.59
1:C:256:THR:HG21	1:C:260:GLY:N	2.17	0.59
1:C:310:PRO:HD3	1:C:644:PHE:HE1	1.67	0.58
1:C:674:GLU:HG3	1:C:705:LYS:HB2	1.85	0.58
1:A:694:MET:HG2	1:A:696:PRO:HD3	1.86	0.58
1:A:359:ARG:NE	1:A:386:LEU:O	2.33	0.58
1:B:674:GLU:HG3	1:B:705:LYS:HB2	1.85	0.58
1:B:425:CYS:HA	1:B:461:VAL:HG13	1.84	0.58
1:C:66:ASN:HB3	1:C:570:ASP:HB3	1.86	0.58
1:A:495:LEU:HD23	1:A:541:SER:OG	2.04	0.58
1:C:694:MET:HG2	1:C:696:PRO:HD3	1.86	0.58
1:B:324:ASN:ND2	2:G:1:NAG:H81	2.19	0.58
2:E:1:NAG:O6	2:E:2:NAG:O5	2.19	0.58
1:A:477:ASP:OD2	1:A:481:SER:OG	2.09	0.58
1:A:117:TYR:O	1:A:568:THR:HG21	2.04	0.57
1:A:256:THR:HG21	1:A:260:GLY:N	2.19	0.57
2:G:1:NAG:H3	2:G:1:NAG:H83	1.87	0.57
1:B:117:TYR:O	1:B:568:THR:HG21	2.04	0.57
1:D:274:GLY:O	1:D:280:LEU:HD12	2.04	0.57
1:D:519:ASP:OD2	1:D:522:GLN:HB2	2.04	0.57
1:A:538:GLY:HA3	1:A:553:TRP:CZ2	2.39	0.57
1:D:694:MET:HG2	1:D:696:PRO:HD3	1.86	0.57
1:B:99:VAL:O	1:B:134:ARG:NH1	2.37	0.57
1:A:572:LYS:HZ2	2:F:2:NAG:H81	1.69	0.57
1:B:383:THR:HG22	1:B:404:TRP:CZ3	2.39	0.57
1:C:545:ALA:O	1:C:546:ARG:HD3	2.05	0.57
1:C:305:SER:HB3	1:C:351:ILE:HD12	1.86	0.56
1:B:225:LEU:HD21	1:B:227:LYS:HE3	1.87	0.56
1:B:673:LYS:HD3	1:B:702:ASP:OD2	2.06	0.56
1:B:694:MET:HG2	1:B:696:PRO:HD3	1.86	0.56
1:A:673:LYS:HD3	1:A:702:ASP:OD2	2.06	0.56
1:C:673:LYS:HD3	1:C:702:ASP:OD2	2.06	0.56
1:D:211:ASN:ND2	1:D:214:GLU:HB3	2.21	0.56
1:C:222:ALA:O	1:C:238:THR:HA	2.06	0.56
1:D:106:PHE:CE1	1:D:157:GLY:HA2	2.41	0.56
1:D:123:ASP:OD1	1:D:125:THR:OG1	2.17	0.55
1:D:593:ASP:OD2	1:D:636:SER:OG	2.17	0.55
1:D:673:LYS:HD3	1:D:702:ASP:OD2	2.06	0.55
1:B:334:GLU:HG3	1:B:340:PHE:CE1	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:HB2	1:A:121:PHE:CD2	2.41	0.55
1:A:287:ASP:HB2	1:A:290:THR:HA	1.88	0.55
1:B:314:GLN:O	1:B:316:GLN:HG3	2.06	0.55
1:B:399:ASP:N	1:B:399:ASP:OD1	2.39	0.55
1:C:211:ASN:ND2	1:C:214:GLU:HB3	2.22	0.55
1:A:150:ILE:HG21	1:A:187:MET:HG3	1.88	0.55
1:B:685:ILE:HB	1:B:688:ASP:HB2	1.89	0.55
1:D:343:ILE:HD11	1:D:360:HIS:CE1	2.42	0.55
1:C:131:THR:HG21	1:C:163:ARG:HD2	1.90	0.54
1:C:461:VAL:HG12	1:C:462:GLY:H	1.71	0.54
1:B:90:VAL:HA	1:B:114:SER:O	2.07	0.54
1:C:685:ILE:HB	1:C:688:ASP:HB2	1.89	0.54
1:A:500:ILE:HD11	1:A:575:LEU:HD12	1.90	0.54
1:B:357:LEU:HD22	1:B:404:TRP:CD2	2.41	0.54
1:D:133:ILE:HD13	1:D:153:ALA:HB2	1.89	0.54
1:C:95:THR:HB	1:C:110:LYS:H	1.71	0.54
1:B:451:ALA:HB1	1:B:454:ILE:HD12	1.89	0.54
1:C:210:LYS:HE2	1:C:217:GLU:OE1	2.08	0.54
1:A:368:GLU:OE1	1:A:368:GLU:N	2.40	0.54
1:A:685:ILE:HB	1:A:688:ASP:HB2	1.89	0.54
1:A:679:THR:OG1	1:A:681:GLY:N	2.37	0.54
1:D:255:ARG:HB2	1:D:266:ILE:HD13	1.90	0.54
1:D:685:ILE:HB	1:D:688:ASP:HB2	1.89	0.54
1:D:81:LEU:HB3	1:D:553:TRP:CZ3	2.43	0.53
1:D:650:GLU:OE2	3:D:807:NAG:N2	2.42	0.53
1:B:593:ASP:OD2	1:B:636:SER:OG	2.17	0.53
1:B:256:THR:HG21	1:B:260:GLY:N	2.24	0.53
1:B:402:GLY:HA2	1:B:641:LEU:HD23	1.89	0.53
1:D:402:GLY:HA2	1:D:641:LEU:HD23	1.90	0.53
1:A:369:THR:O	1:A:432:SER:HB2	2.09	0.52
1:B:538:GLY:HA3	1:B:553:TRP:CZ2	2.43	0.52
1:A:458:HIS:CE1	1:A:492:TYR:HE2	2.27	0.52
1:A:572:LYS:HZ3	2:F:2:NAG:H81	1.74	0.52
1:A:102:VAL:HG23	1:A:103:ILE:HD12	1.92	0.52
1:B:679:THR:OG1	1:B:681:GLY:N	2.37	0.52
1:D:284:VAL:HG21	1:D:712:LEU:HD23	1.90	0.52
1:C:357:LEU:HD12	1:C:358:ASP:N	2.25	0.52
1:B:69:GLN:HG2	1:B:70:HIS:N	2.24	0.52
1:A:62:LYS:HD2	1:A:573:ASP:HB3	1.92	0.52
1:A:68:HIS:O	1:A:567:TYR:HA	2.09	0.52
1:C:324:ASN:HB3	2:K:1:NAG:C7	2.39	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:THR:OG1	1:C:681:GLY:N	2.37	0.52
1:A:78:SER:HB2	1:A:96:THR:OG1	2.10	0.52
1:D:74:ASP:O	1:D:75:LEU:HD23	2.09	0.52
1:A:451:ALA:HB1	1:A:454:ILE:HD12	1.92	0.51
1:D:62:LYS:HD2	1:D:573:ASP:HB3	1.92	0.51
1:C:62:LYS:O	1:C:66:ASN:ND2	2.43	0.51
1:B:293:ARG:NH2	1:B:314:GLN:HA	2.24	0.51
1:A:343:ILE:HD11	1:A:360:HIS:CE1	2.45	0.51
1:B:324:ASN:HB3	2:G:1:NAG:O7	2.10	0.51
1:B:504:ILE:HG12	1:B:514:ILE:HD13	1.92	0.51
1:A:68:HIS:CD2	2:F:1:NAG:H81	2.45	0.51
1:A:106:PHE:HE2	1:B:421:ASN:HD22	1.59	0.51
1:A:148:LYS:HD2	1:A:212:PHE:CE1	2.46	0.51
1:D:196:TYR:O	1:D:197:LEU:HD23	2.11	0.51
1:B:421:ASN:HB3	1:B:424:GLU:HB2	1.92	0.50
1:B:499:GLY:O	1:B:518:THR:HA	2.11	0.50
1:D:679:THR:OG1	1:D:681:GLY:N	2.37	0.50
1:C:83:TRP:CH2	1:C:91:ILE:HD11	2.46	0.50
1:C:519:ASP:HB3	1:C:616:SER:H	1.76	0.50
1:C:224:CYS:HB2	1:C:237:THR:OG1	2.11	0.50
1:A:304:TRP:CB	1:A:712:LEU:HD11	2.42	0.50
1:A:458:HIS:CE1	1:A:492:TYR:CE2	3.00	0.50
1:B:491:TYR:O	1:B:503:ALA:HA	2.12	0.50
1:D:127:LEU:HD21	1:D:174:PHE:HB2	1.94	0.49
1:D:583:ASP:O	1:D:613:ARG:HG3	2.12	0.49
1:C:284:VAL:HG21	1:C:712:LEU:HD23	1.93	0.49
1:A:148:LYS:HB3	1:A:212:PHE:HE1	1.78	0.49
1:B:148:LYS:HE3	1:B:194:SER:OG	2.12	0.49
1:A:314:GLN:O	1:A:316:GLN:HG3	2.12	0.49
1:D:425:CYS:HA	1:D:461:VAL:HG13	1.94	0.49
1:C:645:GLY:O	1:C:658:GLN:HG3	2.13	0.49
1:A:645:GLY:O	1:A:658:GLN:HG3	2.13	0.49
1:D:83:TRP:CZ2	1:D:91:ILE:HD11	2.47	0.49
1:B:334:GLU:HG2	1:B:341:GLY:HA2	1.93	0.49
1:D:131:THR:HG21	1:D:163:ARG:HD2	1.94	0.49
1:D:645:GLY:O	1:D:658:GLN:HG3	2.12	0.49
1:A:425:CYS:HA	1:A:461:VAL:CG1	2.43	0.49
1:A:583:ASP:O	1:A:613:ARG:HG3	2.12	0.49
1:C:593:ASP:OD2	1:C:636:SER:OG	2.17	0.49
1:A:114:SER:HB2	1:A:121:PHE:CE2	2.48	0.49
1:D:399:ASP:N	1:D:399:ASP:OD1	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ILE:HD12	1:B:521:GLY:N	2.28	0.49
1:B:645:GLY:O	1:B:658:GLN:HG3	2.13	0.49
1:D:326:ASP:O	1:D:348:ASP:HA	2.12	0.49
1:C:166:ARG:HD2	1:C:212:PHE:O	2.13	0.49
1:C:583:ASP:O	1:C:613:ARG:HG3	2.13	0.49
1:B:118:GLY:HA3	1:B:568:THR:OG1	2.13	0.48
1:B:504:ILE:CD1	1:B:539:LEU:HD22	2.41	0.48
1:D:522:GLN:NE2	1:D:612:LEU:O	2.46	0.48
1:B:207:TRP:CH2	1:B:218:GLU:HB2	2.48	0.48
1:D:461:VAL:HG12	1:D:462:GLY:H	1.77	0.48
1:B:140:ALA:HB3	1:B:150:ILE:HB	1.94	0.48
1:B:583:ASP:O	1:B:613:ARG:HG3	2.12	0.48
1:D:314:GLN:O	1:D:316:GLN:HG3	2.13	0.48
1:A:456:ILE:HD12	1:A:474:ILE:HD11	1.95	0.48
1:C:495:LEU:HD12	1:C:500:ILE:HB	1.95	0.48
1:A:116:ASP:OD2	1:A:119:LYS:HB3	2.13	0.48
1:A:361:LEU:O	1:A:369:THR:HG22	2.13	0.48
1:D:305:SER:HB3	1:D:351:ILE:HD12	1.94	0.48
1:C:577:ARG:NH2	1:C:618:CYS:HB3	2.29	0.48
1:D:99:VAL:HG12	1:D:134:ARG:HH12	1.79	0.48
1:C:522:GLN:NE2	1:C:612:LEU:O	2.47	0.48
1:A:110:LYS:HB3	1:A:110:LYS:HE3	1.66	0.48
1:A:327:MET:CE	1:A:345:THR:HB	2.44	0.48
1:B:62:LYS:HD2	1:B:573:ASP:HB3	1.96	0.48
1:D:150:ILE:HG12	1:D:189:TYR:OH	2.14	0.48
1:B:411:GLU:OE1	1:B:411:GLU:N	2.41	0.47
1:B:79:VAL:HB	1:B:564:TRP:CZ3	2.49	0.47
1:D:256:THR:HG21	1:D:260:GLY:N	2.28	0.47
1:D:346:SER:HA	1:D:352:VAL:O	2.13	0.47
1:D:577:ARG:NH2	1:D:618:CYS:HB3	2.29	0.47
1:A:304:TRP:CG	1:A:712:LEU:CD1	2.97	0.47
1:A:326:ASP:O	1:A:348:ASP:HA	2.14	0.47
1:A:402:GLY:HA2	1:A:641:LEU:HD23	1.97	0.47
1:B:324:ASN:HB3	2:G:1:NAG:C7	2.44	0.47
1:C:520:GLU:HG3	1:C:612:LEU:HD12	1.96	0.47
1:A:577:ARG:NH2	1:A:618:CYS:HB3	2.29	0.47
1:C:324:ASN:HB3	2:K:1:NAG:O7	2.15	0.47
1:A:132:PHE:CE1	1:A:154:GLU:HB2	2.50	0.47
1:D:570:ASP:HB2	2:J:1:NAG:H81	1.93	0.47
1:D:589:ALA:CB	1:D:602:ILE:HD11	2.45	0.47
1:B:293:ARG:HH22	1:B:314:GLN:HA	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:SER:HB2	1:C:148:LYS:HG2	1.97	0.47
1:C:589:ALA:CB	1:C:602:ILE:HD11	2.45	0.47
1:A:341:GLY:N	1:A:360:HIS:O	2.41	0.46
1:C:407:LEU:HD11	1:C:482:TRP:HE1	1.80	0.46
1:C:480:TYR:CD1	1:C:590:HIS:CD2	3.03	0.46
1:C:70:HIS:CE1	1:C:121:PHE:HB2	2.50	0.46
1:B:67:THR:HG1	1:B:527:TYR:HH	1.59	0.46
1:D:284:VAL:CG2	1:D:712:LEU:HD23	2.45	0.46
1:D:327:MET:HB3	1:D:686:PRO:HG2	1.96	0.46
1:D:352:VAL:HB	1:D:683:ARG:HH12	1.80	0.46
1:A:109:SER:OG	1:A:132:PHE:HA	2.15	0.46
1:A:386:LEU:HD11	1:A:390:ASN:HA	1.97	0.46
1:A:643:ASP:OD1	1:A:644:PHE:N	2.45	0.46
1:B:577:ARG:NH2	1:B:618:CYS:HB3	2.29	0.46
1:B:589:ALA:CB	1:B:602:ILE:HD11	2.45	0.46
1:D:150:ILE:O	1:D:151:LEU:HD12	2.15	0.46
1:D:431:ALA:O	1:D:435:ILE:HG12	2.16	0.46
1:D:504:ILE:HD12	1:D:539:LEU:HD22	1.97	0.46
1:A:463:ASP:O	1:A:467:VAL:HG23	2.15	0.46
1:A:572:LYS:HZ3	2:F:2:NAG:C8	2.27	0.46
1:A:357:LEU:HD12	1:A:358:ASP:N	2.30	0.46
1:C:587:TRP:CD2	1:C:611:ARG:NH2	2.84	0.46
1:A:414:LYS:HE2	1:A:414:LYS:HB3	1.63	0.46
1:A:589:ALA:CB	1:A:602:ILE:HD11	2.45	0.46
1:B:79:VAL:HG21	1:B:564:TRP:CD2	2.51	0.46
1:B:587:TRP:CD2	1:B:611:ARG:NH2	2.84	0.46
1:D:415:CYS:HB3	1:D:425:CYS:HB3	1.89	0.46
1:D:100:PRO:HB2	1:D:103:ILE:HD13	1.97	0.46
1:D:477:ASP:OD1	1:D:477:ASP:N	2.48	0.46
1:D:640:PHE:CZ	1:D:696:PRO:HD2	2.51	0.46
1:C:117:TYR:O	1:C:568:THR:HG21	2.16	0.46
1:B:94:LEU:HD21	1:B:133:ILE:HG21	1.98	0.46
1:A:169:ASP:OD1	1:A:169:ASP:N	2.48	0.45
1:A:348:ASP:OD1	1:A:348:ASP:N	2.47	0.45
1:A:640:PHE:CZ	1:A:696:PRO:HD2	2.51	0.45
1:D:100:PRO:O	1:D:134:ARG:NH1	2.50	0.45
1:C:133:ILE:HD13	1:C:153:ALA:HB2	1.97	0.45
1:C:640:PHE:CZ	1:C:696:PRO:HD2	2.51	0.45
1:A:128:ILE:HG22	1:A:165:PHE:CE2	2.51	0.45
1:B:477:ASP:OD1	1:B:477:ASP:N	2.48	0.45
1:D:89:GLY:HA2	1:D:117:TYR:CD1	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ILE:HD11	1:D:569:VAL:HB	1.98	0.45
1:A:211:ASN:ND2	1:A:214:GLU:HB3	2.31	0.45
1:B:446:LEU:HD12	1:B:447:SER:H	1.82	0.45
1:B:514:ILE:HD13	1:B:514:ILE:HA	1.85	0.45
1:D:255:ARG:NH2	1:D:264:LYS:HD3	2.31	0.45
1:D:587:TRP:CD2	1:D:611:ARG:NH2	2.84	0.45
1:A:111:LEU:HB2	1:A:128:ILE:HD11	1.97	0.45
1:A:357:LEU:HD22	1:A:404:TRP:CG	2.51	0.45
1:A:587:TRP:CD2	1:A:611:ARG:NH2	2.83	0.45
1:B:74:ASP:O	1:B:75:LEU:HD23	2.16	0.45
1:B:284:VAL:HG21	1:B:712:LEU:HD23	1.98	0.45
1:B:458:HIS:CE1	1:B:492:TYR:HE2	2.35	0.45
1:D:340:PHE:O	1:D:362:TYR:HE1	1.99	0.45
1:D:346:SER:HB3	1:D:353:TYR:CE2	2.52	0.45
1:D:378:ARG:HH22	1:D:605:TYR:HB2	1.81	0.45
1:A:119:LYS:HG3	1:A:120:ASN:ND2	2.32	0.45
1:A:407:LEU:HD11	1:A:482:TRP:HE1	1.80	0.45
1:B:192:GLN:HB3	1:B:232:ASN:OD1	2.17	0.45
1:B:640:PHE:CZ	1:B:696:PRO:HD2	2.51	0.45
1:C:345:THR:O	1:C:353:TYR:HA	2.16	0.45
1:B:164:VAL:CG1	1:B:179:LEU:HD11	2.46	0.45
1:B:643:ASP:OD1	1:B:644:PHE:N	2.45	0.45
1:B:110:LYS:HB3	1:B:110:LYS:HE3	1.51	0.45
1:B:461:VAL:HG12	1:B:462:GLY:H	1.81	0.45
1:D:243:SER:HB3	1:C:336:GLY:H	1.82	0.45
1:C:480:TYR:CE1	1:C:590:HIS:CD2	3.05	0.45
1:A:79:VAL:HG21	1:A:564:TRP:CD2	2.52	0.44
1:B:204:ASN:HB3	1:B:223:VAL:O	2.17	0.44
1:B:258:ASP:OD2	1:B:262:THR:OG1	2.30	0.44
1:D:114:SER:HB2	1:D:121:PHE:CD2	2.52	0.44
1:C:514:ILE:HG12	1:C:529:PHE:CD1	2.52	0.44
1:D:359:ARG:O	1:D:385:THR:HB	2.18	0.44
1:C:477:ASP:HA	1:C:587:TRP:CZ3	2.53	0.44
1:A:305:SER:HB3	1:A:351:ILE:HD12	2.00	0.44
1:A:323:ALA:CB	1:A:328:VAL:HG22	2.47	0.44
1:A:284:VAL:HG21	1:A:712:LEU:HD23	2.00	0.44
1:B:501:ILE:O	1:B:516:PHE:HA	2.18	0.44
1:B:520:GLU:OE1	1:B:611:ARG:HG3	2.18	0.44
1:A:141:ILE:HD13	1:A:149:VAL:HG13	1.99	0.44
1:B:190:SER:HB2	1:B:228:TRP:CZ2	2.52	0.44
1:B:415:CYS:O	1:B:420:LYS:NZ	2.25	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HB	1:C:564:TRP:CZ3	2.53	0.44
1:C:314:GLN:O	1:C:316:GLN:HG3	2.17	0.44
1:A:256:THR:HG21	1:A:260:GLY:CA	2.47	0.44
1:B:596:ASP:HA	1:B:599:ASP:HB2	2.00	0.44
1:D:596:ASP:HA	1:D:599:ASP:HB2	2.00	0.44
1:C:150:ILE:O	1:C:151:LEU:HD12	2.18	0.44
1:C:287:ASP:HB2	1:C:290:THR:CG2	2.45	0.44
1:D:102:VAL:HG23	1:D:103:ILE:HD12	2.00	0.44
1:A:148:LYS:HD2	1:A:212:PHE:CD1	2.53	0.43
1:B:66:ASN:HB3	1:B:570:ASP:HB3	2.00	0.43
1:B:70:HIS:NE2	1:B:121:PHE:HB2	2.33	0.43
1:C:500:ILE:HD11	1:C:575:LEU:HD12	1.99	0.43
1:D:472:VAL:HB	1:D:486:LEU:HB2	2.00	0.43
1:B:144:GLU:HG3	1:B:145:ASN:OD1	2.18	0.43
1:A:63:LEU:HD21	1:A:574:ILE:HG13	2.01	0.43
1:A:399:ASP:OD1	1:A:399:ASP:N	2.52	0.43
1:B:346:SER:OG	1:B:350:GLY:HA2	2.18	0.43
1:B:382:ILE:HG12	1:B:396:ILE:HB	2.01	0.43
1:B:495:LEU:HD23	1:B:541:SER:OG	2.18	0.43
1:C:284:VAL:CG2	1:C:712:LEU:HD23	2.48	0.43
1:C:430:HIS:HB3	1:C:441:VAL:HG21	2.00	0.43
1:C:308:GLN:C	1:C:309:LEU:HD12	2.39	0.43
1:C:310:PRO:HD3	1:C:644:PHE:CD1	2.53	0.43
1:C:368:GLU:OE1	1:C:368:GLU:N	2.47	0.43
1:C:596:ASP:HA	1:C:599:ASP:HB2	2.00	0.43
1:A:198:LEU:HD13	1:A:206:LEU:HD11	2.00	0.43
1:B:348:ASP:OD1	1:B:348:ASP:N	2.51	0.43
1:D:387:SER:HB3	1:D:393:GLN:CD	2.39	0.43
1:D:499:GLY:O	1:D:518:THR:HA	2.18	0.43
1:C:78:SER:HB2	1:C:96:THR:OG1	2.19	0.43
1:C:310:PRO:CD	1:C:644:PHE:HE1	2.30	0.43
2:L:1:NAG:H62	2:L:2:NAG:HN2	1.83	0.43
1:A:403:ARG:NH1	1:A:653:SER:HB3	2.34	0.43
1:A:95:THR:HB	1:A:110:LYS:H	1.84	0.43
1:A:140:ALA:HB3	1:A:150:ILE:HB	2.01	0.43
1:A:414:LYS:H	1:A:414:LYS:HG2	1.55	0.43
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.89	0.43
1:A:457:ALA:HA	1:A:492:TYR:OH	2.19	0.43
1:C:114:SER:HB2	1:C:121:PHE:CD2	2.54	0.43
1:A:68:HIS:ND1	1:A:119:LYS:HD3	2.34	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.88	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LEU:HD21	1:D:184:LEU:HA	2.01	0.42
1:A:94:LEU:HD13	1:A:111:LEU:HD13	2.00	0.42
1:A:562:ARG:HE	1:A:562:ARG:HB3	1.67	0.42
1:B:198:LEU:HA	1:B:207:TRP:O	2.19	0.42
1:B:253:LEU:O	1:B:266:ILE:HG12	2.19	0.42
1:B:287:ASP:O	1:B:290:THR:HG22	2.19	0.42
1:A:596:ASP:HA	1:A:599:ASP:HB2	2.00	0.42
1:D:116:ASP:OD1	1:D:116:ASP:N	2.49	0.42
1:C:328:VAL:N	1:C:346:SER:OG	2.52	0.42
1:A:371:PHE:HA	1:A:383:THR:HB	2.01	0.42
1:B:211:ASN:OD1	1:B:211:ASN:N	2.52	0.42
1:C:348:ASP:N	1:C:348:ASP:OD1	2.52	0.42
1:A:361:LEU:HD21	1:A:386:LEU:HB2	2.01	0.42
1:B:228:TRP:CH2	1:B:234:ILE:HD11	2.54	0.42
1:D:148:LYS:HD2	1:D:212:PHE:CD1	2.55	0.42
1:B:133:ILE:HD13	1:B:153:ALA:HB2	2.01	0.42
1:B:370:ASP:HA	1:B:431:ALA:HB3	2.02	0.42
1:C:619:GLN:NE2	1:C:620:ASN:O	2.53	0.42
1:A:368:GLU:HB2	1:A:436:SER:OG	2.20	0.42
1:A:619:GLN:NE2	1:A:620:ASN:O	2.53	0.42
1:D:368:GLU:OE1	1:D:368:GLU:N	2.46	0.42
1:A:90:VAL:HG11	1:A:171:ALA:HB3	2.00	0.42
1:A:196:TYR:CD1	1:A:210:LYS:HA	2.55	0.42
1:A:343:ILE:HD11	1:A:360:HIS:ND1	2.34	0.42
1:A:520:GLU:HG3	1:A:612:LEU:HD12	2.02	0.42
1:B:343:ILE:HD11	1:B:360:HIS:ND1	2.34	0.42
1:B:407:LEU:HD11	1:B:482:TRP:NE1	2.31	0.42
1:B:619:GLN:NE2	1:B:620:ASN:O	2.53	0.42
1:A:81:LEU:HB3	1:A:553:TRP:CZ3	2.55	0.42
1:B:642:CYS:SG	1:B:648:ARG:HG3	2.60	0.42
1:C:256:THR:HG21	1:C:260:GLY:H	1.83	0.42
1:A:642:CYS:SG	1:A:648:ARG:HG3	2.60	0.41
1:B:554:GLY:O	1:B:564:TRP:HA	2.20	0.41
1:D:70:HIS:CE1	1:D:121:PHE:HB2	2.55	0.41
1:D:619:GLN:NE2	1:D:620:ASN:O	2.53	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.85	0.41
1:B:164:VAL:HG13	1:B:179:LEU:HD11	2.02	0.41
1:C:538:GLY:HA3	1:C:553:TRP:CZ2	2.56	0.41
1:A:445:PRO:HA	1:A:457:ALA:HB2	2.02	0.41
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.72	0.41
1:B:549:ASN:OD1	2:H:1:NAG:O5	2.38	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:SER:HB2	1:D:96:THR:OG1	2.19	0.41
1:D:237:THR:HA	1:D:252:GLU:O	2.21	0.41
1:D:487:GLU:O	1:D:490:HIS:HE1	2.03	0.41
1:A:222:ALA:O	1:A:238:THR:HA	2.21	0.41
1:B:446:LEU:HD12	1:B:447:SER:N	2.36	0.41
1:C:605:TYR:HD1	1:C:605:TYR:HA	1.75	0.41
1:A:140:ALA:O	1:A:189:TYR:OH	2.32	0.41
1:B:431:ALA:O	1:B:435:ILE:HG12	2.20	0.41
1:C:397:THR:HG22	1:C:404:TRP:CZ3	2.55	0.41
1:B:425:CYS:HA	1:B:461:VAL:CG1	2.51	0.41
1:B:605:TYR:HD1	1:B:605:TYR:HA	1.75	0.41
1:D:642:CYS:SG	1:D:648:ARG:HG3	2.60	0.41
1:A:167:SER:HB2	1:A:174:PHE:CD2	2.55	0.41
1:A:167:SER:HB2	1:A:174:PHE:CE2	2.55	0.41
1:B:381:TYR:HE1	1:B:400:GLN:HG3	1.85	0.41
1:C:310:PRO:CD	1:C:644:PHE:CE1	3.01	0.41
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.86	0.41
1:C:68:His:CD2	1:C:119:LYS:HD3	2.56	0.41
1:C:327:MET:HB3	1:C:686:PRO:HG2	2.03	0.41
1:A:256:THR:HG23	1:A:262:THR:O	2.21	0.41
1:A:485:MET:O	1:A:486:LEU:HD23	2.21	0.41
1:B:310:PRO:N	1:B:644:PHE:HE1	2.19	0.41
1:D:293:ARG:HH22	1:D:314:GLN:HA	1.86	0.41
1:A:253:LEU:O	1:A:266:ILE:HG12	2.21	0.40
1:C:184:LEU:HD23	1:C:200:LEU:HD23	2.03	0.40
1:C:340:PHE:HA	1:C:360:HIS:O	2.21	0.40
1:B:213:GLY:HA2	1:B:216:TRP:CZ2	2.56	0.40
1:B:221:LYS:HB3	1:B:221:LYS:HE2	1.72	0.40
1:D:480:TYR:CD1	1:D:590:HIS:CD2	3.08	0.40
1:D:679:THR:OG1	1:D:680:ASN:N	2.54	0.40
1:C:143:PRO:HB2	1:C:146:SER:HB3	2.03	0.40
1:C:679:THR:OG1	1:C:680:ASN:N	2.54	0.40
1:B:472:VAL:HB	1:B:486:LEU:HB2	2.04	0.40
1:D:274:GLY:C	1:D:275:LEU:HD12	2.41	0.40
1:C:642:CYS:SG	1:C:648:ARG:HG3	2.60	0.40
1:A:331:HIS:CE1	1:A:341:GLY:HA3	2.57	0.40
1:D:248:LEU:HB3	1:D:271:TYR:CE1	2.57	0.40
1:A:679:THR:OG1	1:A:680:ASN:N	2.54	0.40
1:B:328:VAL:HG11	1:B:353:TYR:OH	2.22	0.40
1:B:473:TYR:CE2	1:B:484:LYS:HB2	2.56	0.40
1:D:343:ILE:HD11	1:D:360:HIS:ND1	2.37	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ILE:HD12	1:D:474:ILE:HD11	2.04	0.40
1:C:643:ASP:OD1	1:C:644:PHE:N	2.45	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:GLN:NE2	2:K:2:NAG:O4[1_554]	1.84	0.36
1:A:581:GLU:OE2	1:C:298:THR:OG1[1_554]	2.12	0.08
1:A:693:GLY:CA	1:C:629:GLN:NE2[1_554]	2.14	0.06

## 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	636/732 (87%)	592 (93%)	42 (7%)	2 (0%)	41	75
1	B	636/732 (87%)	592 (93%)	43 (7%)	1 (0%)	47	79
1	C	634/732 (87%)	596 (94%)	37 (6%)	1 (0%)	47	79
1	D	636/732 (87%)	591 (93%)	44 (7%)	1 (0%)	47	79
All	All	2542/2928 (87%)	2371 (93%)	166 (6%)	5 (0%)	47	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	C	240	VAL
1	B	240	VAL
1	D	240	VAL
1	A	240	VAL



### 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	565/626 (90%)	560 (99%)	5 (1%)	78	88
1	B	565/626 (90%)	557 (99%)	8 (1%)	67	81
1	C	563/626 (90%)	557 (99%)	6 (1%)	73	85
1	D	565/626 (90%)	558 (99%)	7 (1%)	71	84
All	All	2258/2504 (90%)	2232 (99%)	26 (1%)	71	84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	597	TYR
1	A	605	TYR
1	A	707	CYS
1	A	712	LEU
1	A	713	ASN
1	B	338	THR
1	B	397	THR
1	B	432	SER
1	B	552	ILE
1	B	597	TYR
1	B	605	TYR
1	B	707	CYS
1	B	712	LEU
1	D	80	SER
1	D	338	THR
1	D	397	THR
1	D	597	TYR
1	D	605	TYR
1	D	707	CYS
1	D	712	LEU
1	C	315	GLU
1	C	338	THR
1	C	354	SER
1	C	597	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	605	TYR
1	C	707	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	316	GLN
1	B	658	GLN
1	D	316	GLN
1	D	423	ASN
1	D	437	GLN
1	D	619	GLN
1	D	629	GLN
1	D	658	GLN
1	C	68	HIS
1	C	590	HIS
1	C	658	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

24 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	0.59	0	17,19,21	2.34	5 (29%)
2	NAG	E	2	2	14,14,15	0.72	0	17,19,21	2.54	7 (41%)
2	BMA	E	3	2	11,11,12	0.54	0	15,15,17	1.65	5 (33%)
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	1.59	4 (23%)
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	1.42	4 (23%)
2	BMA	F	3	2	11,11,12	0.38	0	15,15,17	1.19	1 (6%)
2	NAG	G	1	1,2	14,14,15	0.60	0	17,19,21	2.39	7 (41%)
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.75	0
2	BMA	G	3	2	11,11,12	0.30	0	15,15,17	1.01	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.70	0	17,19,21	2.65	6 (35%)
2	NAG	H	2	2	14,14,15	0.37	0	17,19,21	1.13	1 (5%)
2	BMA	H	3	2	11,11,12	0.33	0	15,15,17	1.13	1 (6%)
2	NAG	I	1	1,2	14,14,15	0.69	0	17,19,21	1.37	4 (23%)
2	NAG	I	2	2	14,14,15	0.52	0	17,19,21	1.57	2 (11%)
2	BMA	I	3	2	11,11,12	0.42	0	15,15,17	0.94	0
2	NAG	J	1	1,2	14,14,15	0.49	0	17,19,21	1.64	4 (23%)
2	NAG	J	2	2	14,14,15	0.36	0	17,19,21	1.65	4 (23%)
2	BMA	J	3	2	11,11,12	0.38	0	15,15,17	1.17	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.58	0	17,19,21	1.32	3 (17%)
2	NAG	K	2	2	14,14,15	0.56	0	17,19,21	2.26	3 (17%)
2	BMA	K	3	2	11,11,12	0.69	0	15,15,17	1.47	3 (20%)
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	0.86	0
2	NAG	L	2	2	14,14,15	0.40	0	17,19,21	1.50	4 (23%)
2	BMA	L	3	2	11,11,12	0.54	0	15,15,17	1.57	3 (20%)

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	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	NAG	O4-C4-C3	-7.26	93.56	110.35
2	H	1	NAG	C2-N2-C7	7.19	133.15	122.90
2	G	1	NAG	C2-N2-C7	6.75	132.52	122.90
2	E	2	NAG	C1-O5-C5	6.44	120.92	112.19
2	E	1	NAG	O5-C5-C6	5.32	115.55	107.20
2	H	1	NAG	C1-O5-C5	5.25	119.31	112.19
2	E	1	NAG	C4-C3-C2	-4.40	104.56	111.02
2	E	1	NAG	O4-C4-C3	4.32	120.34	110.35
2	F	1	NAG	O5-C5-C6	-4.17	100.66	107.20
2	I	2	NAG	C2-N2-C7	4.14	128.80	122.90
2	K	2	NAG	C4-C3-C2	4.13	117.07	111.02
2	E	2	NAG	C3-C4-C5	-3.94	103.22	110.24
2	G	1	NAG	O6-C6-C5	-3.77	98.35	111.29
2	J	2	NAG	O5-C1-C2	-3.75	105.37	111.29
2	L	3	BMA	O5-C5-C6	3.51	112.70	107.20
2	E	2	NAG	O4-C4-C3	3.42	118.25	110.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C1-O5-C5	3.40	116.80	112.19
2	E	3	BMA	O3-C3-C2	3.30	116.31	109.99
2	E	2	NAG	O5-C1-C2	-3.16	106.31	111.29
2	H	2	NAG	C2-N2-C7	3.15	127.39	122.90
2	E	2	NAG	O3-C3-C4	3.14	117.61	110.35
2	J	1	NAG	C2-N2-C7	3.10	127.31	122.90
2	J	1	NAG	C6-C5-C4	3.03	120.10	113.00
2	L	2	NAG	C2-N2-C7	3.02	127.20	122.90
2	E	2	NAG	C1-C2-N2	2.99	115.59	110.49
2	H	1	NAG	C1-C2-N2	2.97	115.56	110.49
2	L	3	BMA	C1-O5-C5	-2.96	108.19	112.19
2	J	1	NAG	O4-C4-C5	2.93	116.58	109.30
2	L	3	BMA	C1-C2-C3	-2.90	106.10	109.67
2	E	1	NAG	O5-C5-C4	-2.85	103.89	110.83
2	F	1	NAG	O4-C4-C3	2.85	116.93	110.35
2	H	1	NAG	O5-C1-C2	-2.83	106.82	111.29
2	H	1	NAG	O5-C5-C6	-2.82	102.79	107.20
2	J	3	BMA	C1-C2-C3	-2.79	106.23	109.67
2	E	3	BMA	O4-C4-C3	-2.78	103.92	110.35
2	G	1	NAG	C8-C7-N2	2.75	120.75	116.10
2	F	2	NAG	C1-O5-C5	2.72	115.88	112.19
2	L	2	NAG	O4-C4-C5	-2.72	102.54	109.30
2	H	3	BMA	O5-C5-C6	2.72	111.47	107.20
2	K	3	BMA	O2-C2-C3	-2.69	104.74	110.14
2	G	1	NAG	O5-C5-C6	-2.66	103.03	107.20
2	J	2	NAG	C1-C2-N2	2.66	115.02	110.49
2	G	1	NAG	O5-C1-C2	-2.62	107.15	111.29
2	K	1	NAG	O3-C3-C2	2.59	114.82	109.47
2	E	2	NAG	C4-C3-C2	-2.58	107.23	111.02
2	K	3	BMA	C6-C5-C4	2.54	118.95	113.00
2	K	3	BMA	C1-O5-C5	-2.52	108.78	112.19
2	H	1	NAG	C8-C7-N2	2.50	120.33	116.10
2	E	1	NAG	O4-C4-C5	2.44	115.35	109.30
2	F	2	NAG	O5-C5-C6	2.42	111.00	107.20
2	L	2	NAG	O4-C4-C3	-2.42	104.76	110.35
2	I	1	NAG	O4-C4-C3	2.39	115.88	110.35
2	G	1	NAG	O7-C7-N2	-2.39	117.56	121.95
2	E	3	BMA	O5-C1-C2	-2.34	107.17	110.77
2	I	1	NAG	C2-N2-C7	-2.28	119.66	122.90
2	F	3	BMA	O2-C2-C3	-2.27	105.59	110.14
2	G	3	BMA	O5-C5-C6	2.25	110.74	107.20
2	F	1	NAG	O6-C6-C5	-2.24	103.59	111.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C1-O5-C5	2.23	115.22	112.19
2	K	1	NAG	C2-N2-C7	2.21	126.05	122.90
2	J	2	NAG	C3-C4-C5	-2.21	106.30	110.24
2	I	1	NAG	C1-O5-C5	2.14	115.09	112.19
2	J	1	NAG	O5-C1-C2	2.13	114.64	111.29
2	E	3	BMA	O3-C3-C4	-2.12	105.46	110.35
2	G	1	NAG	O4-C4-C3	-2.10	105.49	110.35
2	F	2	NAG	C3-C4-C5	-2.10	106.50	110.24
2	K	1	NAG	O5-C1-C2	-2.07	108.02	111.29
2	I	1	NAG	O5-C5-C6	2.07	110.45	107.20
2	F	1	NAG	O4-C4-C5	-2.03	104.25	109.30
2	F	2	NAG	O5-C1-C2	-2.02	108.10	111.29
2	E	3	BMA	O4-C4-C5	2.02	114.31	109.30
2	L	2	NAG	O5-C1-C2	-2.02	108.10	111.29
2	K	2	NAG	C2-N2-C7	2.00	125.75	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	I	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C8-C7-N2-C2
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	H	1	NAG	O7-C7-N2-C2
2	I	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	G	1	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
2	K	2	NAG	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	L	3	BMA	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C4-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7

There are no ring outliers.

13 monomers are involved in 26 short contacts:

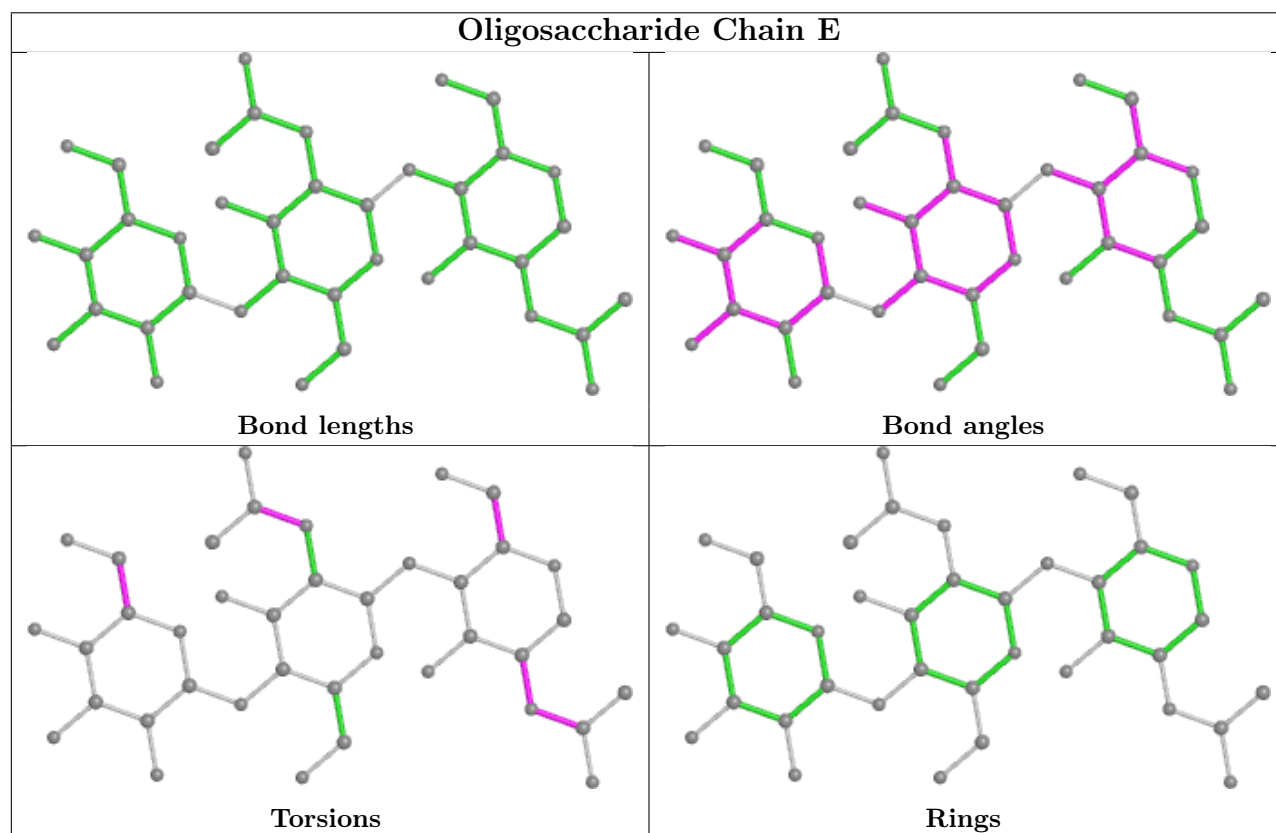
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	4	0
2	E	2	NAG	1	0
2	L	1	NAG	1	0
2	J	1	NAG	3	0
2	K	2	NAG	2	1
2	L	2	NAG	1	0
2	H	2	NAG	2	0
2	E	1	NAG	1	0

*Continued on next page...*

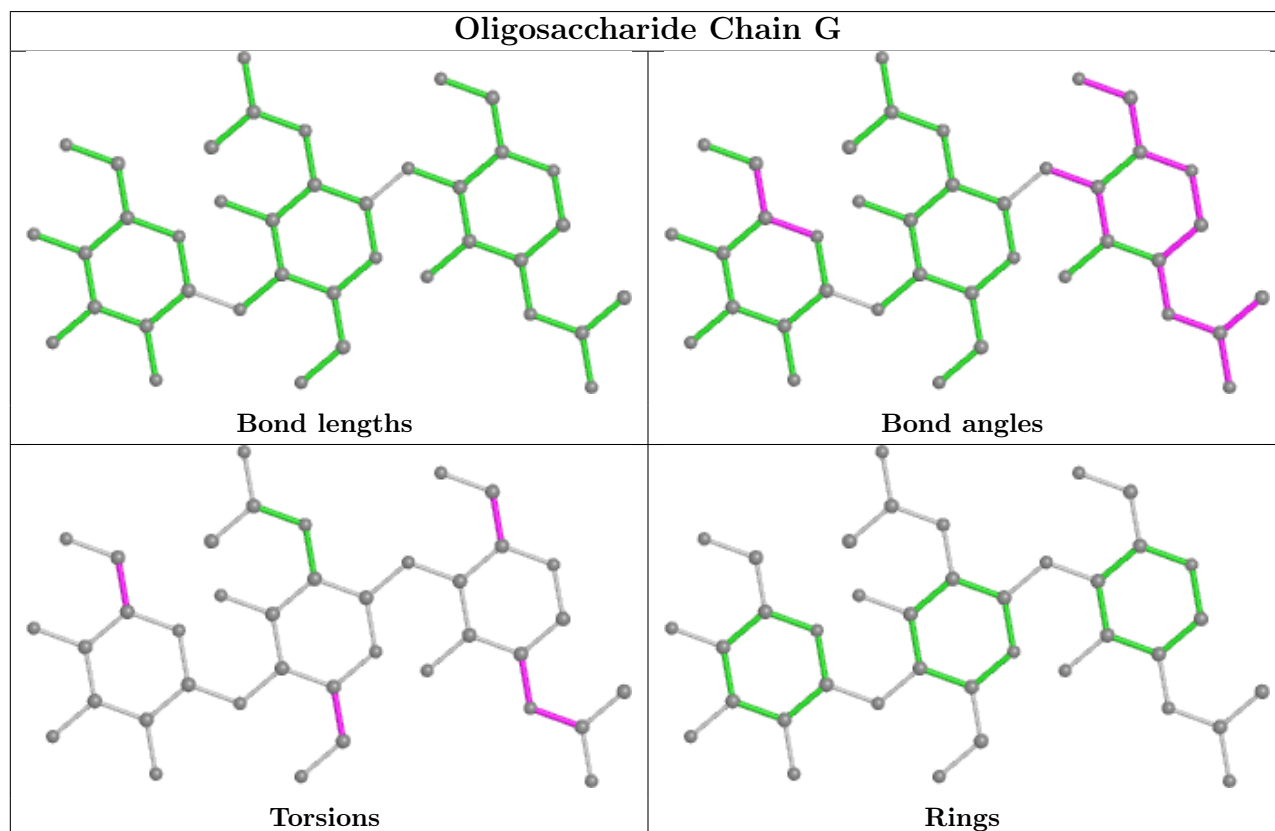
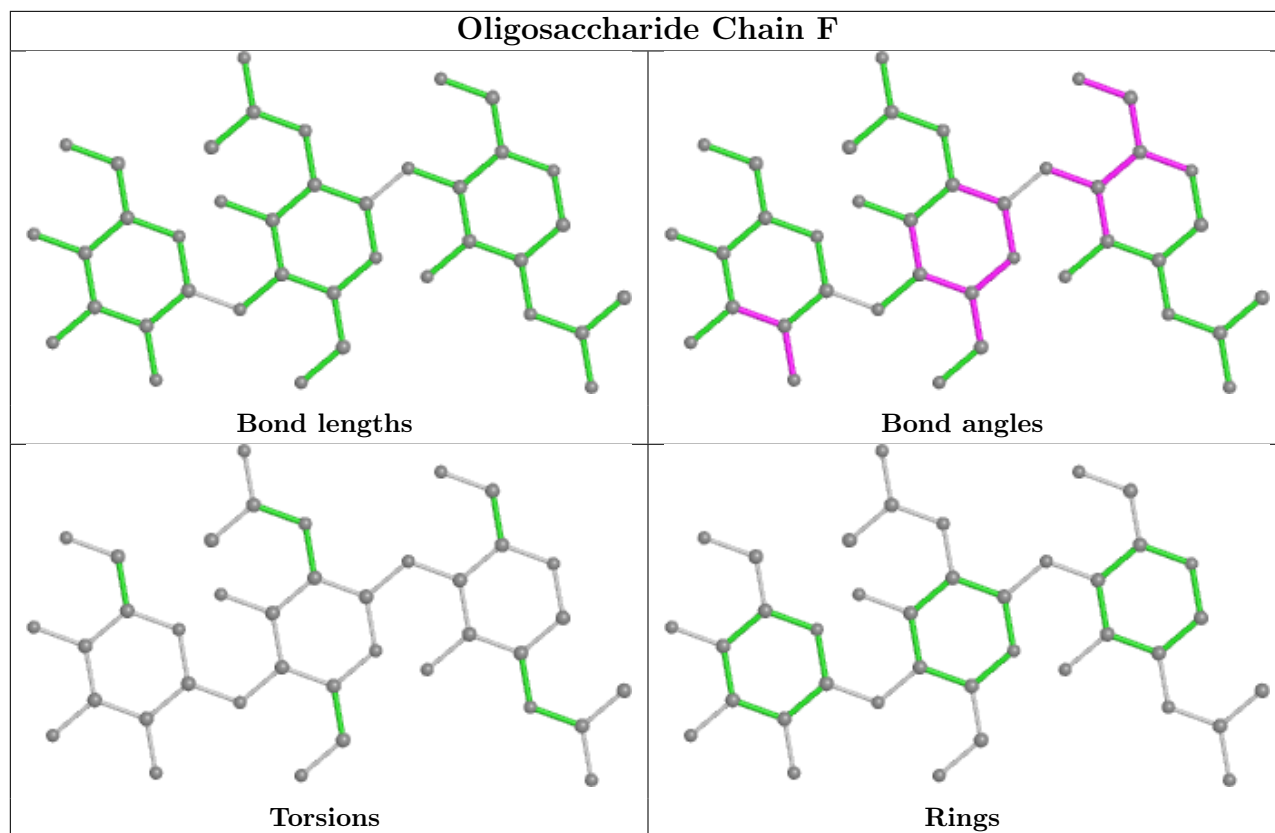
Continued from previous page...

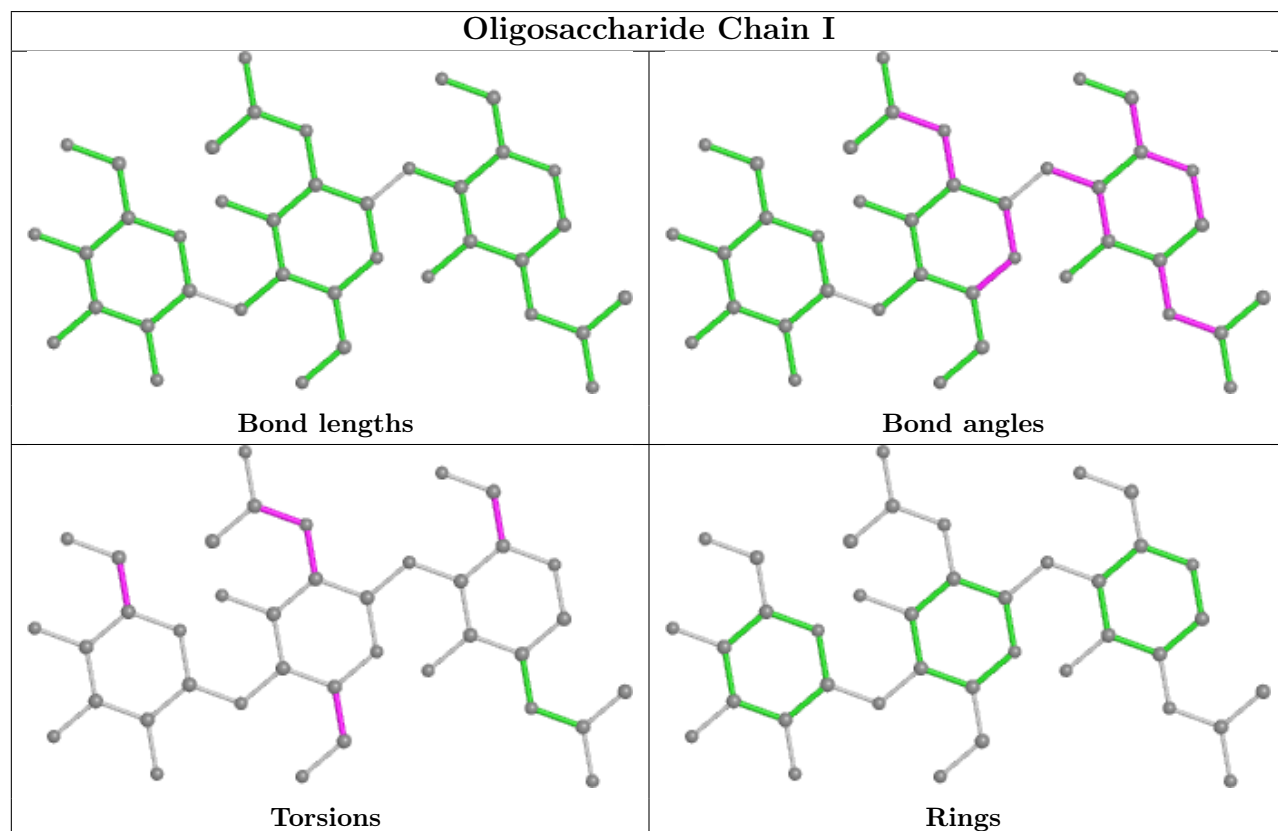
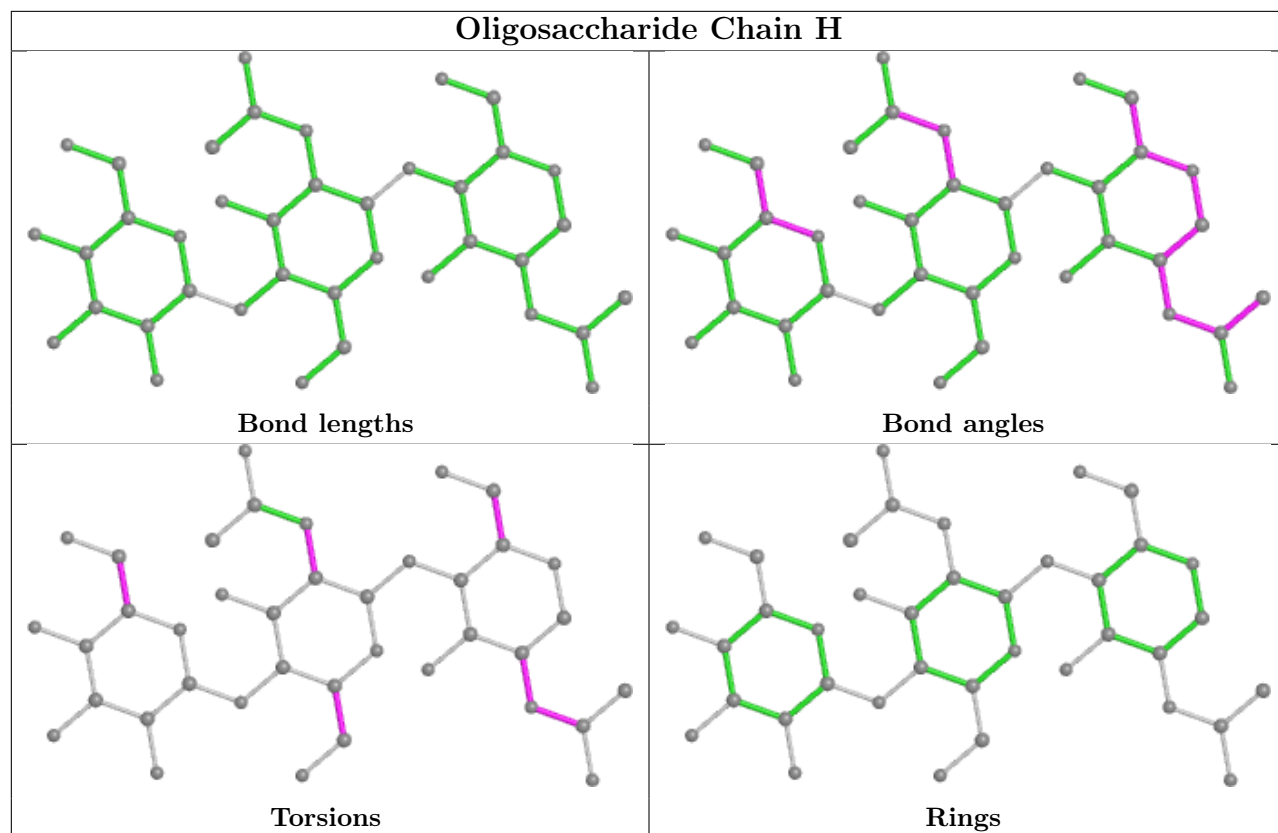
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	F	2	NAG	4	0
2	I	1	NAG	1	0
2	G	1	NAG	6	0
2	K	1	NAG	2	0

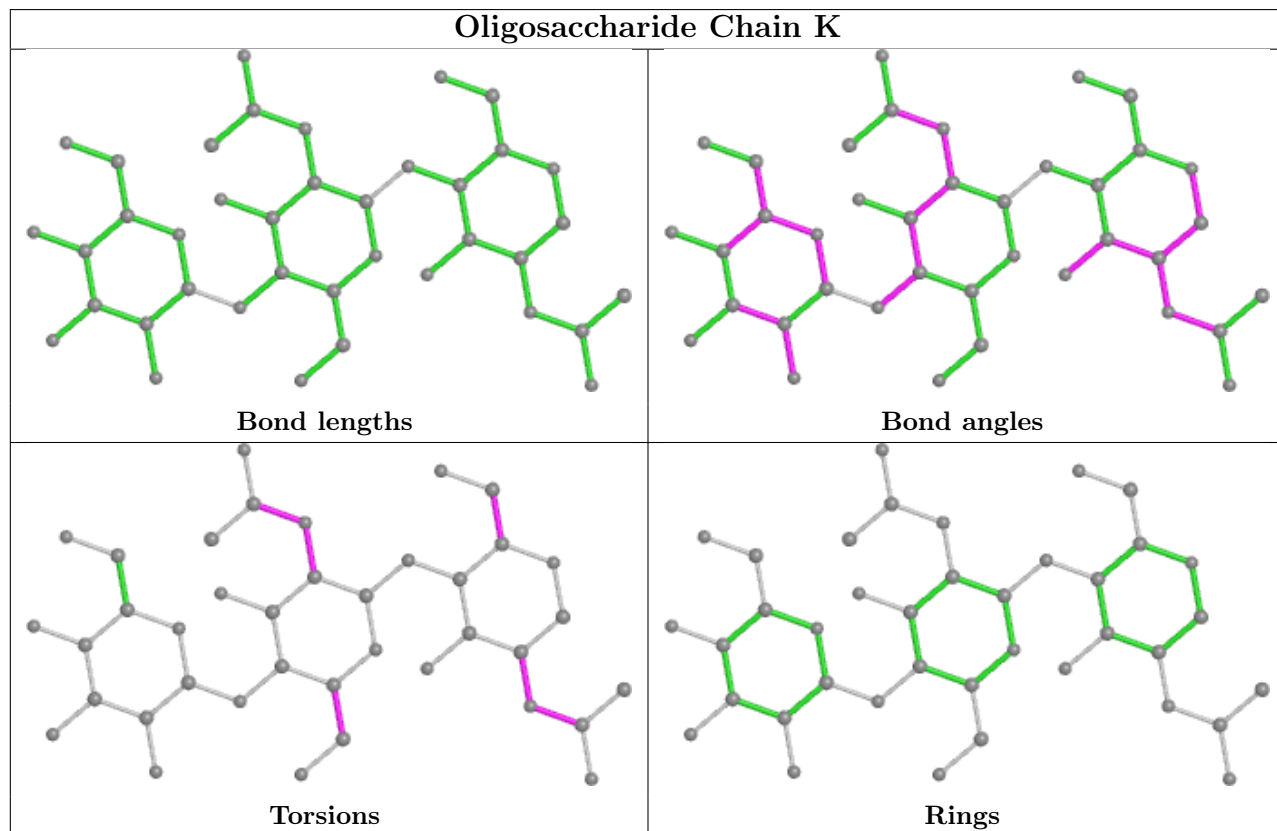
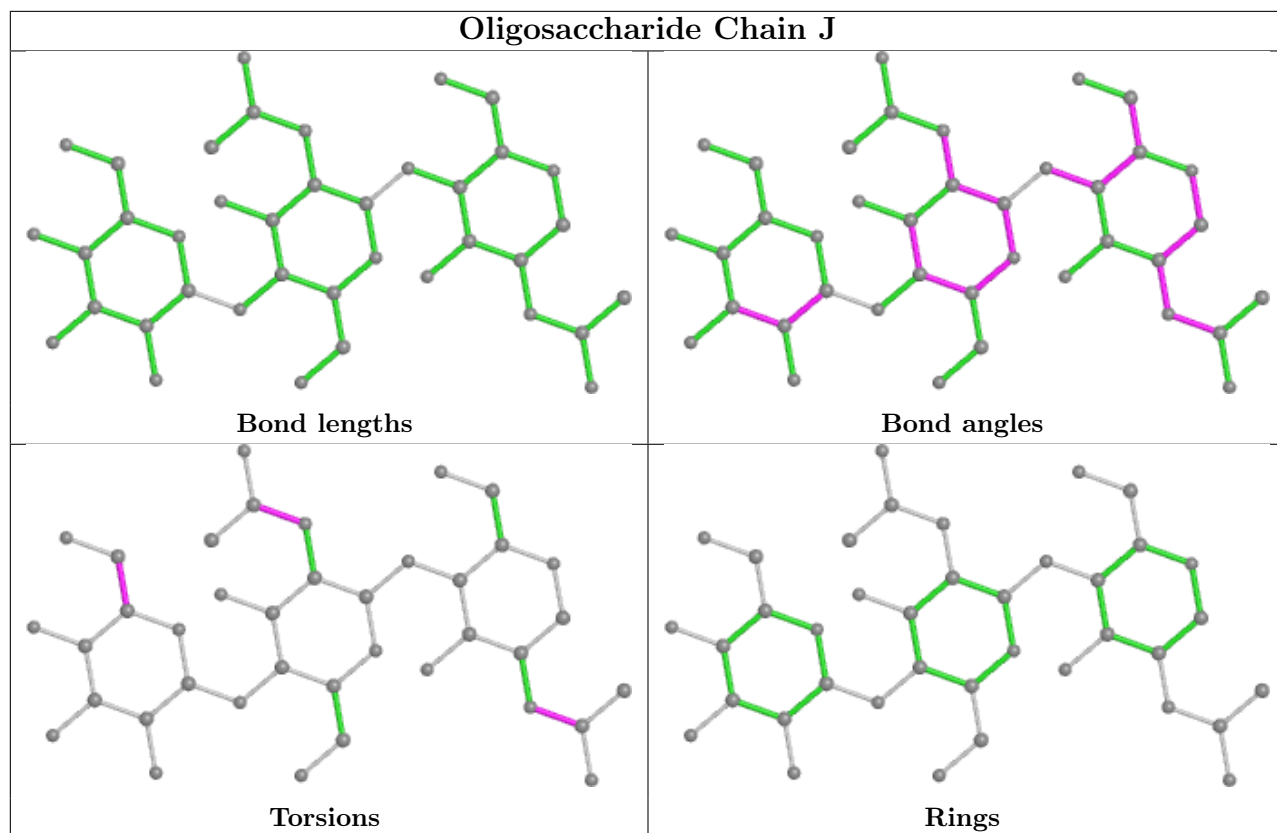
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

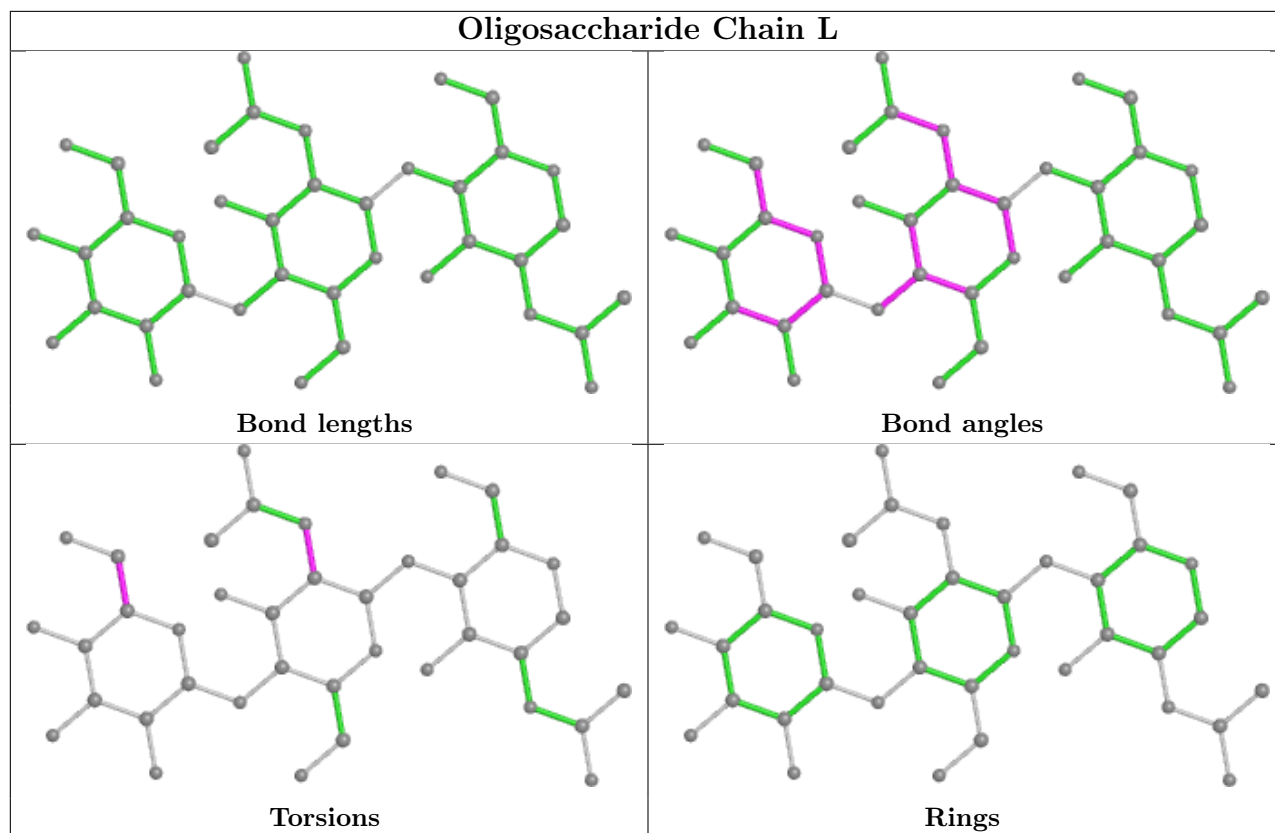












## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	NAG	C	807	1	14,14,15	0.48	0	17,19,21	1.74	5 (29%)
3	NAG	A	807	1	14,14,15	0.45	0	17,19,21	0.90	1 (5%)
3	NAG	D	807	-	14,14,15	0.46	0	17,19,21	0.93	0
3	NAG	B	807	1	14,14,15	0.37	0	17,19,21	0.68	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
3	NAG	C	807	1	-	1/6/23/26	0/1/1/1
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1
3	NAG	D	807	-	-	2/6/23/26	0/1/1/1
3	NAG	B	807	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	807	NAG	O5-C5-C6	3.64	112.91	107.20
3	C	807	NAG	C1-C2-N2	3.27	116.08	110.49
3	C	807	NAG	C6-C5-C4	-2.67	106.74	113.00
3	A	807	NAG	O5-C5-C6	2.67	111.38	107.20
3	C	807	NAG	C2-N2-C7	2.23	126.08	122.90
3	C	807	NAG	O3-C3-C2	-2.10	105.12	109.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	807	NAG	O5-C5-C6-O6
3	D	807	NAG	C4-C5-C6-O6
3	C	807	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	807	NAG	4	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	648/732 (88%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	107, 178, 239, 297	0
1	B	648/732 (88%)	-0.24	4 (0%) <span style="border: 1px solid blue; padding: 2px;">89</span> <span style="border: 1px solid blue; padding: 2px;">84</span>	107, 190, 259, 330	0
1	C	646/732 (88%)	-0.17	6 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">77</span>	115, 205, 289, 342	0
1	D	648/732 (88%)	-0.13	11 (1%) <span style="border: 1px solid blue; padding: 2px;">70</span> <span style="border: 1px solid blue; padding: 2px;">60</span>	133, 224, 288, 377	0
All	All	2590/2928 (88%)	-0.20	21 (0%) <span style="border: 1px solid blue; padding: 2px;">86</span> <span style="border: 1px solid blue; padding: 2px;">79</span>	107, 198, 279, 377	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	TYR	3.6
1	B	623	ASP	3.3
1	B	625	VAL	3.2
1	D	608	GLN	2.8
1	C	520	GLU	2.6
1	C	624	TYR	2.6
1	D	502	VAL	2.5
1	D	627	ALA	2.4
1	B	626	VAL	2.4
1	C	571	PHE	2.3
1	D	311	SER	2.3
1	C	420	LYS	2.2
1	D	628	LYS	2.2
1	C	54	GLY	2.2
1	D	139	MET	2.1
1	D	75	LEU	2.1
1	C	573	ASP	2.1
1	D	625	VAL	2.1
1	D	552	ILE	2.1
1	D	94	LEU	2.0
1	D	626	VAL	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](#)

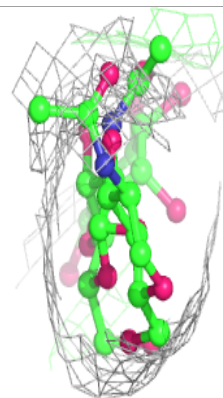
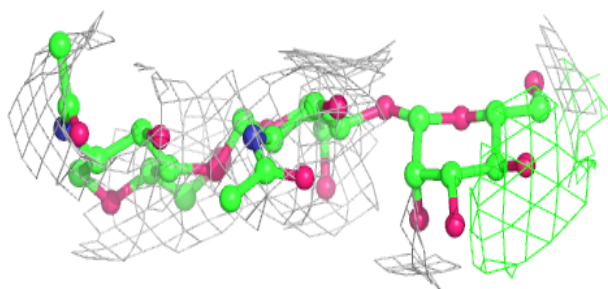
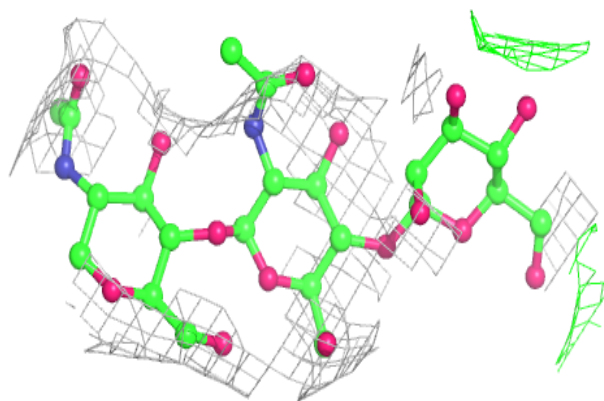
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	BMA	I	3	11/12	0.57	0.45	261,279,288,288	0
2	BMA	G	3	11/12	0.59	0.55	298,309,326,334	0
2	BMA	J	3	11/12	0.68	0.14	261,306,326,336	0
2	BMA	L	3	11/12	0.75	0.23	278,289,293,296	0
2	BMA	K	3	11/12	0.76	0.38	152,196,221,225	0
2	BMA	E	3	11/12	0.80	0.54	206,230,249,249	0
2	BMA	F	3	11/12	0.83	0.23	234,273,285,294	0
2	BMA	H	3	11/12	0.83	0.17	291,303,307,307	0
2	NAG	H	1	14/15	0.84	0.20	265,276,320,355	0
2	NAG	E	2	14/15	0.85	0.26	175,211,235,238	0
2	NAG	J	1	14/15	0.86	0.12	251,284,301,311	0
2	NAG	F	1	14/15	0.87	0.18	152,186,216,223	0
2	NAG	F	2	14/15	0.89	0.19	208,231,258,275	0
2	NAG	G	1	14/15	0.90	0.24	179,207,223,228	0
2	NAG	G	2	14/15	0.90	0.24	178,204,242,277	0
2	NAG	I	2	14/15	0.91	0.22	210,227,245,261	0
2	NAG	L	2	14/15	0.91	0.17	247,259,269,275	0
2	NAG	K	2	14/15	0.91	0.21	176,203,223,227	0
2	NAG	I	1	14/15	0.92	0.22	142,168,192,207	0
2	NAG	K	1	14/15	0.92	0.21	154,172,182,186	0
2	NAG	H	2	14/15	0.93	0.09	257,282,301,305	0
2	NAG	E	1	14/15	0.93	0.28	128,153,176,202	0
2	NAG	J	2	14/15	0.94	0.11	278,294,311,313	0
2	NAG	L	1	14/15	0.95	0.24	229,252,264,284	0

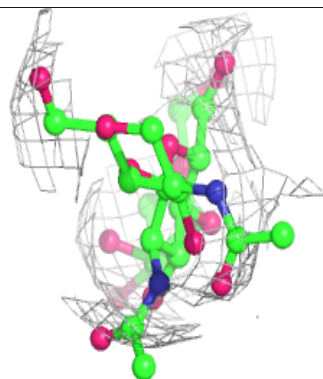
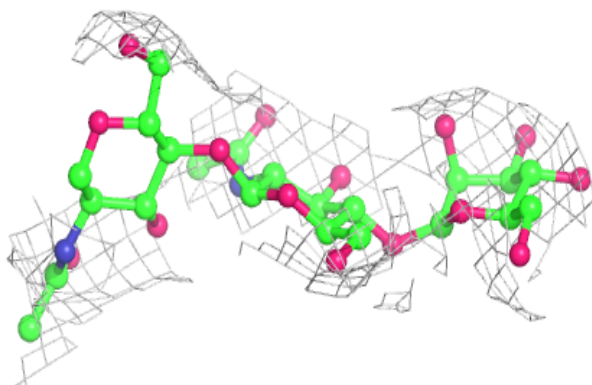
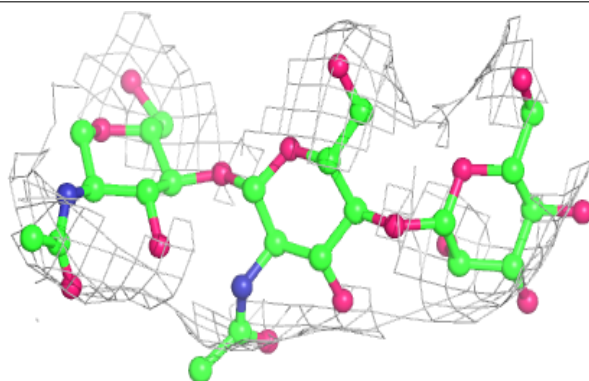
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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:**

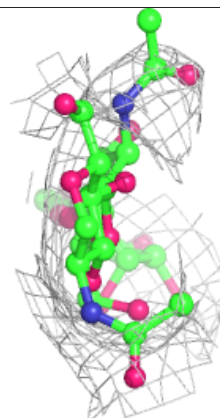
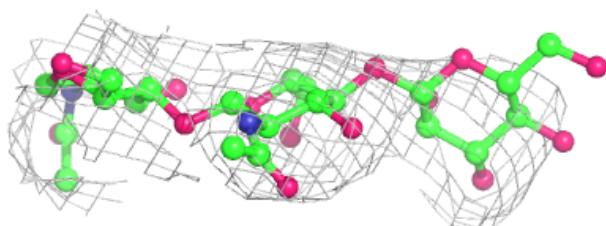
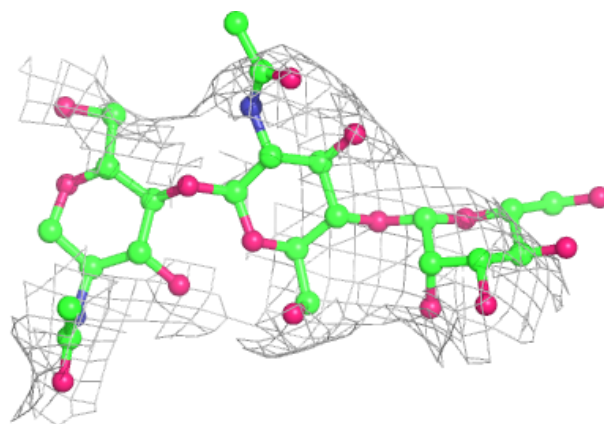
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





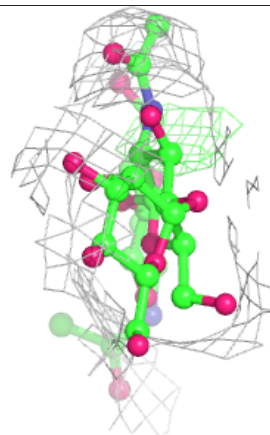
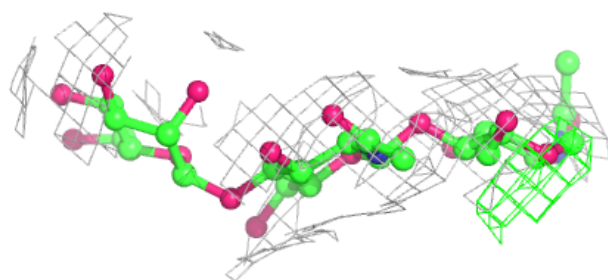
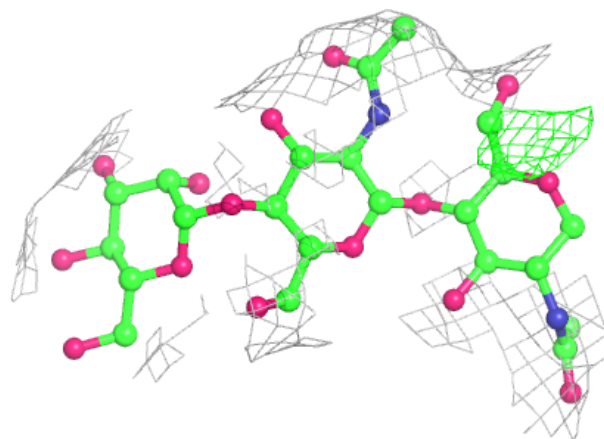
**Electron density around Chain G:**

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

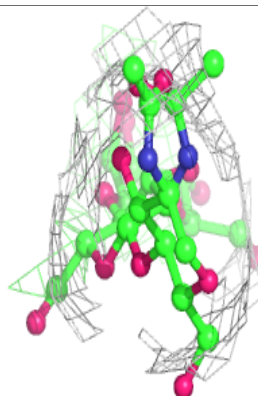
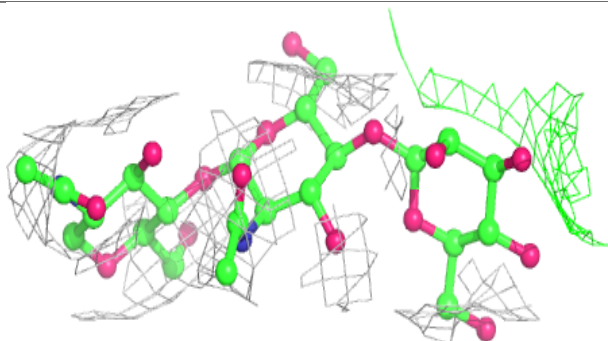
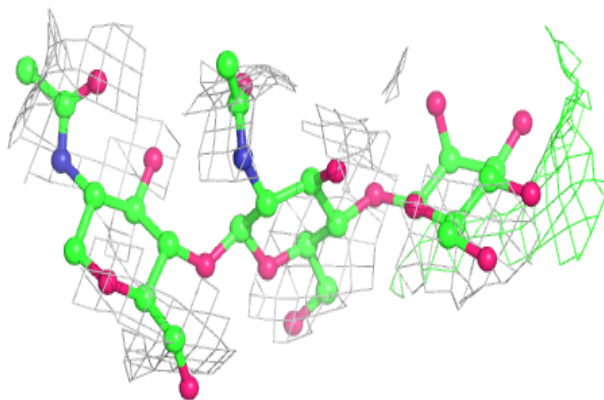


**Electron density around Chain H:**

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

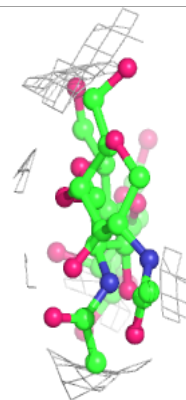
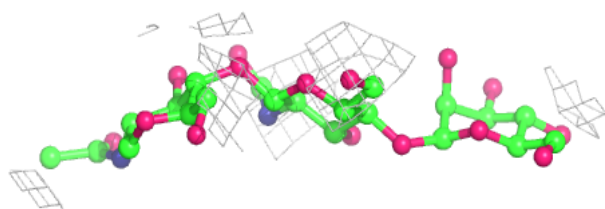
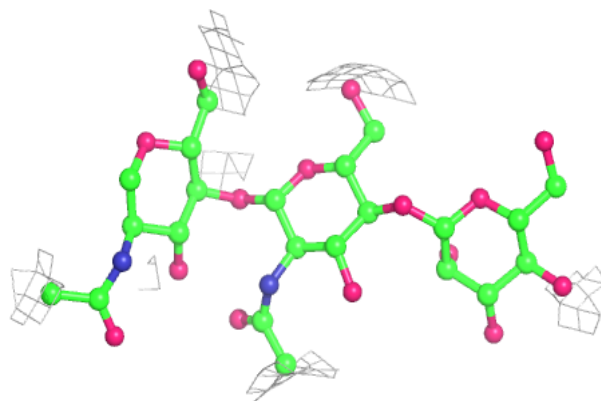
**Electron density around Chain I:**

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

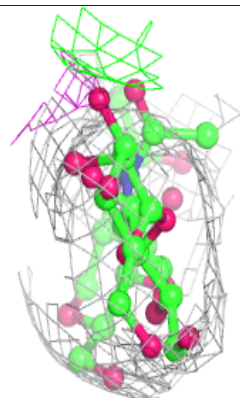
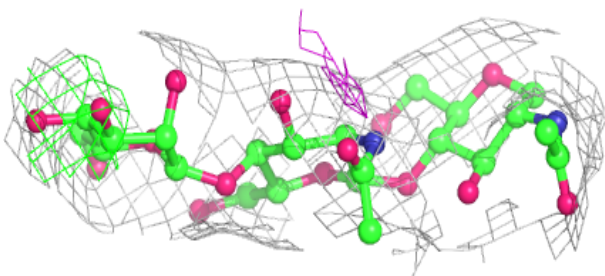
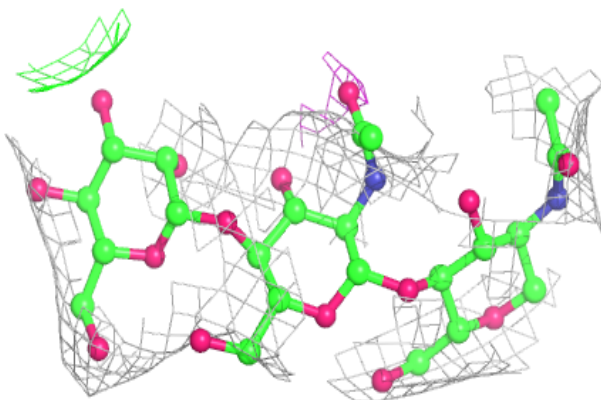


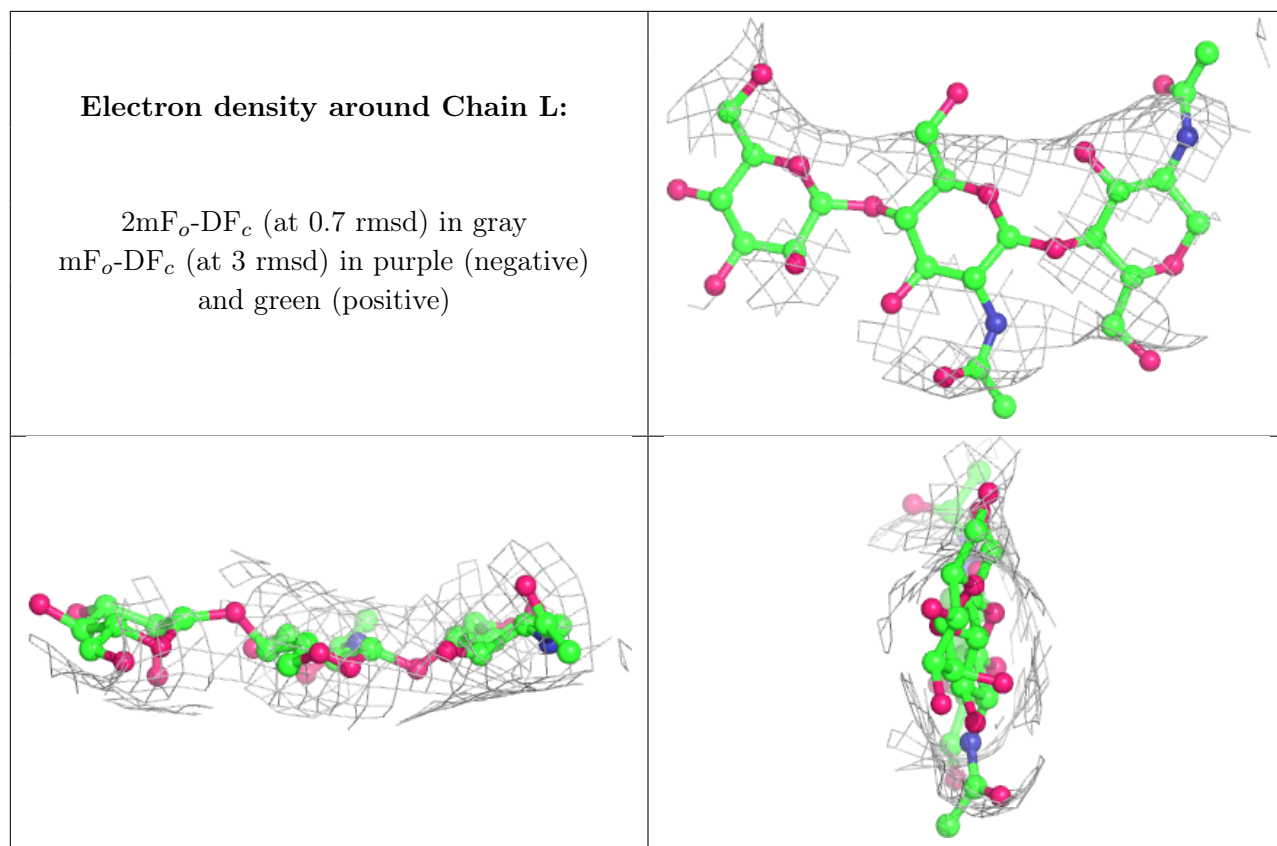
**Electron density around Chain J:**

$2mF_o-DF_c$  (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)





## 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
3	NAG	C	807	14/15	0.88	0.56	170,217,226,230	0
3	NAG	B	807	14/15	0.90	0.35	157,185,210,222	0
3	NAG	A	807	14/15	0.90	0.44	173,194,205,220	0
3	NAG	D	807	14/15	0.94	0.36	182,190,213,220	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.