



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 06:28 pm GMT

PDB ID : 1DZG  
Title : N135Q-S380C-ANTITHROMBIN-III  
Authors : McCoy, A.J.; Huntington, J.A.; Carrell, R.W.  
Deposited on : 2000-02-28  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

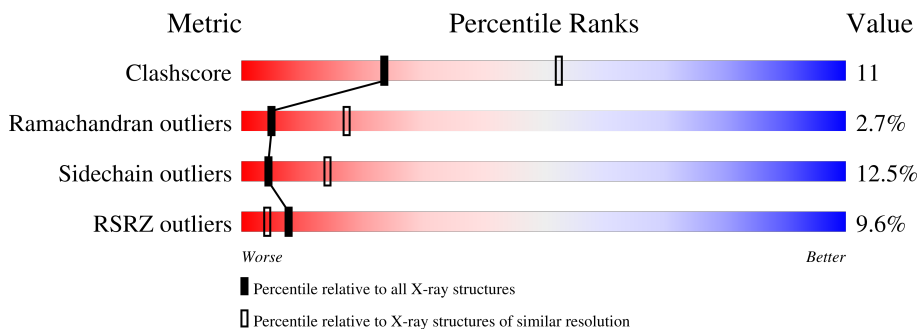
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	I	432	
2	L	432	
3	A	2	
3	B	2	
3	C	2	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2	-	-	-	X
3	NAG	C	2	-	-	-	X
4	NAG	I	861	-	-	-	X
5	GOL	I	901	-	-	-	X
5	GOL	L	901	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6593 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 ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	422	3271	2088	549	616	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	GLN	ASN	engineered mutation	UNP P01008
I	380	CYS	SER	engineered mutation	UNP P01008

- Molecule 2 is a protein called ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	409	3180	2031	525	606	18	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	A	2	28	16	2	10	0	0	0
3	B	2	28	16	2	10	0	0	0
3	C	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O		
4	I	1	14	8	1	5	0	0
4	I	1	14	8	1	5	0	0
4	L	1	14	8	1	5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	I	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	L	1	6	3	3	0	0

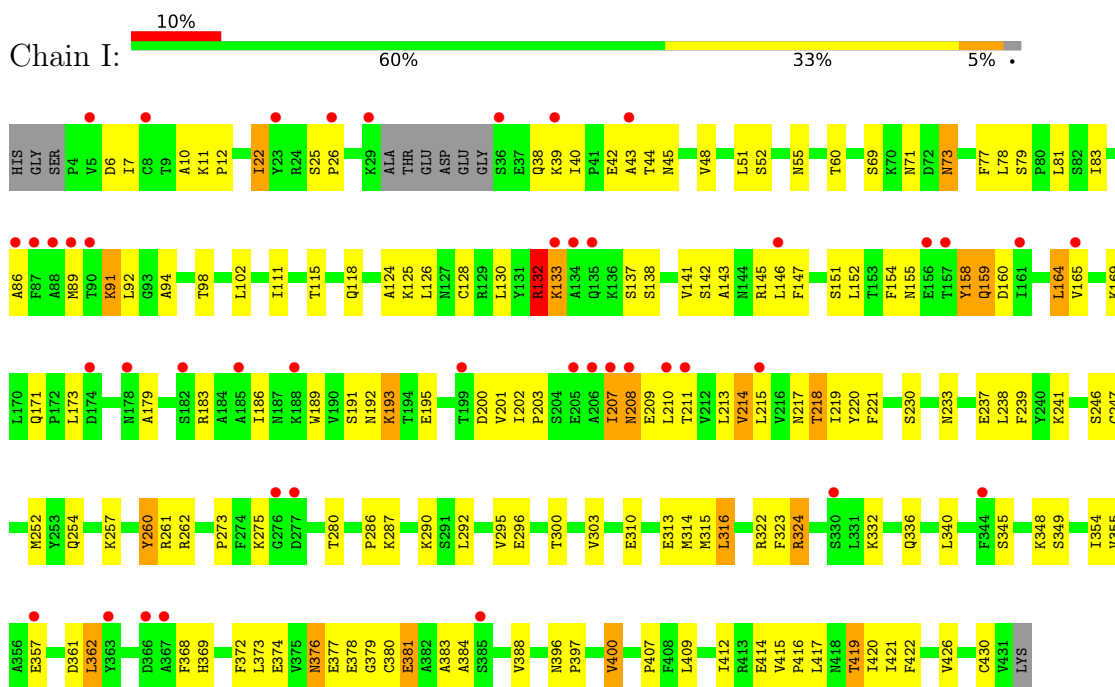
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	O	0	0
			2	2		
6	L	2	Total	O	0	0
			2	2		

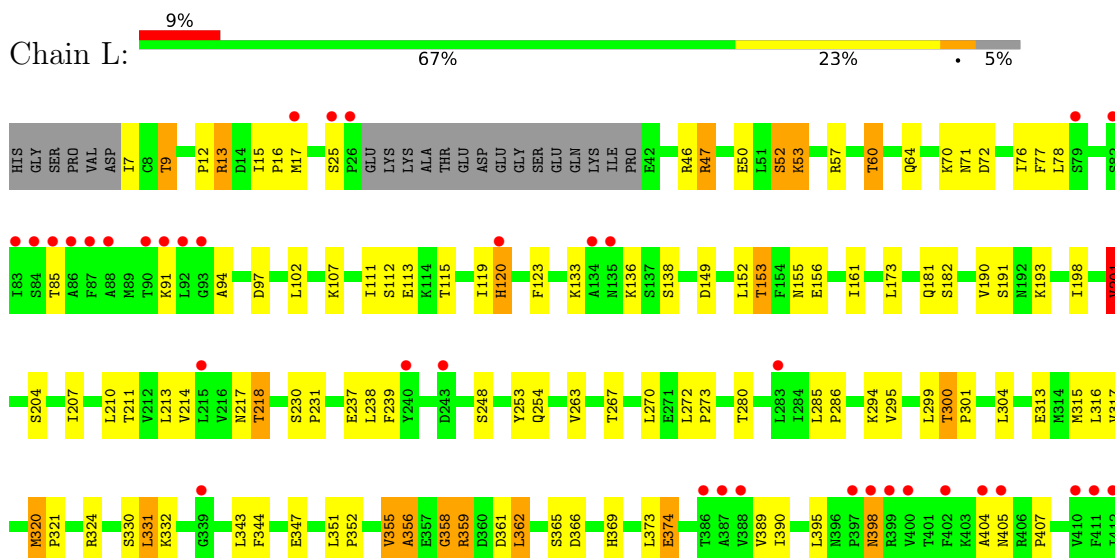
### 3 Residue-property plots

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: ANTITHROMBIN-III



#### • Molecule 2: ANTITHROMBIN-III





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

Chain A:  100%



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

Chain B:  100%



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

Chain C:  100%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.61Å 99.54Å 88.69Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 26.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.80) 97.9 (26.24-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.297 0.245 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL

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	I	0.45	0/3337	1.00	4/4524 (0.1%)
2	L	0.43	0/3245	0.92	1/4398 (0.0%)
All	All	0.44	0/6582	0.96	5/8922 (0.1%)

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
2	L	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	324	ARG	CD-NE-CZ	6.28	132.39	123.60
1	I	260	TYR	CA-CB-CG	6.01	124.81	113.40
1	I	132	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	I	6	ASP	N-CA-CB	5.62	120.71	110.60
2	L	405	ASN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	300	THR	Mainchain

## 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	I	3271	0	3182	85	0
2	L	3180	0	3094	59	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
3	C	28	0	25	1	0
4	I	28	0	26	0	0
4	L	14	0	13	0	0
5	I	6	0	8	2	0
5	L	6	0	8	1	0
6	I	2	0	0	0	0
6	L	2	0	0	0	0
All	All	6593	0	6406	145	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 11.

All (145) 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:I:81:LEU:HD21	1:I:130:LEU:HD21	1.58	0.86
1:I:378:GLU:HG3	1:I:384:ALA:HB3	1.64	0.79
1:I:324:ARG:HE	1:I:372:PHE:HZ	1.36	0.74
2:L:214:VAL:HG22	2:L:389:VAL:HG23	1.70	0.73
1:I:388:VAL:HG22	2:L:317:VAL:HB	1.72	0.72
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.70	0.72
2:L:13:ARG:HH11	2:L:13:ARG:HB2	1.58	0.69
2:L:111:ILE:HD12	2:L:119:ILE:HD12	1.75	0.68
2:L:331:LEU:HD21	2:L:369:HIS:HB2	1.76	0.67
2:L:300:THR:HB	2:L:301:PRO:HD2	1.79	0.63
1:I:45:ASN:HD21	1:I:125:LYS:HD3	1.64	0.62
2:L:17:MET:SD	2:L:120:HIS:HB2	2.39	0.62
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.80	0.62
1:I:7:ILE:HD11	1:I:132:ARG:HE	1.63	0.61
2:L:239:PHE:HE2	2:L:404:ALA:HB1	1.65	0.61
1:I:217:ASN:O	1:I:218:THR:HB	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:261:ARG:HG2	1:I:310:GLU:HB3	1.83	0.60
2:L:60:THR:HG21	2:L:300:THR:HA	1.82	0.60
1:I:126:LEU:HD11	1:I:419:THR:HG21	1.85	0.59
2:L:85:THR:HB	2:L:217:ASN:ND2	2.17	0.59
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.85	0.58
2:L:47:ARG:HD2	2:L:112:SER:HB2	1.85	0.58
2:L:415:VAL:HB	2:L:416:PRO:HD3	1.85	0.58
1:I:164:LEU:HD23	1:I:165:VAL:HG23	1.86	0.57
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.85	0.57
1:I:86:ALA:HB1	1:I:215:LEU:HD21	1.87	0.57
1:I:147:PHE:HB2	1:I:214:VAL:HG23	1.87	0.57
1:I:102:LEU:HG	1:I:340:LEU:HD11	1.87	0.56
1:I:324:ARG:HG3	1:I:374:GLU:HG3	1.88	0.55
2:L:213:LEU:HB3	2:L:390:ILE:HD12	1.88	0.55
1:I:40:ILE:HG23	1:I:44:THR:HB	1.89	0.55
2:L:153:THR:HB	2:L:356:ALA:HB2	1.88	0.54
1:I:86:ALA:HB2	1:I:217:ASN:HB3	1.89	0.54
2:L:213:LEU:HD23	2:L:390:ILE:HD12	1.89	0.54
2:L:355:VAL:HG13	2:L:362:LEU:HD11	1.89	0.54
1:I:361:ASP:O	1:I:362:LEU:C	2.46	0.54
2:L:91:LYS:HG3	2:L:102:LEU:HD13	1.89	0.53
1:I:257:LYS:HE2	1:I:313:GLU:HB3	1.90	0.53
1:I:273:PRO:HB3	1:I:280:THR:HG22	1.91	0.53
1:I:115:THR:HB	1:I:118:GLN:HG3	1.92	0.52
1:I:414:GLU:HB2	1:I:421:ILE:HD11	1.90	0.52
1:I:195:GLU:HG2	1:I:220:TYR:CE2	2.45	0.52
3:C:1:NAG:H62	3:C:2:NAG:C7	2.40	0.52
1:I:316:LEU:HB3	1:I:400:VAL:HG12	1.91	0.52
1:I:11:LYS:HB3	1:I:12:PRO:HD2	1.91	0.51
1:I:146:LEU:HG	1:I:213:LEU:HD22	1.92	0.51
2:L:70:LYS:HD3	2:L:76:ILE:HG12	1.93	0.51
2:L:7:ILE:HG22	2:L:9:THR:HG23	1.94	0.50
1:I:45:ASN:HB3	1:I:48:VAL:HB	1.93	0.50
2:L:304:LEU:HD12	5:L:901:GOL:H12	1.95	0.49
1:I:412:ILE:HB	1:I:422:PHE:HB2	1.93	0.49
1:I:252:MET:SD	1:I:377:GLU:HG3	2.52	0.48
1:I:287:LYS:HG3	1:I:290:LYS:H	1.78	0.48
2:L:193:LYS:HB3	2:L:218:THR:HG21	1.94	0.48
2:L:207:ILE:HG23	2:L:211:THR:HG21	1.96	0.48
2:L:358:GLY:O	2:L:359:ARG:C	2.51	0.48
2:L:190:VAL:HG21	2:L:201:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:355:VAL:CG2	2:L:359:ARG:HB2	2.43	0.48
1:I:195:GLU:HG2	1:I:220:TYR:HE2	1.78	0.48
1:I:345:SER:HB3	1:I:348:LYS:HD2	1.95	0.48
1:I:132:ARG:O	1:I:133:LYS:C	2.51	0.48
2:L:270:LEU:HD21	2:L:272:LEU:HD21	1.95	0.47
1:I:83:ILE:HA	1:I:217:ASN:ND2	2.28	0.47
2:L:253:TYR:O	2:L:254:GLN:HB3	2.14	0.47
1:I:179:ALA:HB1	1:I:208:ASN:HA	1.97	0.47
1:I:207:ILE:HD12	1:I:207:ILE:H	1.80	0.47
1:I:207:ILE:HG23	1:I:211:THR:HG21	1.96	0.47
2:L:191:SER:HA	2:L:198:ILE:O	2.16	0.46
2:L:300:THR:HB	2:L:301:PRO:CD	2.45	0.46
1:I:7:ILE:CD1	1:I:132:ARG:HH21	2.29	0.46
2:L:324:ARG:HB2	2:L:374:GLU:OE1	2.15	0.46
1:I:42:GLU:O	1:I:43:ALA:HB3	2.16	0.46
1:I:420:ILE:HD11	5:I:901:GOL:H2	1.97	0.46
2:L:155:ASN:OD1	2:L:156:GLU:N	2.49	0.46
2:L:407:PRO:HB3	2:L:427:ALA:HB2	1.96	0.46
1:I:376:ASN:ND2	1:I:379:GLY:H	2.14	0.46
2:L:173:LEU:HD13	2:L:182:SER:HB3	1.97	0.45
1:I:145:ARG:HG3	1:I:169:LYS:O	2.16	0.45
1:I:237:GLU:HG2	1:I:238:LEU:H	1.81	0.45
1:I:323:PHE:HE1	1:I:373:LEU:HD23	1.80	0.45
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.51	0.45
1:I:217:ASN:OD1	1:I:369:HIS:HB2	2.16	0.45
1:I:152:LEU:HD13	1:I:354:ILE:HG21	1.97	0.45
2:L:365:SER:OG	2:L:389:VAL:HG13	2.16	0.45
1:I:239:PHE:HB3	1:I:247:CYS:HB3	1.98	0.45
1:I:300:THR:H	1:I:303:VAL:HB	1.81	0.45
2:L:111:ILE:HG22	2:L:112:SER:H	1.82	0.45
2:L:153:THR:CB	2:L:356:ALA:HB2	2.47	0.45
2:L:415:VAL:HB	2:L:416:PRO:CD	2.45	0.45
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.81	0.45
2:L:359:ARG:HG2	2:L:361:ASP:OD2	2.16	0.45
1:I:51:LEU:HG	1:I:55:ASN:ND2	2.31	0.44
1:I:407:PRO:HA	1:I:426:VAL:O	2.17	0.44
1:I:51:LEU:HA	1:I:111:ILE:HD11	2.00	0.44
2:L:267:THR:HA	2:L:286:PRO:HA	1.99	0.44
1:I:25:SER:HB2	1:I:26:PRO:HD2	2.00	0.44
1:I:77:PHE:CE1	1:I:373:LEU:HD22	2.53	0.44
1:I:130:LEU:HD13	1:I:417:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:PHE:O	1:I:155:ASN:C	2.56	0.44
2:L:94:ALA:HA	2:L:351:LEU:HD23	1.98	0.44
2:L:398:ASN:HD22	2:L:398:ASN:H	1.66	0.44
1:I:208:ASN:HB2	1:I:209:GLU:H	1.71	0.44
1:I:202:ILE:HG23	1:I:368:PHE:CE2	2.53	0.43
2:L:152:LEU:HD11	2:L:359:ARG:NH1	2.33	0.43
2:L:71:ASN:ND2	2:L:72:ASP:H	2.16	0.43
1:I:336:GLN:HA	1:I:340:LEU:O	2.18	0.43
1:I:171:GLN:HG3	1:I:173:LEU:HG	2.01	0.43
1:I:189:TRP:O	1:I:193:LYS:HG2	2.19	0.43
1:I:124:ALA:HA	1:I:165:VAL:HG13	2.01	0.43
1:I:230:SER:HB3	1:I:233:ASN:ND2	2.33	0.43
2:L:53:LYS:HG3	2:L:57:ARG:HH21	1.82	0.43
2:L:207:ILE:HG12	2:L:389:VAL:HG21	2.00	0.43
2:L:332:LYS:HG3	2:L:344:PHE:CD2	2.53	0.43
1:I:143:ALA:HB3	1:I:218:THR:HG22	2.01	0.42
3:B:1:NAG:H62	3:B:2:NAG:O7	2.20	0.42
1:I:132:ARG:HA	1:I:132:ARG:HD3	1.46	0.42
1:I:290:LYS:HE2	1:I:295:VAL:HG22	2.01	0.42
1:I:7:ILE:HD11	1:I:132:ARG:NE	2.32	0.42
1:I:261:ARG:HG2	1:I:310:GLU:CB	2.49	0.42
1:I:22:ILE:HG12	1:I:115:THR:CG2	2.50	0.42
2:L:46:ARG:O	2:L:50:GLU:HG3	2.20	0.42
2:L:230:SER:HA	2:L:231:PRO:HD3	1.83	0.42
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.19	0.42
2:L:273:PRO:HA	2:L:280:THR:HG22	2.02	0.42
1:I:221:PHE:HD2	1:I:380:CYS:HG	1.67	0.41
1:I:48:VAL:HG13	1:I:126:LEU:HD13	2.03	0.41
1:I:380:CYS:O	1:I:381:GLU:HB2	2.20	0.41
2:L:355:VAL:HG22	2:L:359:ARG:HB2	2.02	0.41
1:I:45:ASN:ND2	1:I:48:VAL:HG23	2.36	0.41
2:L:320:MET:HA	2:L:321:PRO:HD3	1.92	0.41
1:I:79:SER:OG	1:I:219:ILE:HD12	2.20	0.41
2:L:17:MET:HG3	2:L:161:ILE:HG23	2.01	0.41
1:I:261:ARG:HG2	1:I:310:GLU:CG	2.51	0.41
2:L:52:SER:HB2	2:L:419:THR:HG23	2.03	0.41
2:L:149:ASP:HB3	2:L:152:LEU:HD12	2.03	0.41
2:L:60:THR:O	2:L:64:GLN:HG3	2.21	0.41
1:I:159:GLN:O	1:I:160:ASP:C	2.59	0.41
1:I:420:ILE:HG13	5:I:901:GOL:H12	2.03	0.41
1:I:207:ILE:HA	1:I:211:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:ALA:O	1:I:384:ALA:HB2	2.21	0.40
1:I:292:LEU:O	1:I:296:GLU:HG3	2.21	0.40
2:L:366:ASP:O	2:L:389:VAL:HG12	2.22	0.40
1:I:286:PRO:HB3	1:I:295:VAL:HG21	2.03	0.40
2:L:15:ILE:HA	2:L:16:PRO:HD3	1.98	0.40
2:L:111:ILE:H	2:L:111:ILE:HG13	1.69	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	I	418/432 (97%)	346 (83%)	58 (14%)	14 (3%)	4	13
2	L	405/432 (94%)	357 (88%)	40 (10%)	8 (2%)	7	24
All	All	823/864 (95%)	703 (85%)	98 (12%)	22 (3%)	5	17

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	203	PRO
1	I	332	LYS
2	L	356	ALA
1	I	164	LEU
1	I	362	LEU
2	L	201	VAL
1	I	94	ALA
1	I	133	LYS
1	I	349	SER
2	L	107	LYS
2	L	358	GLY
1	I	218	THR

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Mol	Chain	Res	Type
1	I	357	GLU
1	I	381	GLU
2	L	362	LEU
1	I	10	ALA
1	I	73	ASN
1	I	159	GLN
2	L	12	PRO
2	L	113	GLU
2	L	352	PRO
1	I	207	ILE

### 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	I	350/383 (91%)	306 (87%)	44 (13%)	4	14
2	L	344/383 (90%)	301 (88%)	43 (12%)	4	14
All	All	694/766 (91%)	607 (88%)	87 (12%)	4	14

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	22	ILE
1	I	38	GLN
1	I	39	LYS
1	I	52	SER
1	I	60	THR
1	I	69	SER
1	I	71	ASN
1	I	73	ASN
1	I	78	LEU
1	I	89	MET
1	I	91	LYS
1	I	98	THR
1	I	128	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	132	ARG
1	I	137	SER
1	I	138	SER
1	I	141	VAL
1	I	142	SER
1	I	151	SER
1	I	158	TYR
1	I	183	ARG
1	I	191	SER
1	I	192	ASN
1	I	193	LYS
1	I	200	ASP
1	I	201	VAL
1	I	208	ASN
1	I	210	LEU
1	I	214	VAL
1	I	241	LYS
1	I	246	SER
1	I	254	GLN
1	I	260	TYR
1	I	262	ARG
1	I	275	LYS
1	I	314	MET
1	I	315	MET
1	I	316	LEU
1	I	322	ARG
1	I	355	VAL
1	I	376	ASN
1	I	400	VAL
1	I	419	THR
1	I	430	CYS
2	L	9	THR
2	L	13	ARG
2	L	25	SER
2	L	47	ARG
2	L	52	SER
2	L	53	LYS
2	L	60	THR
2	L	78	LEU
2	L	97	ASP
2	L	115	THR
2	L	120	HIS

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Mol	Chain	Res	Type
2	L	123	PHE
2	L	133	LYS
2	L	136	LYS
2	L	138	SER
2	L	153	THR
2	L	181	GLN
2	L	201	VAL
2	L	204	SER
2	L	210	LEU
2	L	218	THR
2	L	237	GLU
2	L	238	LEU
2	L	248	SER
2	L	263	VAL
2	L	285	LEU
2	L	294	LYS
2	L	295	VAL
2	L	299	LEU
2	L	313	GLU
2	L	315	MET
2	L	316	LEU
2	L	320	MET
2	L	330	SER
2	L	331	LEU
2	L	343	LEU
2	L	347	GLU
2	L	355	VAL
2	L	359	ARG
2	L	374	GLU
2	L	395	LEU
2	L	398	ASN
2	L	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	45	ASN
1	I	159	GLN
1	I	178	ASN
1	I	233	ASN
1	I	254	GLN
1	I	305	GLN

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Mol	Chain	Res	Type
1	I	319	HIS
1	I	376	ASN
1	I	418	ASN
2	L	71	ASN
2	L	171	GLN
2	L	181	GLN
2	L	233	ASN
2	L	254	GLN
2	L	334	GLN
2	L	398	ASN
2	L	418	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1	1,3	14,14,15	1.23	1 (7%)	17,19,21	1.70	3 (17%)
3	NAG	A	2	3	14,14,15	1.29	1 (7%)	17,19,21	0.86	0
3	NAG	B	1	2,3	14,14,15	1.30	1 (7%)	17,19,21	2.23	5 (29%)
3	NAG	B	2	3	14,14,15	1.20	1 (7%)	17,19,21	1.57	4 (23%)
3	NAG	C	1	2,3	14,14,15	1.43	2 (14%)	17,19,21	1.39	2 (11%)
3	NAG	C	2	3	14,14,15	1.29	1 (7%)	17,19,21	1.63	2 (11%)

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	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	2/6/23/26	0/1/1/1
3	NAG	B	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	B	2	3	-	3/6/23/26	0/1/1/1
3	NAG	C	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O7-C7	-3.80	1.14	1.23
3	A	2	NAG	O7-C7	-3.79	1.14	1.23
3	B	1	NAG	O7-C7	-3.79	1.14	1.23
3	B	2	NAG	O7-C7	-3.78	1.14	1.23
3	C	1	NAG	O7-C7	-3.76	1.14	1.23
3	A	1	NAG	O7-C7	-3.74	1.14	1.23
3	C	1	NAG	C2-N2	2.17	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-C2-N2	5.28	119.51	110.49
3	B	1	NAG	C2-N2-C7	4.66	129.53	122.90
3	C	2	NAG	O5-C1-C2	-4.44	104.28	111.29
3	A	1	NAG	C1-O5-C5	4.10	117.75	112.19
3	C	2	NAG	C1-O5-C5	3.47	116.90	112.19
3	B	2	NAG	C1-C2-N2	3.42	116.33	110.49
3	B	2	NAG	C2-N2-C7	3.34	127.66	122.90
3	B	1	NAG	O5-C1-C2	-3.14	106.33	111.29
3	A	1	NAG	C4-C3-C2	-3.14	106.42	111.02
3	B	1	NAG	C1-O5-C5	3.09	116.37	112.19
3	A	1	NAG	O5-C1-C2	-3.08	106.43	111.29
3	C	1	NAG	C4-C3-C2	3.04	115.47	111.02
3	B	2	NAG	O5-C1-C2	-2.80	106.87	111.29
3	B	1	NAG	O5-C5-C6	-2.58	103.16	107.20
3	B	2	NAG	C4-C3-C2	-2.18	107.82	111.02
3	C	1	NAG	O5-C5-C6	-2.15	103.84	107.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

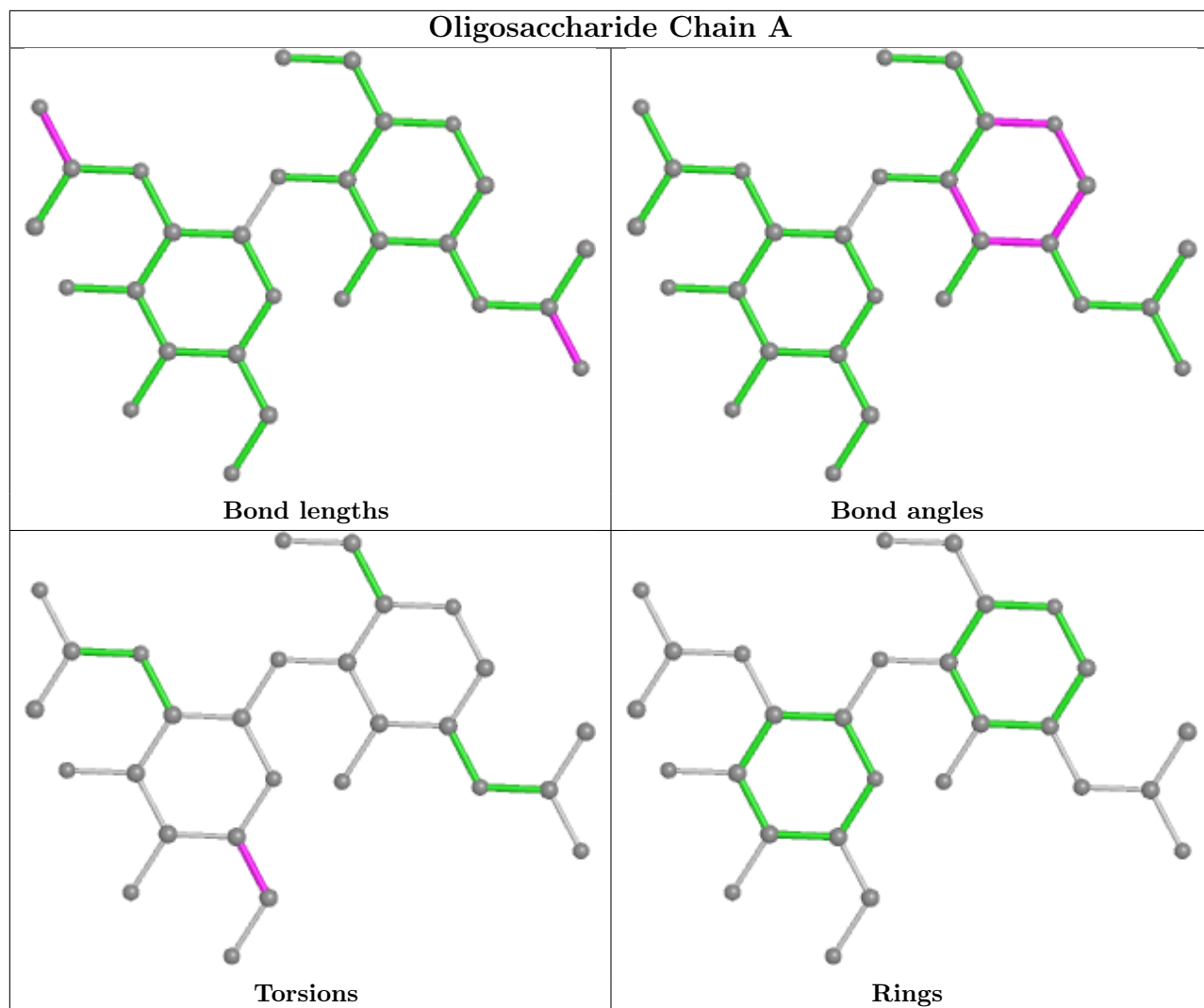
Mol	Chain	Res	Type	Atoms
3	A	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7

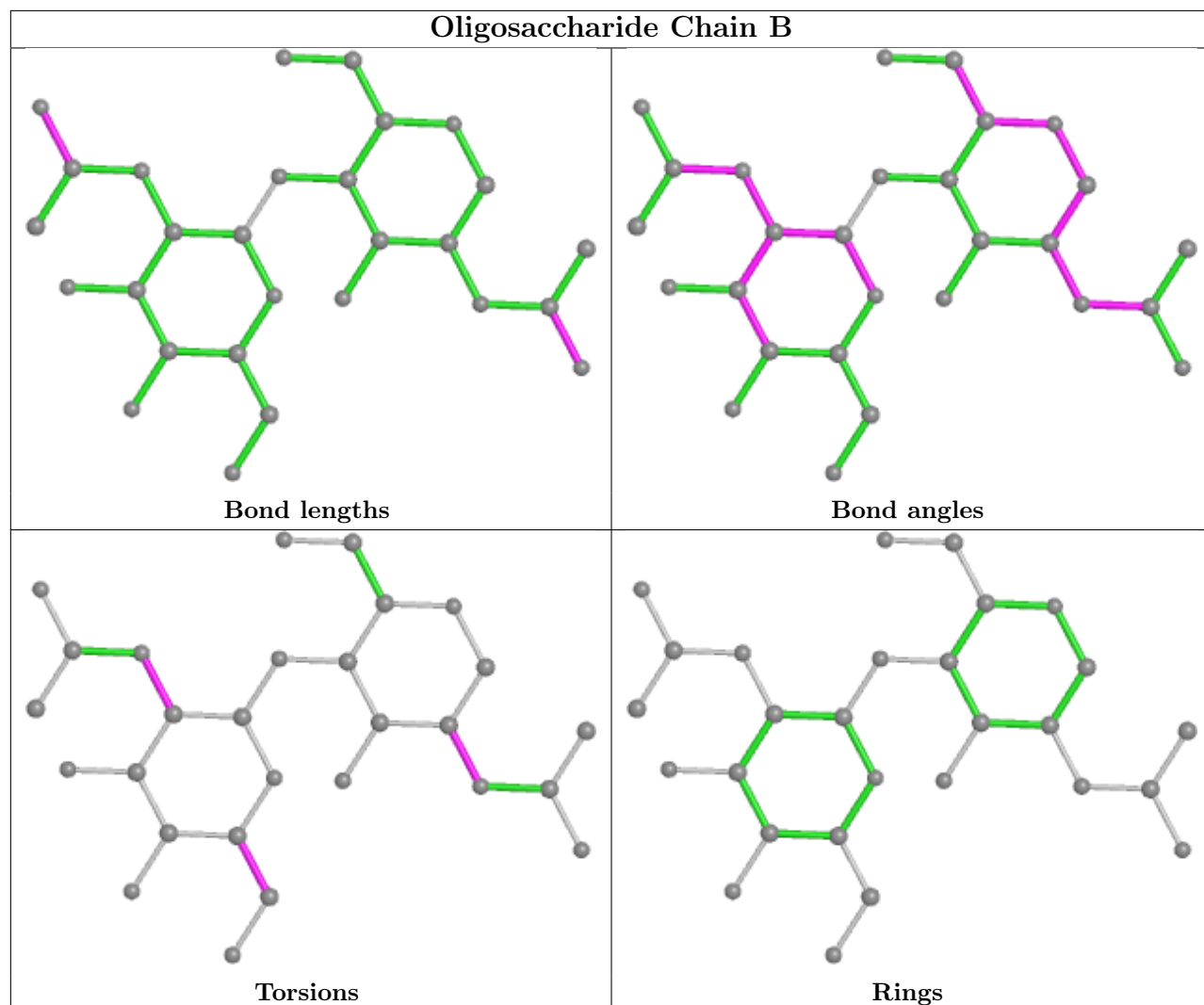
There are no ring outliers.

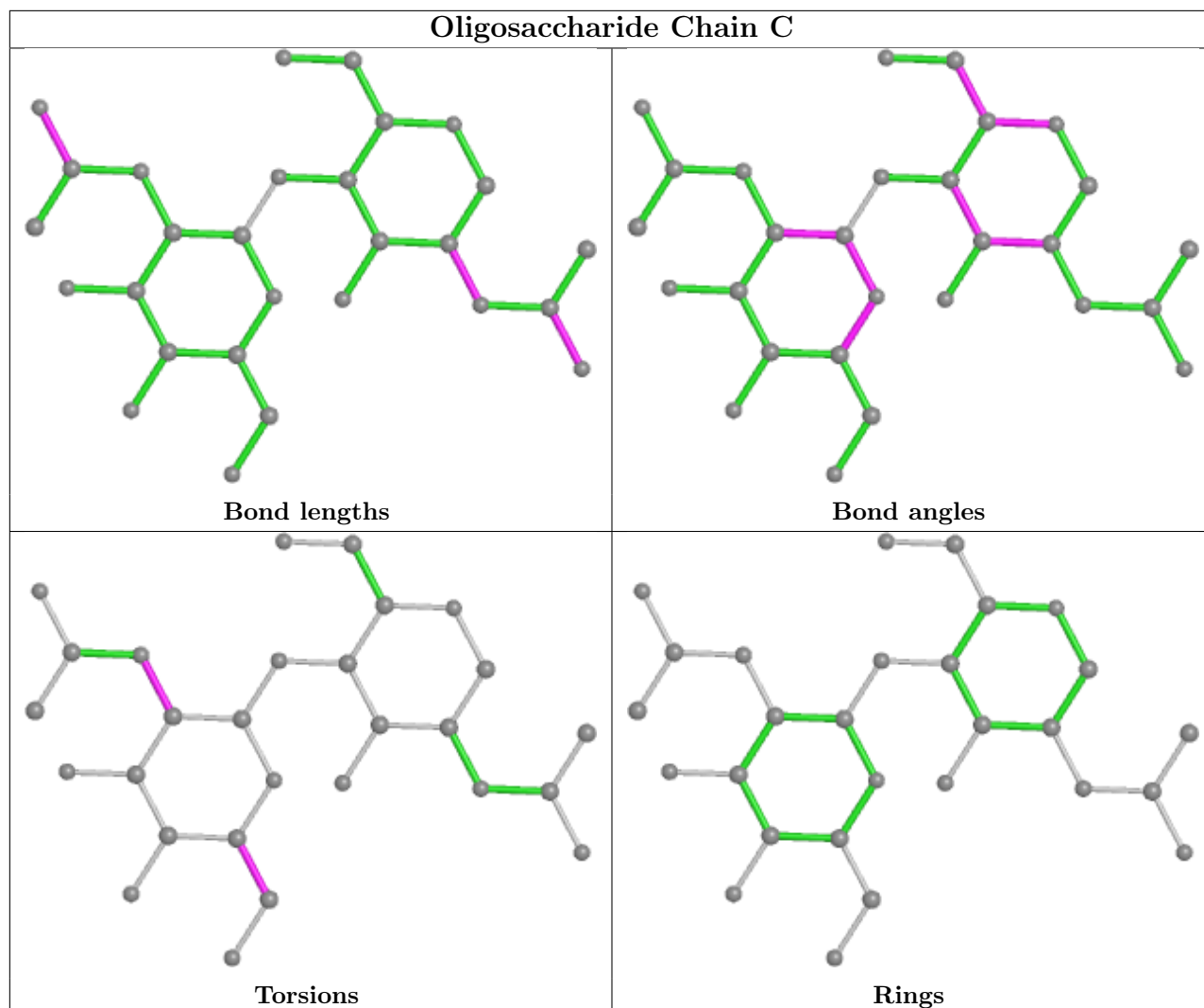
4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NAG	1	0
3	B	1	NAG	1	0
3	C	2	NAG	1	0
3	C	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

5 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	I	861	1	14,14,15	1.20	1 (7%)	17,19,21	0.82	0
4	NAG	I	801	1	14,14,15	1.34	1 (7%)	17,19,21	2.08	3 (17%)
4	NAG	L	861	2	14,14,15	1.20	1 (7%)	17,19,21	0.87	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	L	901	-	5,5,5	0.70	0	5,5,5	0.55	0
5	GOL	I	901	-	5,5,5	0.62	0	5,5,5	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	861	1	-	2/6/23/26	0/1/1/1
4	NAG	I	801	1	-	3/6/23/26	0/1/1/1
4	NAG	L	861	2	-	2/6/23/26	0/1/1/1
5	GOL	L	901	-	-	0/4/4/4	-
5	GOL	I	901	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	801	NAG	O7-C7	-3.91	1.14	1.23
4	I	861	NAG	O7-C7	-3.76	1.14	1.23
4	L	861	NAG	O7-C7	-3.72	1.14	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	801	NAG	C1-O5-C5	4.86	118.78	112.19
4	I	801	NAG	C2-N2-C7	4.72	129.62	122.90
4	I	801	NAG	C1-C2-N2	4.31	117.84	110.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	901	GOL	C1-C2-C3-O3
4	I	861	NAG	O5-C5-C6-O6
4	I	861	NAG	C4-C5-C6-O6
4	I	801	NAG	C1-C2-N2-C7
4	I	801	NAG	C4-C5-C6-O6
4	L	861	NAG	C4-C5-C6-O6
4	L	861	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	801	NAG	O5-C5-C6-O6
5	I	901	GOL	O2-C2-C3-O3
5	I	901	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	901	GOL	1	0
5	I	901	GOL	2	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	I	422/432 (97%)	0.48	43 (10%) <b>6</b> <b>3</b>	39, 82, 125, 145	0
2	L	409/432 (94%)	0.34	37 (9%) <b>9</b> <b>5</b>	35, 68, 116, 156	0
All	All	831/864 (96%)	0.41	80 (9%) <b>8</b> <b>4</b>	35, 75, 122, 156	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	207	ILE	10.4
1	I	174	ASP	6.9
2	L	400	VAL	6.9
2	L	398	ASN	5.1
2	L	90	THR	4.9
1	I	36	SER	4.2
1	I	206	ALA	4.1
1	I	90	THR	4.1
1	I	135	GLN	4.0
1	I	133	LYS	3.7
2	L	399	ARG	3.7
1	I	363	TYR	3.6
2	L	397	PRO	3.5
1	I	161	ILE	3.5
1	I	357	GLU	3.4
1	I	134	ALA	3.4
1	I	43	ALA	3.3
2	L	404	ALA	3.2
2	L	88	ALA	3.1
1	I	8	CYS	3.0
2	L	86	ALA	2.9
2	L	412	ILE	2.8
1	I	5	VAL	2.8
1	I	208	ASN	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	277	ASP	2.8
2	L	134	ALA	2.8
1	I	146	LEU	2.7
1	I	199	THR	2.7
2	L	84	SER	2.7
2	L	402	PHE	2.7
2	L	388	VAL	2.7
1	I	185	ALA	2.7
2	L	85	THR	2.6
1	I	88	ALA	2.6
1	I	367	ALA	2.6
2	L	339	GLY	2.6
1	I	156	GLU	2.6
2	L	92	LEU	2.6
2	L	135	ASN	2.6
2	L	243	ASP	2.5
1	I	210	LEU	2.5
1	I	385	SER	2.5
2	L	25	SER	2.5
1	I	87	PHE	2.5
1	I	215	LEU	2.5
2	L	93	GLY	2.5
2	L	26	PRO	2.5
1	I	26	PRO	2.5
1	I	182	SER	2.4
2	L	386	THR	2.4
1	I	157	THR	2.4
2	L	17	MET	2.4
1	I	344	PHE	2.4
2	L	91	LYS	2.4
1	I	29	LYS	2.4
1	I	165	VAL	2.4
1	I	276	GLY	2.4
2	L	82	SER	2.4
1	I	89	MET	2.3
1	I	86	ALA	2.3
1	I	211	THR	2.3
2	L	283	LEU	2.3
2	L	410	VAL	2.2
1	I	178	ASN	2.2
2	L	120	HIS	2.2
1	I	188	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	330	SER	2.2
1	I	23	TYR	2.2
1	I	205	GLU	2.2
2	L	240	TYR	2.2
2	L	387	ALA	2.1
2	L	215	LEU	2.1
2	L	83	ILE	2.1
2	L	405	ASN	2.1
2	L	87	PHE	2.1
2	L	411	PHE	2.1
1	I	366	ASP	2.1
2	L	79	SER	2.0
2	L	430	CYS	2.0
1	I	39	LYS	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](#)

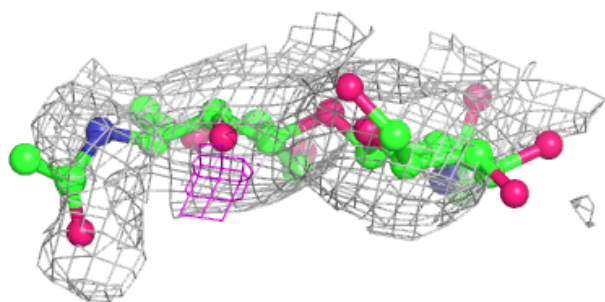
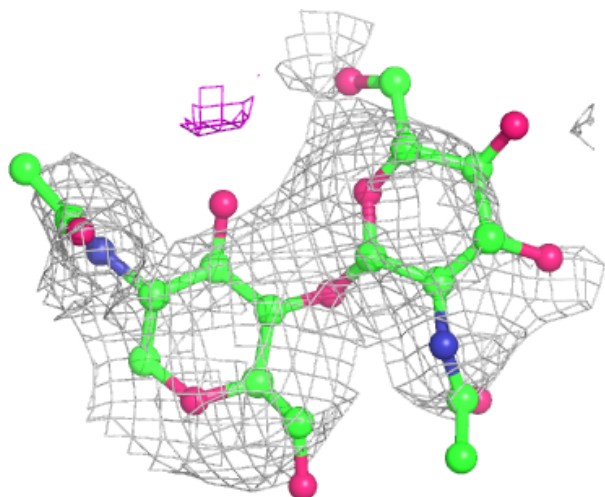
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	NAG	A	1	14/15	0.71	0.37	124,126,130,135	0
3	NAG	A	2	14/15	0.75	0.64	139,142,145,146	0
3	NAG	B	1	14/15	0.76	0.34	120,123,130,137	0
3	NAG	C	2	14/15	0.79	0.47	118,125,127,128	0
3	NAG	B	2	14/15	0.87	0.60	144,148,156,157	0
3	NAG	C	1	14/15	0.89	0.14	87,94,101,108	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.

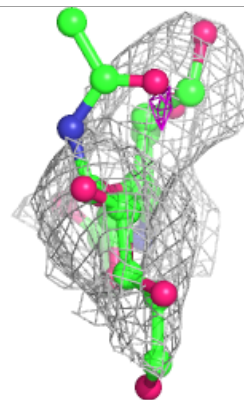
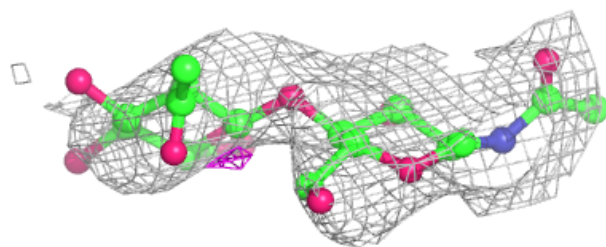
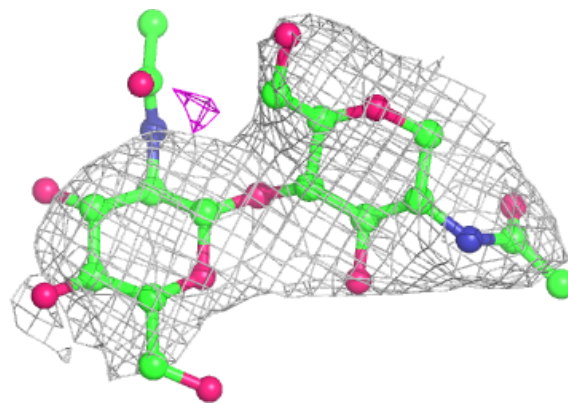
**Electron density around Chain A:**

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

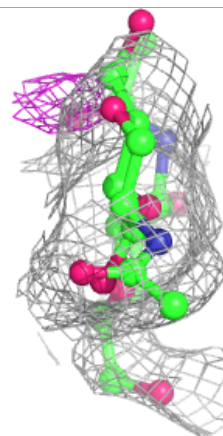
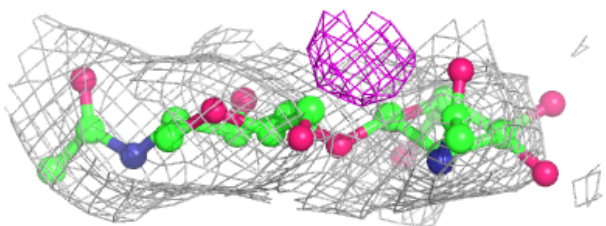
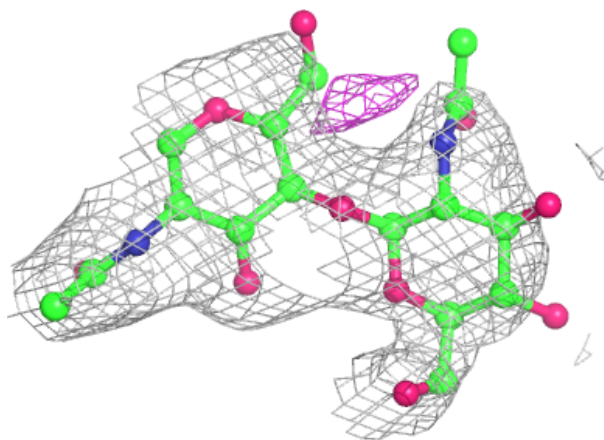


**Electron density around Chain B:**

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

**Electron density around Chain C:**

$2mF_o-DF_c$  (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
4	NAG	L	861	14/15	0.56	0.36	118,120,124,126	0
4	NAG	I	861	14/15	0.61	0.43	147,150,154,154	0
5	GOL	L	901	6/6	0.61	0.42	76,81,85,88	0
5	GOL	I	901	6/6	0.75	0.61	91,93,94,94	0
4	NAG	I	801	14/15	0.89	0.38	128,132,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.