



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:28 PM EDT

PDB ID : 1FQ5  
Title : X-ray structure of a cyclic statine inhibitor PD-129,541 bound to yeast proteinase A  
Authors : Cronin, N.B.; Badasso, M.O.; Tickle, I.J.; Dreyer, T.; Hoover, D.J.; Rosati, R.L.; Humblet, C.C.; Lunney, E.A.; Cooper, J.B.  
Deposited on : 2000-09-03  
Resolution : 2.40 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

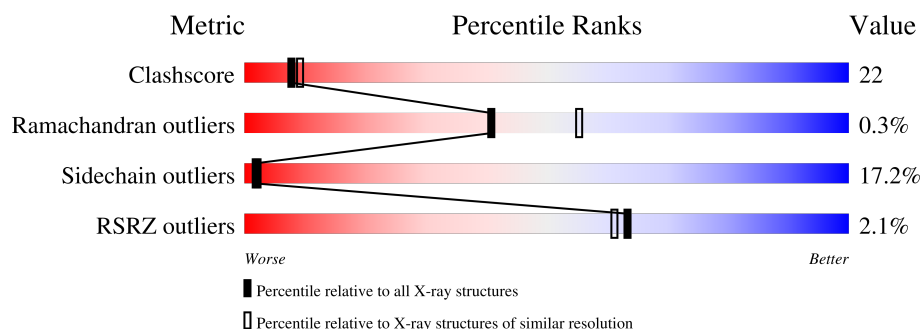
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	329	
2	B	5	

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	MAN	B	3	X	-	-	-
2	MAN	B	4	X	-	X	-
3	NAG	A	337	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2770 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.

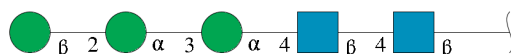
- Molecule 1 is a protein called SACCHAROPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2528	1618	396	508	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	conflict	UNP P07267

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



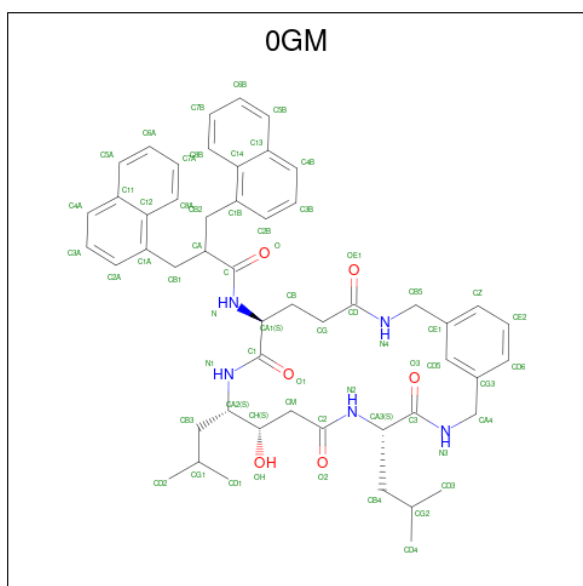
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N-[(5S,9S,10S,13S)-9-hydroxy-5,10-bis(2-methylpropyl)-4,7,12,16-tetraoxo-3,6,11,17-tetraazabicyclo[17.3.1]tricoso-1(23),19,21-trien-13-yl]-3-(naphthalen-1-yl)-2-(naphthalen-1-ylmethyl)propanamide (three-letter code: OGM) (formula: C<sub>51</sub>H<sub>61</sub>N<sub>5</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			62	51	5	6		

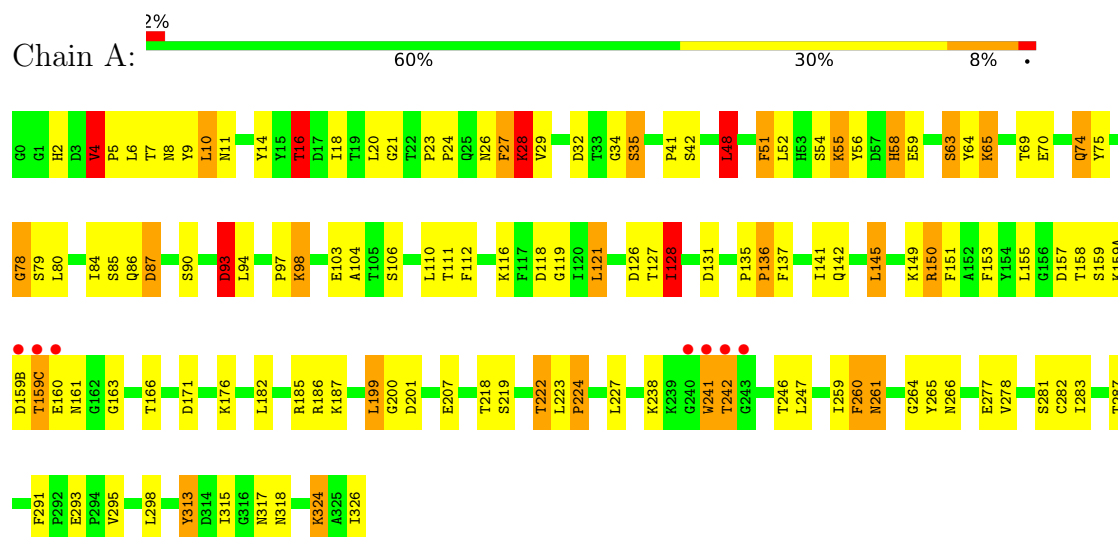
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total 105	O 105	0	0

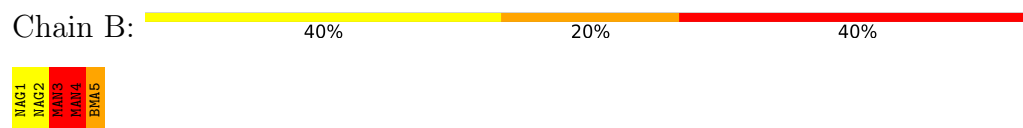
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: SACCHAROPEPSIN



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.30Å 87.30Å 110.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.90 – 2.40 12.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.90-2.40) 89.9 (12.81-2.41)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.41Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.200 , 0.280 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 104.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.70	0/2592	1.56	40/3526 (1.1%)

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
1	A	4	0

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	TRP	CA-CB-CG	18.73	149.29	113.70
1	A	93	ASP	CB-CG-OD1	-11.52	107.94	118.30
1	A	4	VAL	CA-CB-CG2	9.95	125.82	110.90
1	A	153	PHE	CZ-CE2-CD2	8.72	130.56	120.10
1	A	186	ARG	CA-CB-CG	8.34	131.75	113.40
1	A	153	PHE	CG-CD2-CE2	-8.16	111.82	120.80
1	A	128	ILE	CB-CG1-CD1	-7.28	93.53	113.90
1	A	28	LYS	CD-CE-NZ	7.08	128.00	111.70
1	A	278	VAL	CA-CB-CG2	6.97	121.35	110.90
1	A	48	LEU	CB-CG-CD1	6.92	122.77	111.00
1	A	94	LEU	CB-CG-CD1	-6.80	99.43	111.00
1	A	116	LYS	CD-CE-NZ	6.74	127.20	111.70
1	A	182	LEU	CB-CG-CD2	6.63	122.27	111.00
1	A	78	GLY	C-N-CA	6.49	137.92	121.70
1	A	63	SER	N-CA-CB	6.45	120.17	110.50
1	A	155	LEU	CA-CB-CG	6.34	129.89	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	103	GLU	CA-CB-CG	6.24	127.13	113.40
1	A	200	GLY	C-N-CA	6.23	137.27	121.70
1	A	199	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	A	87	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	150	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	112	PHE	N-CA-CB	5.95	121.30	110.60
1	A	16	THR	CA-CB-CG2	5.86	120.61	112.40
1	A	145	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	A	186	ARG	CG-CD-NE	5.75	123.88	111.80
1	A	227	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	A	242	THR	CA-C-N	5.56	127.32	116.20
1	A	126	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	207	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	A	34	GLY	C-N-CA	5.32	135.01	121.70
1	A	199	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	295	VAL	CA-CB-CG1	-5.22	103.06	110.90
1	A	260	PHE	O-C-N	5.17	130.98	122.70
1	A	93	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	20	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	186	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	160	GLU	CB-CA-C	5.10	120.60	110.40
1	A	74	GLN	C-N-CA	5.07	134.38	121.70
1	A	171	ASP	CB-CG-OD1	5.06	122.85	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	16	THR	CB
1	A	63	SER	CA
1	A	112	PHE	CA
1	A	160	GLU	CA

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2400	99	3
2	B	61	0	50	12	0
3	A	14	0	13	4	0
4	A	62	0	61	7	0
5	A	105	0	0	6	3
All	All	2770	0	2524	113	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 22.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HB2	1:A:55:LYS:NZ	1.47	1.12
1:A:69:THR:HB	1:A:84:ILE:HD13	1.28	1.09
1:A:242:THR:O	1:A:242:THR:HG22	1.50	1.07
1:A:55:LYS:HB2	1:A:55:LYS:HZ3	1.02	1.05
1:A:242:THR:O	1:A:242:THR:CG2	2.16	0.91
1:A:86:GLN:HE21	1:A:98:LYS:HA	1.37	0.88
1:A:4:VAL:HG23	1:A:16:THR:HG21	1.59	0.84
1:A:259:ILE:HD13	3:A:337:NAG:H62	1.60	0.84
2:B:3:MAN:H3	2:B:3:MAN:O2	1.78	0.83
1:A:246:THR:HG22	1:A:283:ILE:HG22	1.59	0.82
1:A:69:THR:HB	1:A:84:ILE:CD1	2.09	0.81
1:A:5:PRO:O	1:A:16:THR:HG23	1.81	0.80
2:B:4:MAN:C2	2:B:5:BMA:C1	2.59	0.79
1:A:2:HIS:HD2	1:A:93:ASP:HB3	1.50	0.77
1:A:86:GLN:O	1:A:87:ASP:HB2	1.85	0.76
1:A:137:PHE:HE2	1:A:315:ILE:HG21	1.50	0.76
1:A:74:GLN:HG3	1:A:74:GLN:O	1.85	0.75
1:A:2:HIS:HD2	1:A:93:ASP:CB	2.00	0.75
1:A:261:ASN:HD22	1:A:261:ASN:C	1.93	0.72
1:A:2:HIS:CD2	1:A:93:ASP:HB3	2.25	0.71
1:A:51:PHE:C	1:A:51:PHE:CD1	2.64	0.71
1:A:324:LYS:HG2	5:A:549:HOH:O	1.90	0.70
2:B:4:MAN:C2	2:B:4:MAN:O2	2.40	0.70
1:A:41:PRO:HB2	1:A:55:LYS:HG3	1.74	0.70
1:A:41:PRO:HG2	1:A:54:SER:O	1.93	0.68
1:A:23:PRO:HB2	1:A:24:PRO:HD2	1.76	0.68
1:A:80:LEU:HD12	1:A:104:ALA:HB2	1.75	0.67
2:B:3:MAN:O2	2:B:3:MAN:C1	2.42	0.67
2:B:4:MAN:O2	2:B:4:MAN:C1	2.43	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:OD2	1:A:35:SER:HB2	1.94	0.67
5:A:657:HOH:O	2:B:5:BMA:H5	1.95	0.67
1:A:261:ASN:HD21	1:A:264:GLY:H	1.43	0.67
2:B:3:MAN:O2	2:B:3:MAN:C2	2.43	0.66
1:A:42:SER:O	1:A:55:LYS:HG2	1.94	0.66
1:A:86:GLN:NE2	1:A:98:LYS:HB3	2.11	0.66
1:A:259:ILE:HD13	3:A:337:NAG:C6	2.27	0.64
1:A:55:LYS:NZ	1:A:55:LYS:CB	2.40	0.64
1:A:137:PHE:HE2	1:A:315:ILE:CG2	2.10	0.64
1:A:86:GLN:HE21	1:A:98:LYS:CA	2.09	0.64
1:A:10:LEU:O	1:A:11:ASN:HB2	1.96	0.63
1:A:128:ILE:O	1:A:128:ILE:HG12	1.98	0.63
2:B:3:MAN:O2	2:B:3:MAN:C3	2.48	0.62
1:A:259:ILE:CD1	3:A:337:NAG:H62	2.28	0.62
2:B:4:MAN:O2	2:B:4:MAN:C3	2.49	0.61
1:A:313:TYR:N	1:A:313:TYR:CD1	2.72	0.58
1:A:127:THR:HG21	5:A:653:HOH:O	2.03	0.57
1:A:218:THR:HG23	4:A:338:0GM:O	2.04	0.57
4:A:338:0GM:C2A	4:A:338:0GM:HB2	2.33	0.56
1:A:69:THR:O	1:A:84:ILE:HD12	2.04	0.56
1:A:69:THR:CB	1:A:84:ILE:HD13	2.18	0.56
1:A:145:LEU:HD23	1:A:145:LEU:N	2.18	0.56
1:A:84:ILE:HG22	1:A:85:SER:N	2.21	0.55
1:A:261:ASN:ND2	1:A:264:GLY:H	2.05	0.55
2:B:4:MAN:O2	2:B:4:MAN:O5	2.25	0.55
1:A:201:ASP:HB2	5:A:557:HOH:O	2.07	0.54
1:A:65:LYS:O	1:A:65:LYS:HG3	2.04	0.54
1:A:10:LEU:HD13	5:A:501:HOH:O	2.07	0.53
1:A:141:ILE:HD13	1:A:149:LYS:HD3	1.91	0.52
1:A:261:ASN:C	1:A:261:ASN:ND2	2.62	0.52
2:B:4:MAN:C3	2:B:5:BMA:C1	2.88	0.52
1:A:48:LEU:HD11	1:A:52:LEU:HD11	1.92	0.52
1:A:51:PHE:CD1	1:A:51:PHE:O	2.63	0.52
1:A:9:TYR:CZ	1:A:10:LEU:HD22	2.46	0.51
1:A:58:HIS:HB2	1:A:64:TYR:CG	2.45	0.51
1:A:55:LYS:HB2	1:A:55:LYS:HZ2	1.62	0.51
1:A:157:ASP:HB3	1:A:159(A):LYS:HB3	1.93	0.51
1:A:4:VAL:CG2	1:A:16:THR:HG21	2.38	0.49
1:A:7:THR:O	1:A:14:TYR:HA	2.13	0.49
1:A:150:ARG:NH2	5:A:571:HOH:O	2.45	0.48
1:A:75:TYR:HB2	1:A:78:GLY:O	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:MAN:O2	2:B:4:MAN:C4	2.62	0.47
1:A:277:GLU:HG3	1:A:282:CYS:SG	2.54	0.47
1:A:84:ILE:HD11	1:A:131:ASP:OD2	2.15	0.47
1:A:16:THR:O	1:A:28:LYS:HA	2.15	0.47
1:A:84:ILE:CG2	1:A:85:SER:N	2.77	0.47
1:A:21:GLY:HA2	1:A:87:ASP:OD1	2.14	0.47
1:A:222:THR:HA	1:A:287:THR:O	2.15	0.47
1:A:58:HIS:HD2	1:A:59:GLU:H	1.63	0.46
1:A:317:ASN:HD22	1:A:317:ASN:HA	1.34	0.46
1:A:29:VAL:HA	1:A:119:GLY:O	2.15	0.46
1:A:74:GLN:O	4:A:338:0GM:H13	2.16	0.46
1:A:137:PHE:CE2	1:A:315:ILE:HG21	2.40	0.46
1:A:27:PHE:HZ	1:A:56:TYR:HB2	1.80	0.46
1:A:6:LEU:HB2	1:A:163:GLY:HA3	1.98	0.46
1:A:121:LEU:C	1:A:121:LEU:HD12	2.36	0.46
1:A:86:GLN:HE21	1:A:98:LYS:CB	2.28	0.46
1:A:97:PRO:C	1:A:98:LYS:HG2	2.35	0.45
1:A:317:ASN:O	1:A:318:ASN:HB2	2.16	0.45
1:A:218:THR:HG23	4:A:338:0GM:HA1	2.00	0.44
1:A:159(A):LYS:HG2	1:A:159(B):ASP:N	2.31	0.44
1:A:58:HIS:CD2	1:A:58:HIS:H	2.36	0.43
1:A:135:PRO:HA	1:A:136:PRO:HD3	1.76	0.43
4:A:338:0GM:C12	4:A:338:0GM:H8B	2.47	0.43
1:A:151:PHE:HA	1:A:166:THR:O	2.19	0.43
1:A:23:PRO:CB	1:A:24:PRO:HD2	2.46	0.42
1:A:42:SER:HB3	1:A:104:ALA:O	2.20	0.42
1:A:42:SER:C	1:A:55:LYS:HG2	2.40	0.42
1:A:86:GLN:HE21	1:A:98:LYS:HB3	1.81	0.42
1:A:23:PRO:CB	1:A:24:PRO:CD	2.97	0.42
1:A:260:PHE:O	1:A:266:ASN:HA	2.20	0.42
1:A:27:PHE:CD1	1:A:27:PHE:N	2.89	0.41
1:A:58:HIS:HB2	1:A:64:TYR:CD2	2.56	0.41
1:A:266:ASN:ND2	3:A:337:NAG:C7	2.83	0.41
1:A:8:ASN:OD1	1:A:8:ASN:C	2.59	0.41
1:A:84:ILE:CG2	1:A:85:SER:H	2.33	0.41
1:A:10:LEU:O	1:A:11:ASN:CB	2.66	0.41
1:A:2:HIS:CD2	1:A:93:ASP:CB	2.89	0.40
1:A:291:PHE:CZ	4:A:338:0GM:HB5	2.56	0.40
1:A:261:ASN:HA	1:A:265:TYR:O	2.21	0.40
1:A:18:ILE:HG12	1:A:29:VAL:CG2	2.52	0.40
1:A:128:ILE:HG12	4:A:338:0GM:HD4B	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:CD1	1:A:104:ALA:HB2	2.49	0.40
1:A:223:LEU:O	1:A:224:PRO:C	2.58	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:149:LYS:CE	5:A:616:HOH:O[3_565]	0.79	1.41
1:A:149:LYS:NZ	5:A:616:HOH:O[3_565]	0.89	1.31
1:A:149:LYS:CD	5:A:616:HOH:O[3_565]	1.76	0.44

## 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	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	41 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159(C)	THR

### 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	268/268 (100%)	222 (83%)	46 (17%)	<b>2</b> <b>2</b>

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	10	LEU
1	A	16	THR
1	A	26	ASN
1	A	27	PHE
1	A	28	LYS
1	A	35	SER
1	A	48	LEU
1	A	51	PHE
1	A	55	LYS
1	A	58	HIS
1	A	63	SER
1	A	65	LYS
1	A	70	GLU
1	A	79	SER
1	A	90	SER
1	A	93	ASP
1	A	98	LYS
1	A	106	SER
1	A	110	LEU
1	A	111	THR
1	A	118	ASP
1	A	121	LEU
1	A	128	ILE
1	A	136	PRO
1	A	142	GLN
1	A	158	THR
1	A	159	SER
1	A	159(C)	THR
1	A	161	ASN
1	A	176	LYS
1	A	185	ARG
1	A	187	LYS
1	A	199	LEU
1	A	219	SER
1	A	222	THR
1	A	224	PRO
1	A	238	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	241	TRP
1	A	247	LEU
1	A	261	ASN
1	A	281	SER
1	A	293	GLU
1	A	313	TYR
1	A	324	LYS
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	43	ASN
1	A	58	HIS
1	A	86	GLN
1	A	142	GLN
1	A	161	ASN
1	A	232	ASN
1	A	261	ASN
1	A	317	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](#)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	B	1	2,1	14,14,15	1.16	1 (7%)	17,19,21	2.18	5 (29%)
2	NAG	B	2	2	14,14,15	1.18	1 (7%)	17,19,21	2.28	6 (35%)
2	MAN	B	3	2	11,11,12	14.30	2 (18%)	15,15,17	6.99	4 (26%)
2	MAN	B	4	2	11,11,12	13.93	4 (36%)	15,15,17	7.10	8 (53%)
2	BMA	B	5	2	11,11,12	1.57	1 (9%)	15,15,17	4.37	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	MAN	B	3	2	2/2/4/5	2/2/19/22	0/1/1/1
2	MAN	B	4	2	2/2/4/5	2/2/19/22	0/1/1/1
2	BMA	B	5	2	-	1/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	MAN	O2-C2	47.34	2.43	1.43
2	B	4	MAN	O2-C2	45.83	2.40	1.43
2	B	4	MAN	C2-C3	-4.39	1.46	1.52
2	B	5	BMA	C2-C3	-4.13	1.46	1.52
2	B	4	MAN	C4-C3	-2.84	1.45	1.52
2	B	2	NAG	C1-C2	-2.49	1.48	1.52
2	B	3	MAN	O5-C1	2.15	1.47	1.43
2	B	4	MAN	O4-C4	2.03	1.47	1.43
2	B	1	NAG	O5-C5	2.00	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MAN	O2-C2-C1	-18.47	71.37	109.15
2	B	3	MAN	O2-C2-C3	-18.25	73.59	110.14
2	B	4	MAN	O2-C2-C1	-17.86	72.60	109.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	O2-C2-C3	-16.92	76.25	110.14
2	B	5	BMA	C1-O5-C5	11.68	128.02	112.19
2	B	5	BMA	C1-C2-C3	9.60	121.46	109.67
2	B	4	MAN	C2-C3-C4	7.74	124.29	110.89
2	B	3	MAN	C1-O5-C5	6.36	120.80	112.19
2	B	5	BMA	C2-C3-C4	5.70	120.76	110.89
2	B	4	MAN	C1-C2-C3	5.46	116.37	109.67
2	B	2	NAG	C1-O5-C5	5.09	119.09	112.19
2	B	4	MAN	O3-C3-C2	5.06	119.69	109.99
2	B	1	NAG	C1-O5-C5	4.83	118.74	112.19
2	B	2	NAG	C2-N2-C7	-4.80	116.07	122.90
2	B	1	NAG	O5-C1-C2	-4.43	104.29	111.29
2	B	4	MAN	O5-C1-C2	3.62	116.36	110.77
2	B	2	NAG	O5-C1-C2	3.29	116.48	111.29
2	B	5	BMA	O2-C2-C3	3.25	116.64	110.14
2	B	1	NAG	C2-N2-C7	-3.10	118.49	122.90
2	B	2	NAG	C3-C4-C5	-2.88	105.09	110.24
2	B	1	NAG	O5-C5-C6	-2.88	102.70	107.20
2	B	1	NAG	C3-C4-C5	-2.48	105.82	110.24
2	B	2	NAG	O5-C5-C6	-2.47	103.33	107.20
2	B	4	MAN	C1-O5-C5	2.25	115.25	112.19
2	B	2	NAG	O6-C6-C5	-2.17	103.83	111.29
2	B	4	MAN	O6-C6-C5	-2.12	104.01	111.29
2	B	3	MAN	C2-C3-C4	2.08	114.50	110.89

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3	MAN	C1
2	B	3	MAN	C3
2	B	4	MAN	C3
2	B	4	MAN	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	3	MAN	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

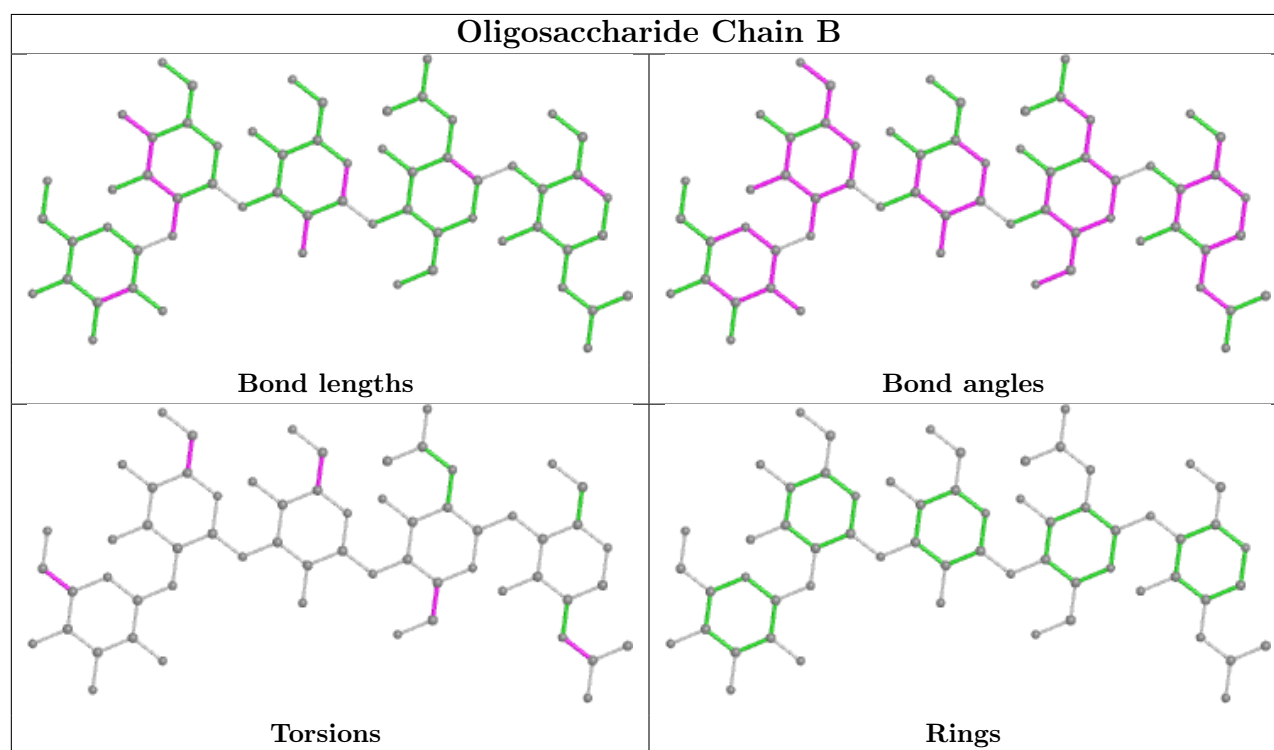
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	BMA	3	0
2	B	4	MAN	7	0
2	B	3	MAN	4	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](#)

2 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	0GM	A	338	-	67,67,67	1.72	4 (5%)	88,92,92	3.12	31 (35%)
3	NAG	A	337	1	14,14,15	0.96	0	17,19,21	2.38	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0GM	A	338	-	-	11/63/63/63	0/5/6/6
3	NAG	A	337	1	1/1/5/7	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	338	0GM	C1-N1	11.13	1.58	1.34
4	A	338	0GM	C14-C13	-3.04	1.37	1.43
4	A	338	0GM	C2B-C1B	2.57	1.42	1.37
4	A	338	0GM	CA4-N3	-2.06	1.42	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	338	0GM	CA2-N1-C1	-12.94	100.21	123.07
4	A	338	0GM	CE1-CB5-N4	12.49	139.80	113.05
4	A	338	0GM	C3A-C4A-C11	8.11	133.13	120.44
4	A	338	0GM	O1-C1-N1	8.03	137.81	122.93
4	A	338	0GM	CA1-C1-N1	-6.99	101.38	116.70
4	A	338	0GM	C4A-C11-C12	-6.53	110.53	119.12
4	A	338	0GM	CA4-N3-C3	6.12	131.14	122.34
3	A	337	NAG	O5-C5-C4	5.73	124.77	110.83
4	A	338	0GM	CZ-CE1-CD5	4.63	125.03	118.54
4	A	338	0GM	C4A-C3A-C2A	-4.60	113.66	120.99
3	A	337	NAG	C1-O5-C5	4.53	118.33	112.19
4	A	338	0GM	C1A-CB1-CA	-4.52	108.32	114.05
4	A	338	0GM	CG3-CA4-N3	4.40	122.47	113.05
4	A	338	0GM	CB5-CE1-CD5	-3.84	112.35	120.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	337	NAG	C2-N2-C7	-3.81	117.47	122.90
4	A	338	0GM	CA1-N-C	3.50	129.16	121.67
4	A	338	0GM	CZ-CE2-CD6	-3.30	115.56	120.25
3	A	337	NAG	O5-C1-C2	3.03	116.07	111.29
4	A	338	0GM	CE2-CD6-CG3	3.02	125.27	120.63
4	A	338	0GM	CM-C2-N2	2.93	120.17	116.33
4	A	338	0GM	C5A-C11-C12	2.90	122.93	119.12
4	A	338	0GM	O-C-N	2.72	127.96	122.93
3	A	337	NAG	O3-C3-C4	-2.69	104.12	110.35
4	A	338	0GM	C7B-C6B-C5B	-2.65	116.72	120.44
4	A	338	0GM	CA-C-N	-2.59	111.73	116.21
3	A	337	NAG	O5-C5-C6	-2.45	103.37	107.20
4	A	338	0GM	CG-CD-N4	2.37	120.41	116.42
4	A	338	0GM	C1A-C12-C11	2.37	121.92	118.98
4	A	338	0GM	OE1-CD-CG	-2.33	117.76	122.02
4	A	338	0GM	CB2-C1B-C2B	-2.32	115.90	119.86
4	A	338	0GM	O2-C2-CM	-2.30	118.13	121.50
4	A	338	0GM	CG-CB-CA1	-2.24	108.97	113.16
4	A	338	0GM	C5B-C13-C4B	-2.16	118.15	123.19
4	A	338	0GM	C6B-C7B-C8B	2.07	123.34	120.44
4	A	338	0GM	CB1-C1A-C12	-2.04	117.54	120.76
4	A	338	0GM	CD6-CG3-CD5	-2.03	115.69	118.54
4	A	338	0GM	CB-CA1-N	2.02	114.96	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	337	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	338	0GM	N1-CA2-CB3-CG1
4	A	338	0GM	CB3-CA2-CH-OH
4	A	338	0GM	CB3-CA2-CH-CM
3	A	337	NAG	O7-C7-N2-C2
3	A	337	NAG	C8-C7-N2-C2
3	A	337	NAG	O5-C5-C6-O6
3	A	337	NAG	C1-C2-N2-C7
4	A	338	0GM	CA2-CB3-CG1-CD1
4	A	338	0GM	CA1-CB-CG-CD
4	A	338	0GM	CA2-CB3-CG1-CD2

*Continued on next page...*

*Continued from previous page...*

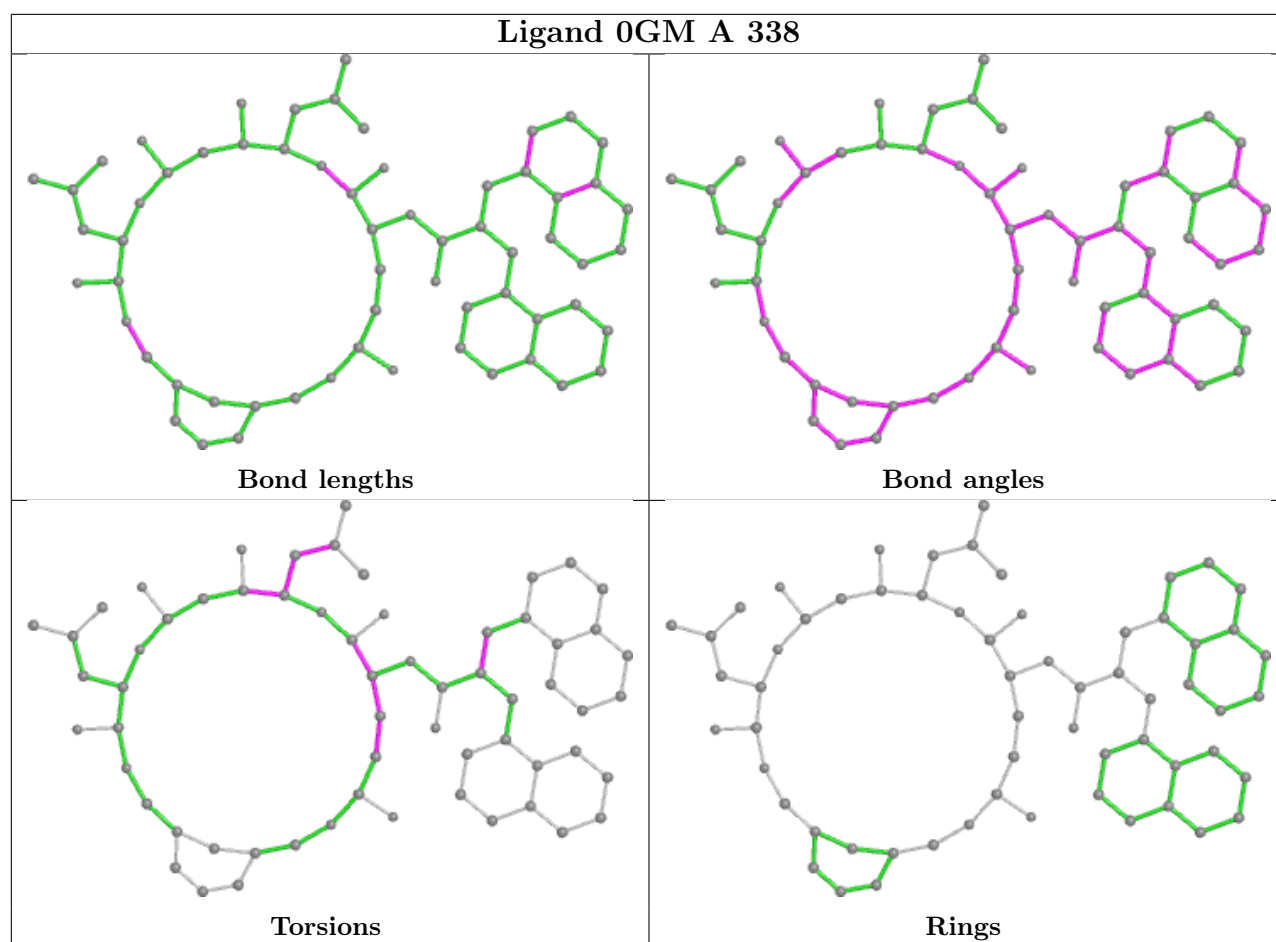
Mol	Chain	Res	Type	Atoms
4	A	338	0GM	O1-C1-CA1-N
4	A	338	0GM	N1-CA2-CH-OH
4	A	338	0GM	N1-C1-CA1-N
4	A	338	0GM	N-CA1-CB-CG
4	A	338	0GM	C-CA-CB2-C1B
3	A	337	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	338	0GM	7	0
3	A	337	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	329/329 (100%)	-0.72	7 (2%) 63 61	11, 34, 76, 141	4 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	TRP	12.3
1	A	242	THR	5.6
1	A	243	GLY	5.2
1	A	160	GLU	3.6
1	A	240	GLY	2.7
1	A	159(B)	ASP	2.5
1	A	159(C)	THR	2.1

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

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

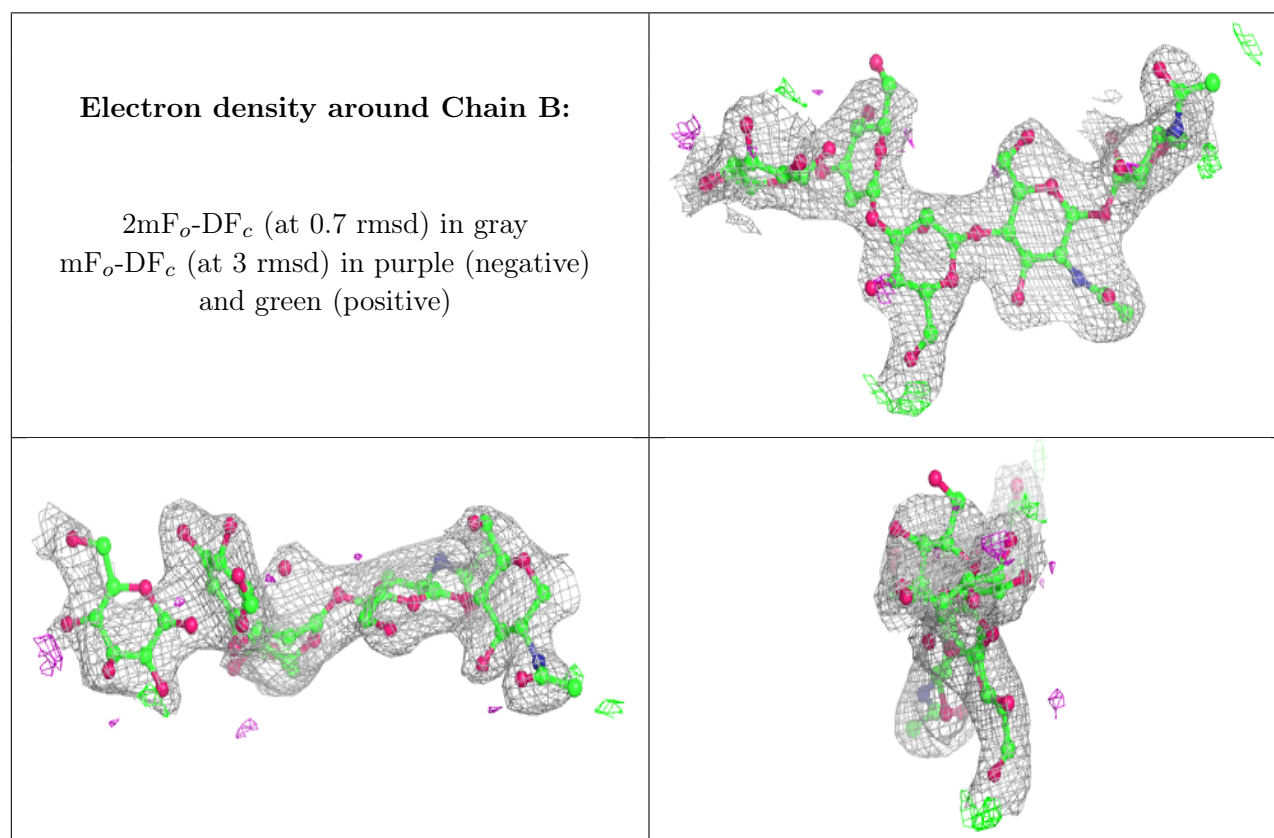
### 6.3 Carbohydrates [i](#)

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	B	5	11/12	0.79	0.28	39,86,157,157	0
2	MAN	B	3	11/12	0.90	0.18	31,53,80,103	0
2	NAG	B	1	14/15	0.93	0.17	33,49,89,124	0
2	MAN	B	4	11/12	0.95	0.14	38,52,153,157	0
2	NAG	B	2	14/15	0.97	0.10	21,35,68,143	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.



## 6.4 Ligands ⓘ

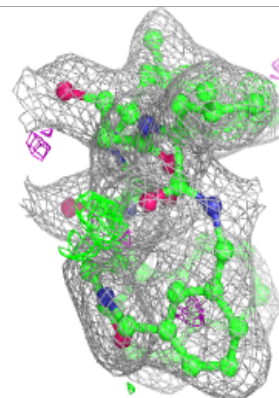
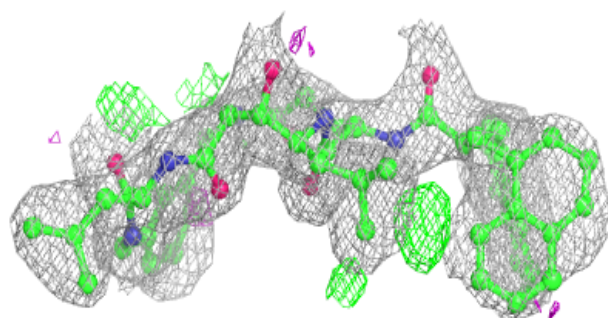
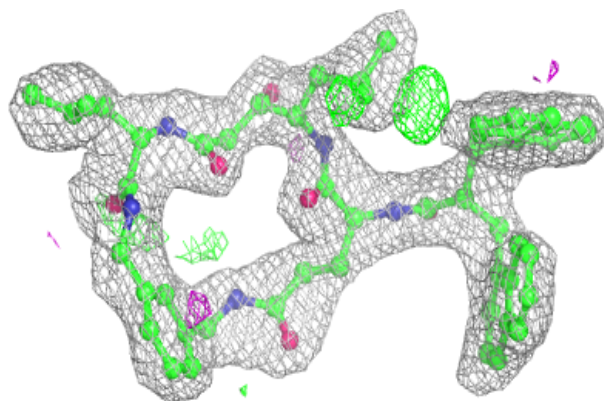
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	337	14/15	0.82	0.21	44,64,120,134	0
4	OGM	A	338	62/62	0.89	0.17	20,43,80,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 0GM A 338:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.