



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:25 PM BST

PDB ID : 1FQ4  
Title : CRYSTAL STRUCTURE OF A COMPLEX BETWEEN HYDROXYETHYLENE INHIBITOR CP-108,420 AND YEAST ASPARTIC PROTEINASE A  
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Deposited on : 2000-09-03  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

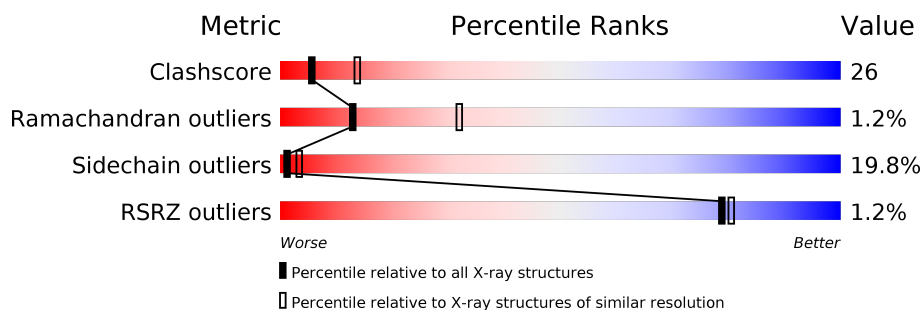
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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
3	2Y2	A	338	X	-	-	-
4	NAG	A	337	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2749 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.

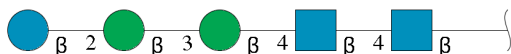
- Molecule 1 is a protein called SACCHAROPEPSIN.

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

There is a discrepancy between the modelled and reference sequences:

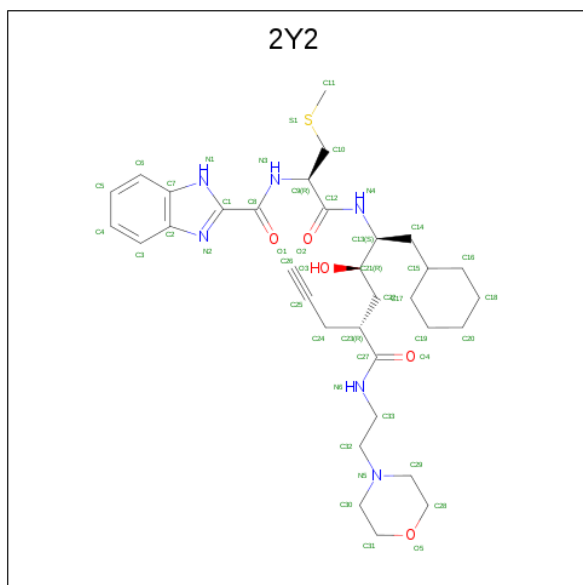
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	conflict	UNP P07267

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



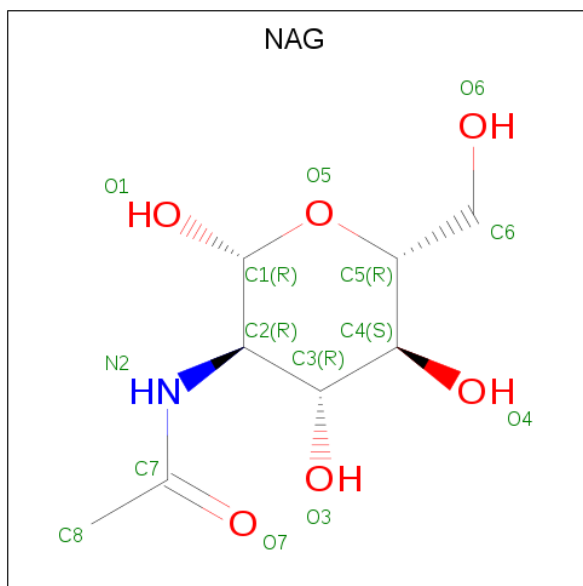
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

- Molecule 3 is N-[(2R)-1-{{(2S,3R,5R)-1-cyclohexyl-3-hydroxy-5-{{2-(morpholin-4-yl)ethyl}carbonyl}oct-7-yn-2-yl}amino}-3-(methylsulfonyl)-1-oxopropan-2-yl]-1H-benzimidazole-2-carboxamide (three-letter code: 2Y2) (formula: C<sub>33</sub>H<sub>48</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	45	33	6	5	1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

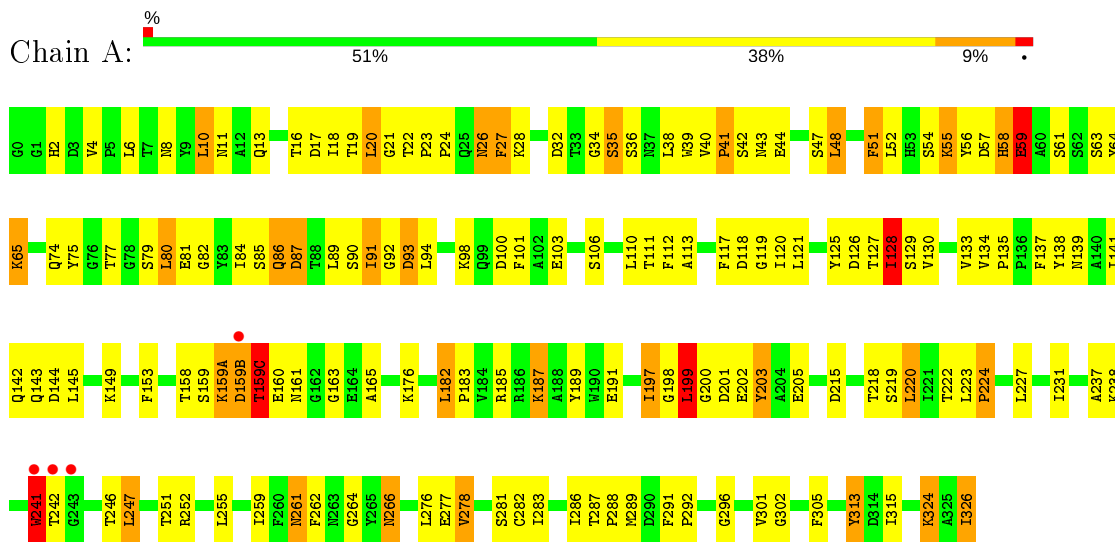
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	101	Total 101	O 101	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-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)-beta-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, $\alpha$ , $\beta$ , $\gamma$	86.91Å 86.91Å 110.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.20 – 2.70 15.16 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.20-2.70) 97.9 (15.16-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.73Å)	Xtrriage
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.170 , (Not available) 0.162 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 90.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: BGC, BMA, 2Y2, 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	0.66	0/2592	1.39	25/3526 (0.7%)

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	2	0

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	278	VAL	CA-CB-CG1	8.88	124.22	110.90
1	A	241	TRP	CA-CB-CG	7.31	127.60	113.70
1	A	128	ILE	CB-CG1-CD1	-7.26	93.57	113.90
1	A	200	GLY	C-N-CA	6.62	138.24	121.70
1	A	153	PHE	CG-CD2-CE2	-6.42	113.73	120.80
1	A	130	VAL	CA-CB-CG2	-6.41	101.29	110.90
1	A	241	TRP	N-CA-CB	6.27	121.89	110.60
1	A	34	GLY	C-N-CA	6.19	137.18	121.70
1	A	220	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	252	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	187	LYS	CD-CE-NZ	-5.80	98.36	111.70
1	A	145	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	159(C)	THR	C-N-CA	5.73	136.02	121.70
1	A	94	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	A	203	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	40	VAL	CA-CB-CG1	-5.66	102.41	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	A	199	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	160	GLU	N-CA-CB	5.37	120.27	110.60
1	A	159(C)	THR	O-C-N	5.35	131.27	122.70
1	A	266	ASN	C-N-CA	5.15	134.58	121.70
1	A	153	PHE	CB-CG-CD2	-5.09	117.23	120.80
1	A	93	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	A	197	ILE	O-C-N	-5.03	114.64	123.20
1	A	153	PHE	O-C-N	5.00	130.70	122.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	160	GLU	CA
1	A	241	TRP	CA

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	2528	0	2401	120	1
2	B	61	0	51	1	0
3	A	45	0	47	19	0
4	A	14	0	13	3	0
5	A	101	0	0	3	0
All	All	2749	0	2512	132	1

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 26.

All (132) 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)
3:A:338:2Y2:C27	3:A:338:2Y2:N6	1.76	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:338:2Y2:C27	3:A:338:2Y2:C33	2.30	1.08
3:A:338:2Y2:C23	3:A:338:2Y2:N6	2.23	1.01
1:A:242:THR:CG2	1:A:242:THR:O	2.09	0.99
1:A:261:ASN:C	1:A:261:ASN:HD22	1.69	0.95
1:A:242:THR:HG22	1:A:242:THR:O	1.66	0.92
3:A:338:2Y2:C22	3:A:338:2Y2:N6	2.37	0.88
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.57	0.86
1:A:16:THR:HG22	1:A:17:ASP:H	1.39	0.86
1:A:23:PRO:HB2	1:A:24:PRO:HD2	1.58	0.86
1:A:86:GLN:O	1:A:87:ASP:HB2	1.74	0.85
1:A:218:THR:HG23	3:A:338:2Y2:H9	1.59	0.82
1:A:10:LEU:O	1:A:11:ASN:HB2	1.81	0.80
1:A:41:PRO:HG2	1:A:54:SER:O	1.85	0.75
1:A:58:HIS:HB2	1:A:64:TYR:CD2	2.22	0.75
1:A:38:LEU:HD13	1:A:121:LEU:HG	1.68	0.74
1:A:32:ASP:OD2	1:A:35:SER:HB2	1.88	0.74
3:A:338:2Y2:C27	3:A:338:2Y2:C32	2.66	0.73
1:A:43:ASN:ND2	1:A:57:ASP:HA	2.04	0.72
1:A:48:LEU:HD11	1:A:52:LEU:CD1	2.20	0.72
1:A:259:ILE:CD1	4:A:337:NAG:H62	2.20	0.72
1:A:27:PHE:HZ	1:A:56:TYR:HB2	1.55	0.72
1:A:261:ASN:ND2	1:A:261:ASN:C	2.42	0.69
1:A:42:SER:HB2	1:A:103:GLU:CB	2.24	0.68
2:B:3:BMA:O2	2:B:4:BMA:C1	2.42	0.67
1:A:26:ASN:HD22	1:A:27:PHE:N	1.92	0.67
1:A:227:LEU:O	1:A:231:ILE:HD12	1.94	0.67
1:A:21:GLY:HA2	1:A:87:ASP:OD1	1.95	0.67
1:A:159(A):LYS:HG2	1:A:159(B):ASP:N	2.11	0.66
1:A:199:LEU:HD23	1:A:199:LEU:O	1.96	0.66
1:A:261:ASN:HD21	1:A:264:GLY:H	1.41	0.65
3:A:338:2Y2:H22A	3:A:338:2Y2:N6	2.12	0.65
3:A:338:2Y2:C22	3:A:338:2Y2:HN6	2.10	0.65
1:A:139:ASN:O	1:A:143:GLN:HG3	1.96	0.64
1:A:313:TYR:CD1	1:A:313:TYR:N	2.67	0.63
1:A:13:GLN:NE2	3:A:338:2Y2:H4	2.14	0.62
1:A:242:THR:HG23	1:A:242:THR:O	1.96	0.62
1:A:16:THR:HG22	1:A:17:ASP:N	2.13	0.62
1:A:27:PHE:CZ	1:A:56:TYR:HB2	2.35	0.60
1:A:48:LEU:HD11	1:A:52:LEU:HD11	1.83	0.59
1:A:23:PRO:HB2	1:A:24:PRO:CD	2.32	0.58
1:A:23:PRO:CB	1:A:24:PRO:CD	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PRO:CB	1:A:24:PRO:HD2	2.28	0.57
1:A:77:THR:HG23	3:A:338:2Y2:H10	1.87	0.57
1:A:51:PHE:C	1:A:51:PHE:CD1	2.77	0.57
1:A:19:THR:OG1	1:A:90:SER:HB3	2.04	0.57
1:A:39:TRP:CE2	1:A:80:LEU:HD11	2.41	0.56
1:A:16:THR:O	1:A:28:LYS:HA	2.05	0.56
1:A:43:ASN:HA	1:A:55:LYS:HD2	1.88	0.55
1:A:77:THR:HG23	3:A:338:2Y2:C10	2.36	0.55
1:A:84:ILE:CG2	1:A:85:SER:N	2.70	0.55
1:A:81:GLU:HB2	1:A:106:SER:HB3	1.88	0.55
1:A:18:ILE:HD13	1:A:89:LEU:CD1	2.37	0.54
1:A:287:THR:HG23	1:A:288:PRO:HD2	1.90	0.54
3:A:338:2Y2:HN6	3:A:338:2Y2:H22	1.71	0.54
1:A:189:TYR:CE1	3:A:338:2Y2:C26	2.91	0.54
1:A:261:ASN:HD22	1:A:262:PHE:N	2.06	0.53
1:A:125:TYR:O	1:A:128:ILE:HG22	2.08	0.53
3:A:338:2Y2:C27	3:A:338:2Y2:H32A	2.39	0.53
1:A:223:LEU:O	1:A:224:PRO:C	2.45	0.53
1:A:185:ARG:HG2	1:A:191:GLU:HG2	1.90	0.52
1:A:48:LEU:HD11	1:A:52:LEU:HD12	1.92	0.52
1:A:80:LEU:HD23	1:A:112:PHE:CE2	2.45	0.52
1:A:149:LYS:HB3	1:A:315:ILE:HG23	1.91	0.52
1:A:128:ILE:O	1:A:128:ILE:HG12	2.09	0.52
1:A:259:ILE:HD12	4:A:337:NAG:H62	1.92	0.52
3:A:338:2Y2:C27	3:A:338:2Y2:H33	2.31	0.51
1:A:39:TRP:CZ2	1:A:120:ILE:HD12	2.45	0.51
1:A:112:PHE:HB3	5:A:606:HOH:O	2.10	0.51
1:A:38:LEU:O	1:A:39:TRP:HB3	2.11	0.51
1:A:324:LYS:HG2	5:A:549:HOH:O	2.10	0.50
1:A:277:GLU:HG3	1:A:282:CYS:SG	2.51	0.50
1:A:127:THR:O	1:A:127:THR:HG22	2.12	0.50
1:A:301:VAL:HG12	1:A:305:PHE:HB3	1.94	0.50
1:A:137:PHE:HE2	1:A:315:ILE:HG21	1.76	0.50
1:A:110:LEU:O	1:A:113:ALA:HB3	2.12	0.49
1:A:56:TYR:CE1	1:A:58:HIS:HB3	2.47	0.49
1:A:18:ILE:HD13	1:A:89:LEU:HD11	1.95	0.48
1:A:58:HIS:HD2	1:A:59:GLU:H	1.61	0.48
1:A:251:THR:O	1:A:255:LEU:HG	2.14	0.48
1:A:326:ILE:OXT	1:A:326:ILE:HG22	2.12	0.48
1:A:135:PRO:HG2	1:A:138:TYR:CD1	2.49	0.48
1:A:326:ILE:OXT	1:A:326:ILE:CG2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:CD1	1:A:117:PHE:O	2.67	0.48
1:A:86:GLN:HG3	1:A:100:ASP:OD1	2.14	0.48
1:A:58:HIS:HB2	1:A:64:TYR:CG	2.47	0.47
1:A:237:ALA:HB2	1:A:247:LEU:HD22	1.96	0.47
1:A:48:LEU:O	1:A:48:LEU:HD12	2.15	0.47
1:A:133:VAL:O	1:A:135:PRO:HD3	2.15	0.47
1:A:84:ILE:HG22	1:A:85:SER:N	2.31	0.46
1:A:222:THR:HA	1:A:287:THR:O	2.15	0.46
1:A:4:VAL:HG22	1:A:165:ALA:HB3	1.97	0.46
1:A:36:SER:HB2	1:A:128:ILE:HG23	1.96	0.46
1:A:82:GLY:HA3	1:A:103:GLU:O	2.14	0.46
1:A:65:LYS:O	1:A:65:LYS:HG3	2.11	0.46
1:A:159(A):LYS:HB2	1:A:159(A):LYS:HE2	1.72	0.46
1:A:77:THR:OG1	3:A:338:2Y2:H19	2.16	0.46
1:A:126:ASP:O	1:A:129:SER:HB3	2.16	0.45
1:A:39:TRP:O	1:A:119:GLY:HA3	2.17	0.45
1:A:84:ILE:HA	1:A:101:PHE:O	2.17	0.45
1:A:2:HIS:CD2	1:A:93:ASP:HB3	2.52	0.45
1:A:292:PRO:O	1:A:292:PRO:HG2	2.17	0.45
1:A:315:ILE:HD13	1:A:315:ILE:HG21	1.54	0.45
1:A:128:ILE:HD12	1:A:128:ILE:HG21	1.48	0.44
1:A:35:SER:OG	1:A:75:TYR:HE1	2.00	0.44
1:A:77:THR:CG2	3:A:338:2Y2:H10A	2.46	0.44
1:A:291:PHE:O	1:A:296:GLY:HA3	2.18	0.44
1:A:91:ILE:O	1:A:92:GLY:C	2.53	0.44
1:A:128:ILE:HG23	1:A:128:ILE:HD13	1.64	0.44
1:A:198:GLY:HA3	1:A:203:TYR:HD1	1.83	0.43
1:A:246:THR:HG22	1:A:283:ILE:HG22	2.01	0.43
1:A:26:ASN:HD22	1:A:27:PHE:H	1.66	0.43
1:A:266:ASN:HD21	4:A:337:NAG:H3	1.53	0.43
1:A:215:ASP:O	1:A:302:GLY:HA2	2.19	0.43
1:A:80:LEU:CD2	1:A:112:PHE:CE2	3.01	0.43
3:A:338:2Y2:H29A	3:A:338:2Y2:H33A	1.46	0.43
1:A:58:HIS:HB2	1:A:64:TYR:CE2	2.53	0.42
1:A:13:GLN:NE2	3:A:338:2Y2:C4	2.83	0.42
1:A:199:LEU:HD23	1:A:199:LEU:C	2.40	0.42
1:A:41:PRO:HD3	1:A:118:ASP:O	2.19	0.42
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.53	0.42
1:A:159(B):ASP:HB2	1:A:159(C):THR:H	1.70	0.42
1:A:223:LEU:HD12	1:A:286:ILE:HG23	2.02	0.41
1:A:141:ILE:HG21	1:A:141:ILE:HD13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HA	1:A:23:PRO:HA	1.78	0.41
1:A:16:THR:CG2	1:A:17:ASP:H	2.21	0.41
1:A:48:LEU:CD1	1:A:52:LEU:HD12	2.50	0.41
1:A:6:LEU:HD23	1:A:6:LEU:HA	1.78	0.41
1:A:8:ASN:C	1:A:8:ASN:OD1	2.59	0.40
1:A:182:LEU:HA	1:A:183:PRO:HD2	1.90	0.40
1:A:127:THR:HG21	5:A:653:HOH:O	2.20	0.40
1:A:6:LEU:HB2	1:A:163:GLY:CA	2.51	0.40

All (1) 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:205:GLU:OE2	1:A:205:GLU:OE2[5_675]	2.16	0.04

## 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%)	17 (5%)	4 (1%)	13 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	TRP
1	A	59	GLU
1	A	87	ASP
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%)	215 (80%)	53 (20%)	<b>1</b> <b>3</b>

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	20	LEU
1	A	26	ASN
1	A	27	PHE
1	A	35	SER
1	A	41	PRO
1	A	44	GLU
1	A	47	SER
1	A	48	LEU
1	A	51	PHE
1	A	55	LYS
1	A	58	HIS
1	A	59	GLU
1	A	61	SER
1	A	63	SER
1	A	65	LYS
1	A	74	GLN
1	A	79	SER
1	A	80	LEU
1	A	86	GLN
1	A	91	ILE
1	A	98	LYS
1	A	111	THR
1	A	128	ILE
1	A	142	GLN
1	A	144	ASP
1	A	158	THR
1	A	159	SER
1	A	159(A)	LYS
1	A	159(B)	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	159(C)	THR
1	A	161	ASN
1	A	176	LYS
1	A	182	LEU
1	A	187	LYS
1	A	197	ILE
1	A	199	LEU
1	A	201	ASP
1	A	202	GLU
1	A	219	SER
1	A	220	LEU
1	A	224	PRO
1	A	238	LYS
1	A	241	TRP
1	A	247	LEU
1	A	261	ASN
1	A	276	LEU
1	A	278	VAL
1	A	281	SER
1	A	289	MET
1	A	313	TYR
1	A	324	LYS
1	A	326	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2	HIS
1	A	13	GLN
1	A	26	ASN
1	A	58	HIS
1	A	86	GLN
1	A	142	GLN
1	A	232	ASN
1	A	250	ASN
1	A	254	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	1,2	14,14,15	1.14	1 (7%)	17,19,21	1.98	6 (35%)
2	NAG	B	2	2	14,14,15	0.94	0	17,19,21	1.97	5 (29%)
2	BMA	B	3	2	11,11,12	1.09	0	15,15,17	2.84	7 (46%)
2	BMA	B	4	2	11,11,12	1.27	1 (9%)	15,15,17	2.07	1 (6%)
2	BGC	B	5	2	11,11,12	1.72	5 (45%)	15,15,17	3.44	6 (40%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	B	5	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	BGC	O3-C3	2.83	1.49	1.43
2	B	5	BGC	O2-C2	2.50	1.48	1.43
2	B	5	BGC	O5-C1	2.40	1.47	1.43
2	B	5	BGC	C2-C3	-2.24	1.49	1.52
2	B	4	BMA	O4-C4	2.24	1.48	1.43
2	B	1	NAG	O4-C4	2.20	1.48	1.43
2	B	5	BGC	O4-C4	2.01	1.47	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	BGC	C1-C2-C3	7.63	119.05	109.67
2	B	3	BMA	O5-C5-C4	-6.85	94.17	110.83
2	B	4	BMA	O5-C5-C4	6.59	126.85	110.83
2	B	5	BGC	C1-O5-C5	6.41	120.88	112.19
2	B	3	BMA	C1-O5-C5	5.52	119.67	112.19
2	B	5	BGC	O5-C5-C4	5.52	124.25	110.83
2	B	5	BGC	C2-C3-C4	5.16	119.82	110.89
2	B	1	NAG	C1-O5-C5	4.86	118.77	112.19
2	B	2	NAG	C1-O5-C5	4.51	118.30	112.19
2	B	1	NAG	O5-C5-C4	3.44	119.19	110.83
2	B	2	NAG	C8-C7-N2	-2.91	111.18	116.10
2	B	3	BMA	C3-C4-C5	-2.73	105.37	110.24
2	B	2	NAG	O5-C5-C6	-2.72	102.95	107.20
2	B	2	NAG	C3-C4-C5	-2.70	105.42	110.24
2	B	3	BMA	O6-C6-C5	2.62	120.30	111.29
2	B	3	BMA	C1-C2-C3	2.60	112.86	109.67
2	B	2	NAG	C2-N2-C7	-2.39	119.50	122.90
2	B	1	NAG	O3-C3-C4	-2.26	105.14	110.35
2	B	3	BMA	O5-C1-C2	2.21	114.18	110.77
2	B	5	BGC	O3-C3-C4	-2.21	105.25	110.35
2	B	1	NAG	O5-C1-C2	-2.17	107.85	111.29
2	B	5	BGC	O2-C2-C1	-2.13	104.79	109.15
2	B	1	NAG	C8-C7-N2	-2.12	112.51	116.10
2	B	1	NAG	C2-N2-C7	-2.09	119.92	122.90
2	B	3	BMA	O5-C5-C6	2.05	110.41	107.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2

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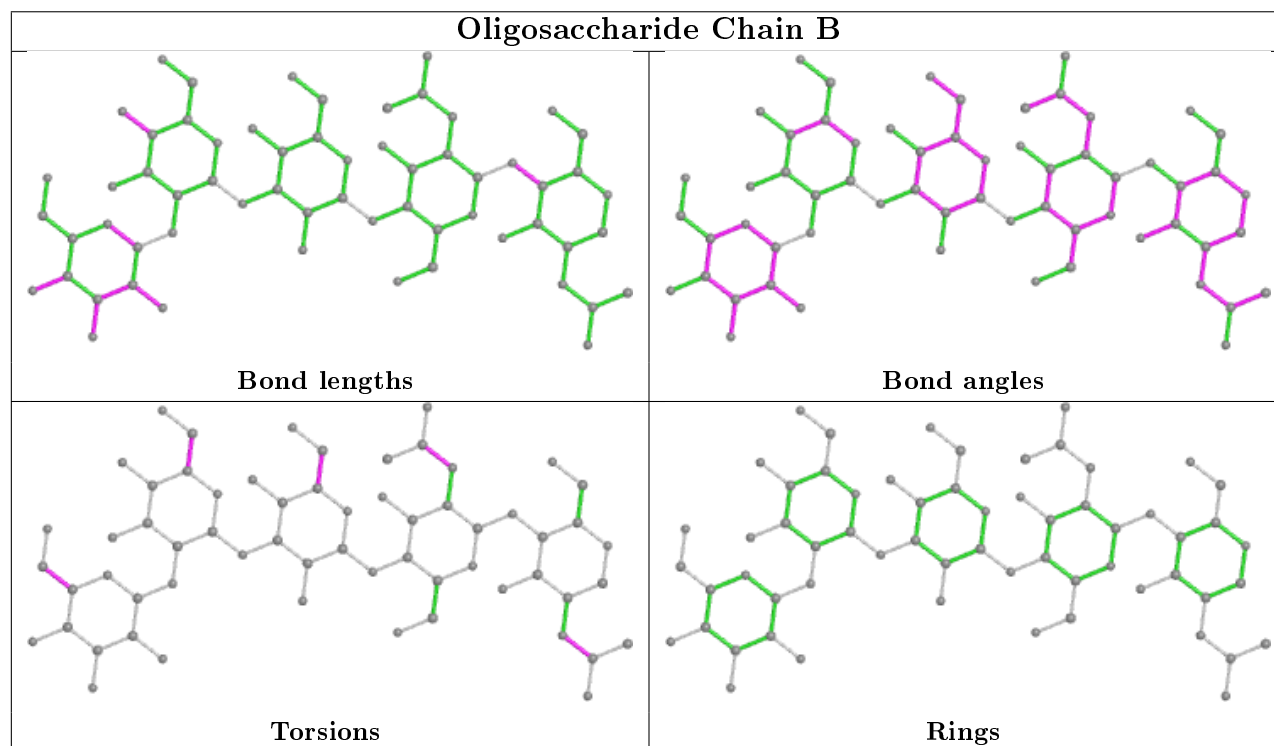
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	5	BGC	O5-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
2	B	5	BGC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BMA	1	0
2	B	3	BMA	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](#)

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
3	2Y2	A	338	-	46,48,48	3.24	6 (13%)	49,63,63	5.33	16 (32%)
4	NAG	A	337	1	14,14,15	1.32	2 (14%)	17,19,21	2.66	7 (41%)

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	2Y2	A	338	-	1/1/9/12	20/39/60/60	0/4/4/4
4	NAG	A	337	1	1/1/5/7	6/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	338	2Y2	C27-N6	19.64	1.76	1.33
3	A	338	2Y2	C24-C23	-4.76	1.47	1.54
3	A	338	2Y2	C24-C25	4.51	1.55	1.47
3	A	338	2Y2	C6-C7	-3.70	1.35	1.41
3	A	338	2Y2	C22-C23	-3.46	1.45	1.53
4	A	337	NAG	O5-C1	2.51	1.47	1.43
4	A	337	NAG	O5-C5	2.41	1.48	1.43
3	A	338	2Y2	C7-N1	-2.25	1.31	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	338	2Y2	C23-C27-N6	-22.85	86.33	115.99
3	A	338	2Y2	C24-C25-C26	-18.43	147.50	177.66
3	A	338	2Y2	C33-N6-C27	-17.55	91.29	122.59
3	A	338	2Y2	O4-C27-N6	7.21	138.48	122.99
4	A	337	NAG	O5-C5-C4	5.97	125.36	110.83
3	A	338	2Y2	O4-C27-C23	-5.97	114.35	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	338	2Y2	C22-C23-C27	5.43	119.05	109.44
4	A	337	NAG	O5-C1-C2	-5.39	102.78	111.29
4	A	337	NAG	C2-N2-C7	-3.63	117.74	122.90
3	A	338	2Y2	C14-C13-N4	3.50	114.72	110.18
4	A	337	NAG	O5-C5-C6	-3.30	102.03	107.20
4	A	337	NAG	O3-C3-C4	-2.91	103.63	110.35
3	A	338	2Y2	O5-C31-C30	2.84	118.05	111.80
3	A	338	2Y2	C33-C32-N5	-2.73	106.09	112.88
3	A	338	2Y2	O1-C8-N3	2.56	127.17	122.45
3	A	338	2Y2	C11-S1-C10	-2.55	96.62	101.30
3	A	338	2Y2	C1-N1-C7	2.53	108.81	103.78
3	A	338	2Y2	C30-N5-C29	2.43	114.30	108.83
3	A	338	2Y2	C1-N2-C2	2.39	108.52	103.78
4	A	337	NAG	C8-C7-N2	-2.38	112.07	116.10
3	A	338	2Y2	C14-C15-C17	2.29	116.72	111.73
3	A	338	2Y2	C18-C16-C15	-2.23	107.94	112.15
4	A	337	NAG	O7-C7-N2	2.12	125.86	121.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	338	2Y2	C23
4	A	337	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	338	2Y2	S1-C10-C9-N3
3	A	338	2Y2	N4-C13-C21-C22
3	A	338	2Y2	C13-C21-C22-C23
3	A	338	2Y2	C22-C23-C24-C25
3	A	338	2Y2	C27-C23-C24-C25
3	A	338	2Y2	C22-C23-C27-N6
3	A	338	2Y2	C33-C32-N5-C29
3	A	338	2Y2	O4-C27-N6-C33
4	A	337	NAG	C8-C7-N2-C2
4	A	337	NAG	O5-C5-C6-O6
4	A	337	NAG	O7-C7-N2-C2
4	A	337	NAG	C3-C2-N2-C7
3	A	338	2Y2	O2-C12-C9-N3
3	A	338	2Y2	N4-C13-C14-C15
3	A	338	2Y2	N4-C13-C21-O3

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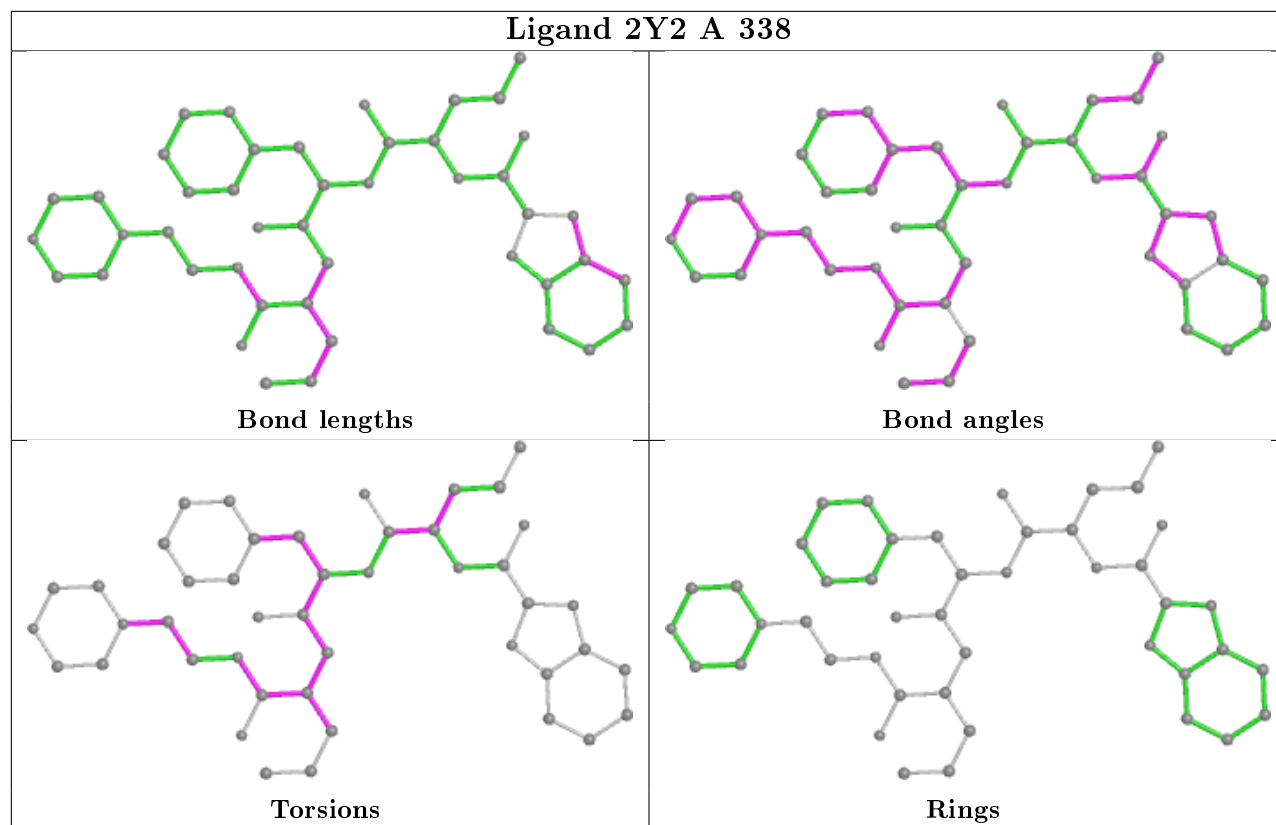
Mol	Chain	Res	Type	Atoms
4	A	337	NAG	C1-C2-N2-C7
3	A	338	2Y2	N4-C12-C9-N3
3	A	338	2Y2	C22-C23-C27-O4
3	A	338	2Y2	N5-C32-C33-N6
3	A	338	2Y2	O3-C21-C22-C23
3	A	338	2Y2	C14-C13-C21-C22
3	A	338	2Y2	C13-C14-C15-C16
3	A	338	2Y2	C13-C14-C15-C17
3	A	338	2Y2	C21-C22-C23-C24
3	A	338	2Y2	S1-C10-C9-C12
4	A	337	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	338	2Y2	19	0
4	A	337	NAG	3	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%)	-0.89	4 (1%) 79 80	5, 28, 66, 96	4 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	6.3
1	A	243	GLY	4.3
1	A	241	TRP	4.2
1	A	159(B)	ASP	2.4

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

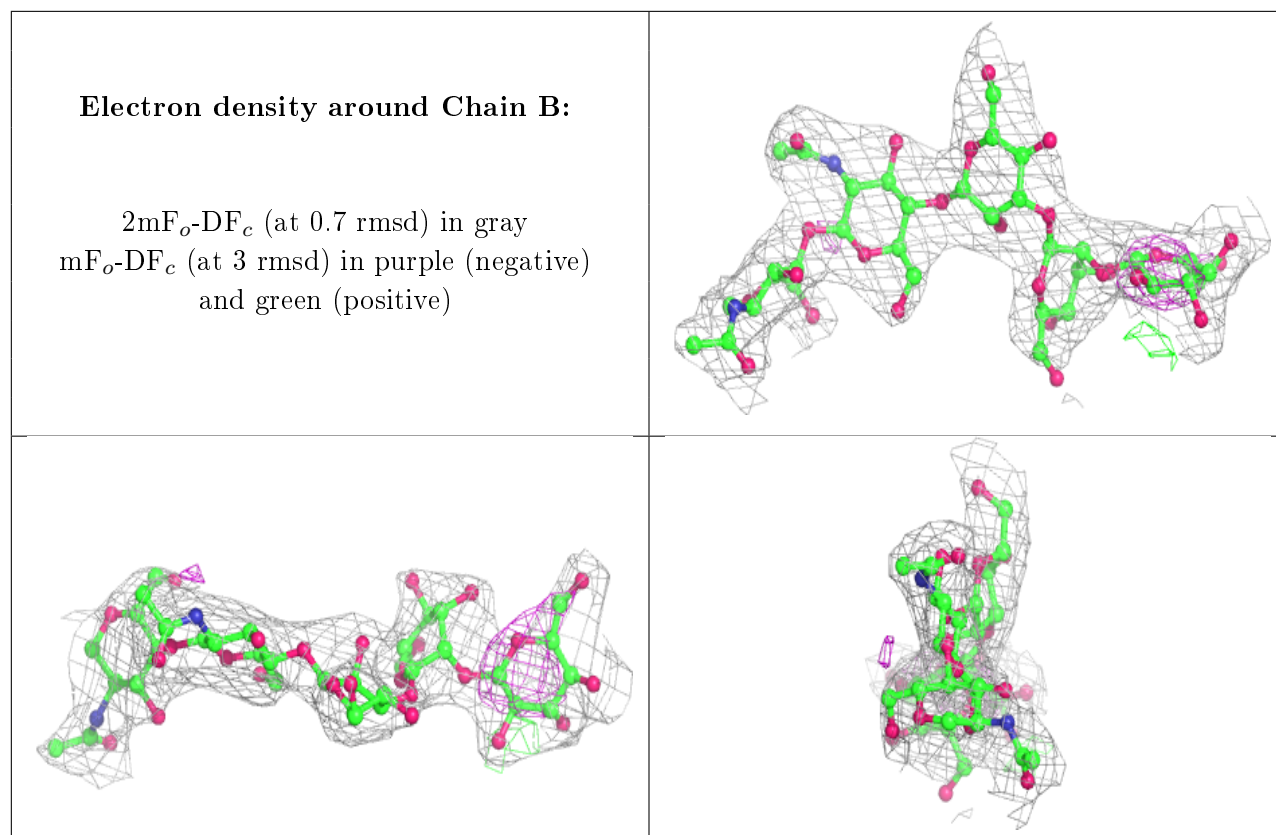
There are no non-standard protein/DNA/RNA residues in this entry.

### 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	BGC	B	5	11/12	0.79	0.30	11,38,76,82	0
2	BMA	B	3	11/12	0.91	0.21	29,49,69,73	0
2	BMA	B	4	11/12	0.92	0.20	27,45,58,86	0
2	NAG	B	1	14/15	0.94	0.16	32,63,88,103	0
2	NAG	B	2	14/15	0.97	0.11	13,29,44,70	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.



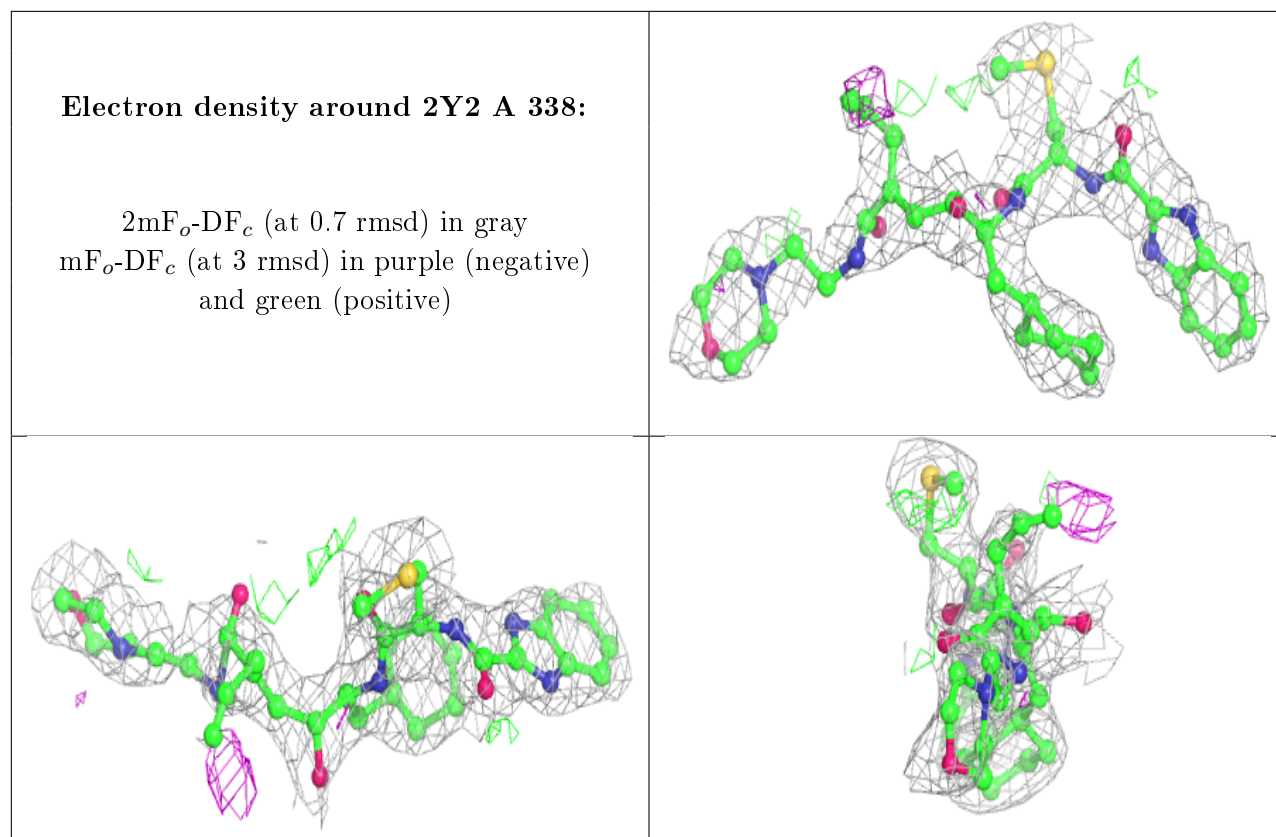
## 6.4 Ligands [i](#)

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	A	337	14/15	0.82	0.19	32,59,151,158	0
3	2Y2	A	338	45/45	0.94	0.18	18,43,97,158	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.