Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:28 PM EDT

PDB ID	:	2JXR
Title	:	STRUCTURE OF YEAST PROTEINASE A
Authors	:	Aguilar, C.F.; Badasso, M.; Dreyer, T.; Cronin, N.B.; Newman, M.P.; Cooper, J.B.; Hoover, D.J.; Wood, S.P.; Johnson, M.S.; Blundell, T.L.
Deposited on	:	1997-04-24
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

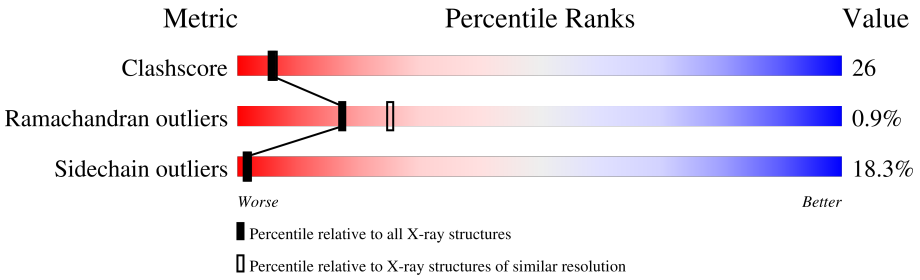
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	45% 40% 11% ·
2	B	5	40% 60%

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	5	X	-	-	-
4	NAG	A	337	X	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2768 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.

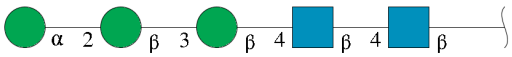
- Molecule 1 is a protein called PROTEINASE A.

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:

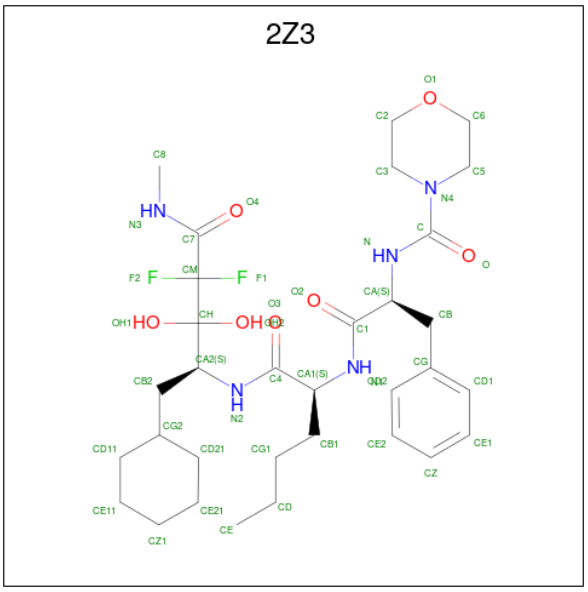
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	engineered mutation	UNP P07267

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(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.



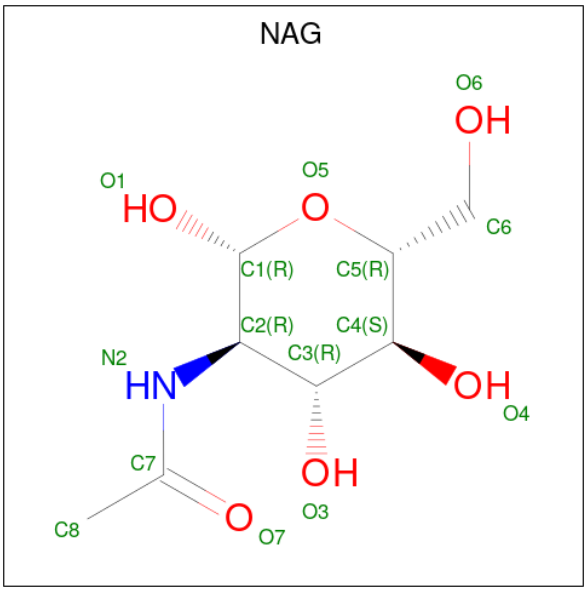
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is N-(morpholin-4-ylcarbonyl)-L-phenylalanyl-N-[(1R)-1-(cyclohexylmethyl)-3,3-difluoro-2,2-dihydroxy-4-(methylamino)-4-oxobutyl]-L-norleucinamide (three-letter code: 2Z3) (formula: $C_{32}H_{49}F_2N_5O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			46	32	2	5	7		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		

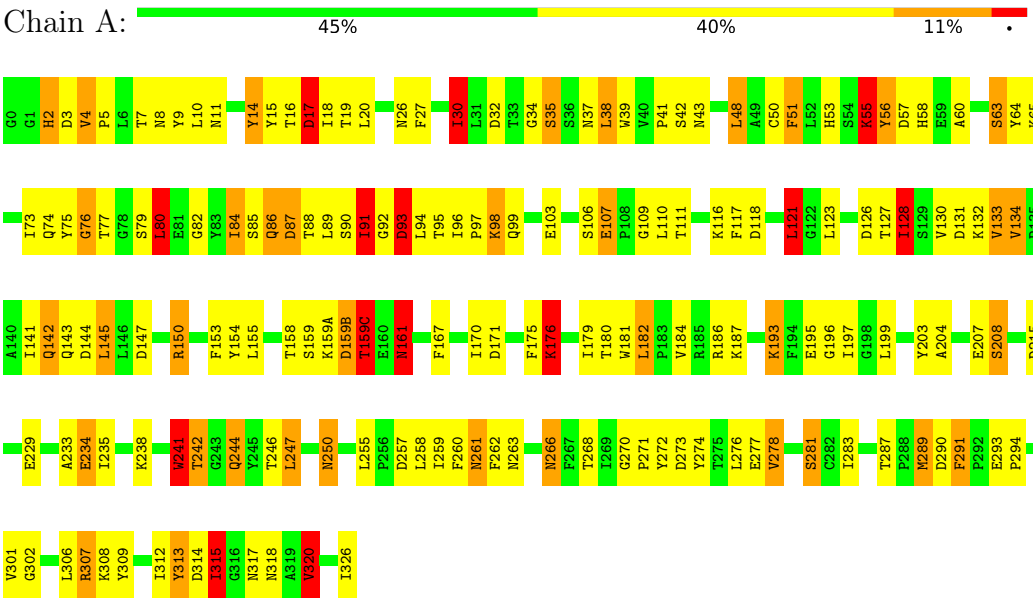
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEINASE A

Chain A:



• Molecule 2: alpha-D-mannopyranose-(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

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.70Å 86.70Å 110.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.193 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2768	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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, MAN, BMA, 2Z3

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	1.23	7/2592 (0.3%)	2.28	105/3526 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	5	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	PHE	CE2-CZ	6.31	1.49	1.37
1	A	301	VAL	CB-CG1	-6.11	1.40	1.52
1	A	63	SER	CA-CB	-5.82	1.44	1.52
1	A	175	PHE	CE1-CZ	5.78	1.48	1.37
1	A	229	GLU	CB-CG	5.72	1.63	1.52
1	A	208	SER	CB-OG	5.29	1.49	1.42
1	A	242	THR	N-CA	-5.05	1.36	1.46

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH1	-21.91	109.34	120.30
1	A	244	GLN	CA-CB-CG	17.52	151.94	113.40
1	A	4	VAL	CA-CB-CG2	15.27	133.81	110.90
1	A	320	VAL	CG1-CB-CG2	14.34	133.84	110.90
1	A	241	TRP	C-N-CA	13.45	155.32	121.70
1	A	215	ASP	CB-CG-OD1	11.55	128.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	CB-CG-OD1	-11.39	108.05	118.30
1	A	290	ASP	CB-CG-OD2	-11.04	108.36	118.30
1	A	176	LYS	CA-CB-CG	10.85	137.26	113.40
1	A	186	ARG	CA-CB-CG	10.35	136.16	113.40
1	A	215	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	186	ARG	CG-CD-NE	10.00	132.80	111.80
1	A	34	GLY	C-N-CA	9.74	146.05	121.70
1	A	193	LYS	CA-CB-CG	9.27	133.78	113.40
1	A	278	VAL	CA-CB-CG2	9.10	124.56	110.90
1	A	309	TYR	CG-CD1-CE1	-8.99	114.11	121.30
1	A	132	LYS	CD-CE-NZ	8.98	132.34	111.70
1	A	150	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	3	ASP	CB-CG-OD1	8.79	126.22	118.30
1	A	80	LEU	CA-CB-CG	8.69	135.28	115.30
1	A	38	LEU	CB-CG-CD1	8.68	125.75	111.00
1	A	175	PHE	CG-CD1-CE1	8.57	130.23	120.80
1	A	301	VAL	CA-CB-CG2	-8.46	98.22	110.90
1	A	307	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	203	TYR	CB-CG-CD2	8.36	126.01	121.00
1	A	258	LEU	CB-CG-CD2	-8.29	96.91	111.00
1	A	94	LEU	CB-CG-CD2	-8.27	96.95	111.00
1	A	175	PHE	CD1-CE1-CZ	-8.04	110.46	120.10
1	A	121	LEU	C-N-CA	8.01	139.12	122.30
1	A	184	VAL	CA-CB-CG1	7.89	122.73	110.90
1	A	289	MET	CG-SD-CE	7.87	112.79	100.20
1	A	60	ALA	O-C-N	7.87	135.29	122.70
1	A	315	ILE	CB-CG1-CD1	-7.83	91.99	113.90
1	A	291	PHE	CG-CD2-CE2	7.82	129.40	120.80
1	A	107	GLU	C-N-CD	7.75	144.67	128.40
1	A	63	SER	N-CA-CB	7.69	122.03	110.50
1	A	145	LEU	CB-CG-CD2	-7.65	97.99	111.00
1	A	281	SER	N-CA-CB	7.64	121.97	110.50
1	A	313	TYR	CB-CG-CD2	7.55	125.53	121.00
1	A	134	VAL	CG1-CB-CG2	-7.47	98.95	110.90
1	A	308	LYS	CD-CE-NZ	7.37	128.66	111.70
1	A	171	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	154	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	A	133	VAL	CA-CB-CG1	-7.25	100.03	110.90
1	A	247	LEU	CB-CG-CD1	-7.17	98.81	111.00
1	A	128	ILE	CB-CG1-CD1	-7.12	93.96	113.90
1	A	278	VAL	CG1-CB-CG2	-7.09	99.56	110.90
1	A	43	ASN	N-CA-CB	7.04	123.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	LYS	CD-CE-NZ	-6.85	95.94	111.70
1	A	193	LYS	CG-CD-CE	6.84	132.42	111.90
1	A	274	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	A	159(B)	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	277	GLU	CA-CB-CG	6.71	128.17	113.40
1	A	91	ILE	CA-C-N	6.71	129.61	116.20
1	A	161	ASN	N-CA-CB	6.61	122.50	110.60
1	A	56	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	A	121	LEU	CB-CG-CD2	-6.59	99.80	111.00
1	A	266	ASN	O-C-N	6.55	133.18	122.70
1	A	91	ILE	C-N-CA	-6.43	108.79	122.30
1	A	15	TYR	CG-CD1-CE1	-6.35	116.22	121.30
1	A	57	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	17	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	30	ILE	CB-CG1-CD1	6.28	131.49	113.90
1	A	14	TYR	CG-CD2-CE2	-6.25	116.30	121.30
1	A	150	ARG	CB-CG-CD	-6.22	95.43	111.60
1	A	180	THR	O-C-N	6.20	132.62	122.70
1	A	126	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	307	ARG	NH1-CZ-NH2	6.15	126.17	119.40
1	A	153	PHE	O-C-N	6.12	132.49	122.70
1	A	131	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	2	HIS	CA-CB-CG	-6.02	103.36	113.60
1	A	145	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	A	306	LEU	O-C-N	-5.94	113.20	122.70
1	A	193	LYS	CB-CG-CD	5.88	126.89	111.60
1	A	86	GLN	CA-CB-CG	5.86	126.29	113.40
1	A	255	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	302	GLY	C-N-CA	5.82	136.25	121.70
1	A	250	ASN	CA-CB-CG	5.81	126.19	113.40
1	A	244	GLN	CB-CA-C	5.80	122.01	110.40
1	A	92	GLY	C-N-CA	5.70	135.95	121.70
1	A	94	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	A	260	PHE	O-C-N	5.67	131.77	122.70
1	A	55	LYS	CA-CB-CG	5.67	125.87	113.40
1	A	159(A)	LYS	CA-CB-CG	5.64	125.81	113.40
1	A	309	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	155	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	76	GLY	C-N-CA	5.60	135.70	121.70
1	A	154	TYR	N-CA-CB	5.55	120.59	110.60
1	A	233	ALA	C-N-CA	5.49	135.43	121.70
1	A	208	SER	CA-CB-OG	-5.46	96.45	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	87	ASP	C-N-CA	-5.32	108.41	121.70
1	A	301	VAL	C-N-CA	5.30	133.43	122.30
1	A	318	ASN	CA-C-O	5.30	131.23	120.10
1	A	167	PHE	O-C-N	-5.26	114.26	123.20
1	A	123	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	313	TYR	CD1-CE1-CZ	5.16	124.44	119.80
1	A	207	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	153	PHE	CB-CG-CD1	-5.12	117.21	120.80
1	A	155	LEU	O-C-N	-5.11	114.51	123.20
1	A	155	LEU	CB-CG-CD1	5.11	119.69	111.00
1	A	272	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
1	A	250	ASN	N-CA-CB	5.07	119.73	110.60
1	A	153	PHE	CA-C-N	-5.03	106.14	117.20
1	A	274	TYR	CA-CB-CG	5.00	122.90	113.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	16	THR	CB
1	A	43	ASN	CA
1	A	63	SER	CA
1	A	161	ASN	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	2398	129	0
2	B	61	0	52	3	0
3	A	46	0	49	4	0
4	A	14	0	12	10	0
5	A	119	0	0	7	0
All	All	2768	0	2511	132	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 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)
1:A:242:THR:CG2	1:A:242:THR:O	1.97	1.13
1:A:242:THR:O	1:A:242:THR:HG22	1.50	1.10
1:A:4:VAL:HG23	1:A:16:THR:HG21	1.30	1.09
1:A:84:ILE:HD12	1:A:84:ILE:N	1.75	1.00
1:A:128:ILE:O	1:A:128:ILE:HG12	1.64	0.96
1:A:84:ILE:N	1:A:84:ILE:CD1	2.36	0.87
1:A:86:GLN:O	1:A:87:ASP:HB2	1.71	0.87
1:A:84:ILE:CD1	1:A:84:ILE:H	1.89	0.86
1:A:246:THR:HG22	1:A:283:ILE:HG22	1.57	0.85
1:A:5:PRO:O	1:A:16:THR:HG23	1.80	0.80
1:A:2:HIS:HD2	1:A:93:ASP:HB3	1.50	0.77
1:A:38:LEU:HD13	1:A:121:LEU:HB2	1.64	0.77
1:A:121:LEU:CD1	1:A:136:PRO:HG2	2.15	0.76
1:A:48:LEU:HD12	1:A:48:LEU:O	1.86	0.76
1:A:276:LEU:HD23	1:A:278:VAL:CG1	2.16	0.76
1:A:69:THR:HB	1:A:84:ILE:HD13	1.68	0.75
2:B:3:BMA:O2	2:B:4:BMA:C1	2.35	0.74
1:A:242:THR:O	1:A:242:THR:HG23	1.88	0.73
1:A:128:ILE:O	1:A:128:ILE:CG1	2.35	0.73
1:A:2:HIS:HD2	1:A:93:ASP:CB	2.02	0.73
1:A:96:ILE:N	1:A:96:ILE:HD12	2.05	0.72
1:A:4:VAL:CG2	1:A:16:THR:HG21	2.16	0.71
1:A:259:ILE:HD13	4:A:337:NAG:H5	1.73	0.70
1:A:259:ILE:CD1	4:A:337:NAG:H62	2.21	0.69
1:A:48:LEU:HD12	1:A:48:LEU:C	2.11	0.69
1:A:86:GLN:NE2	1:A:98:LYS:HB3	2.08	0.69
1:A:320:VAL:HG12	1:A:320:VAL:O	1.95	0.67
1:A:133:VAL:HG12	1:A:134:VAL:N	2.10	0.67
1:A:2:HIS:CD2	1:A:93:ASP:HB3	2.31	0.66
1:A:259:ILE:HD11	4:A:337:NAG:H62	1.78	0.66
1:A:121:LEU:HD11	1:A:136:PRO:HG2	1.78	0.66
1:A:53:HIS:HB3	1:A:118:ASP:OD1	1.95	0.65
1:A:95:THR:C	1:A:96:ILE:HD12	2.17	0.65
1:A:50:CYS:SG	1:A:107:GLU:HG3	2.37	0.64
1:A:84:ILE:HG22	1:A:85:SER:N	2.13	0.63
1:A:51:PHE:O	1:A:51:PHE:CD1	2.51	0.63
1:A:4:VAL:HG23	1:A:16:THR:CG2	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HB2	3:A:327:2Z3:H31	1.83	0.61
1:A:259:ILE:HD13	4:A:337:NAG:C5	2.29	0.61
1:A:58:HIS:HB2	1:A:64:TYR:CD1	2.36	0.61
1:A:222:THR:HA	1:A:287:THR:O	2.01	0.61
1:A:65:LYS:HB3	1:A:86:GLN:HG2	1.81	0.60
1:A:96:ILE:CG2	1:A:139:ASN:HD22	2.14	0.60
1:A:84:ILE:H	1:A:84:ILE:HD13	1.66	0.60
1:A:30:ILE:HD12	1:A:117:PHE:CG	2.37	0.59
1:A:77:THR:O	1:A:77:THR:OG1	2.20	0.58
1:A:82:GLY:HA3	1:A:103:GLU:O	2.03	0.58
1:A:30:ILE:CD1	1:A:117:PHE:CD2	2.88	0.57
1:A:32:ASP:OD2	1:A:35:SER:HB2	2.05	0.57
1:A:142:GLN:OE1	2:B:4:BMA:H62	2.04	0.57
1:A:69:THR:HB	1:A:84:ILE:CD1	2.34	0.57
1:A:39:TRP:CD2	1:A:80:LEU:HD21	2.40	0.57
1:A:96:ILE:HG22	1:A:139:ASN:HD22	1.68	0.57
1:A:259:ILE:HD13	4:A:337:NAG:C6	2.35	0.56
1:A:67:ASN:C	1:A:67:ASN:OD1	2.43	0.55
1:A:51:PHE:CD1	1:A:51:PHE:C	2.80	0.55
1:A:259:ILE:HD13	4:A:337:NAG:H62	1.87	0.55
1:A:9:TYR:CG	1:A:116:LYS:HD2	2.42	0.55
1:A:7:THR:O	1:A:14:TYR:HA	2.08	0.53
1:A:39:TRP:CE2	1:A:80:LEU:HD21	2.45	0.52
1:A:41:PRO:HD3	1:A:118:ASP:O	2.09	0.52
1:A:193:LYS:HE2	1:A:195:GLU:OE2	2.10	0.52
1:A:30:ILE:HD12	1:A:117:PHE:CD2	2.45	0.51
1:A:86:GLN:HE21	1:A:98:LYS:HA	1.76	0.51
1:A:195:GLU:HB2	1:A:261:ASN:ND2	2.26	0.51
1:A:84:ILE:HD12	1:A:84:ILE:H	1.52	0.50
1:A:16:THR:HG22	1:A:17:ASP:H	1.77	0.50
1:A:73:ILE:CG2	1:A:80:LEU:CD1	2.90	0.50
1:A:97:PRO:C	1:A:98:LYS:HG3	2.32	0.50
1:A:133:VAL:CG1	1:A:134:VAL:N	2.75	0.49
1:A:313:TYR:N	1:A:313:TYR:CD1	2.79	0.49
1:A:58:HIS:HB2	1:A:64:TYR:CG	2.46	0.49
1:A:276:LEU:HD23	1:A:278:VAL:HG13	1.91	0.49
1:A:259:ILE:HG21	4:A:337:NAG:H5	1.95	0.49
1:A:89:LEU:HG	1:A:90:SER:N	2.27	0.49
1:A:96:ILE:N	1:A:96:ILE:CD1	2.75	0.48
1:A:73:ILE:HG22	1:A:80:LEU:HD13	1.95	0.47
1:A:84:ILE:CG2	1:A:85:SER:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:O	1:A:141:ILE:HG13	2.15	0.47
1:A:19:THR:OG1	1:A:90:SER:HB3	2.14	0.46
1:A:137:PHE:HE2	1:A:315:ILE:HG22	1.80	0.46
1:A:208:SER:O	1:A:297:PRO:HG2	2.16	0.46
1:A:219:SER:CB	3:A:327:2Z3:H31	2.45	0.46
1:A:234:GLU:HG3	5:A:557:HOH:O	2.16	0.46
1:A:266:ASN:OD1	4:A:337:NAG:H2	2.16	0.46
1:A:42:SER:O	1:A:55:LYS:HG2	2.16	0.46
5:A:563:HOH:O	2:B:4:BMA:H3	2.16	0.45
1:A:56:TYR:HD2	1:A:103:GLU:OE1	1.99	0.45
1:A:10:LEU:O	1:A:11:ASN:HB2	2.16	0.45
4:A:337:NAG:O7	4:A:337:NAG:C1	2.58	0.44
1:A:69:THR:O	1:A:84:ILE:HD13	2.16	0.44
1:A:147:ASP:HB2	5:A:558:HOH:O	2.17	0.44
1:A:176:LYS:HE3	1:A:176:LYS:HB2	1.63	0.44
1:A:261:ASN:HD22	1:A:261:ASN:C	2.20	0.44
1:A:291:PHE:HZ	3:A:327:2Z3:HE11	1.83	0.44
1:A:69:THR:C	1:A:84:ILE:HD13	2.38	0.44
1:A:8:ASN:OD1	1:A:8:ASN:C	2.56	0.43
1:A:76:GLY:HA3	3:A:327:2Z3:HD21	2.00	0.43
1:A:86:GLN:NE2	1:A:98:LYS:HA	2.33	0.43
1:A:127:THR:HG21	5:A:653:HOH:O	2.18	0.43
1:A:181:TRP:C	1:A:182:LEU:HD13	2.39	0.43
1:A:139:ASN:O	1:A:143:GLN:HG3	2.18	0.43
1:A:266:ASN:ND2	4:A:337:NAG:C7	2.80	0.43
1:A:289:MET:HG2	1:A:291:PHE:CE2	2.54	0.43
1:A:86:GLN:O	1:A:87:ASP:CB	2.46	0.43
1:A:317:ASN:HD22	1:A:317:ASN:HA	1.41	0.42
1:A:307:ARG:HH11	1:A:307:ARG:HD3	1.45	0.42
1:A:314:ASP:OD1	1:A:314:ASP:C	2.58	0.42
1:A:9:TYR:CE1	1:A:116:LYS:HE2	2.54	0.42
1:A:141:ILE:HD13	1:A:141:ILE:HG21	1.84	0.42
1:A:271:PRO:HD2	5:A:529:HOH:O	2.19	0.42
1:A:69:THR:CB	1:A:84:ILE:HD13	2.46	0.42
1:A:179:ILE:HD13	1:A:312:ILE:CD1	2.50	0.41
1:A:262:PHE:O	1:A:263:ASN:CB	2.67	0.41
1:A:315:ILE:HD12	5:A:559:HOH:O	2.20	0.41
1:A:137:PHE:HE2	1:A:315:ILE:CG2	2.33	0.41
1:A:86:GLN:HE22	1:A:98:LYS:HB3	1.82	0.41
1:A:159(B):ASP:HB3	1:A:159(C):THR:H	1.41	0.41
1:A:196:GLY:HA2	1:A:204:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:HE21	1:A:142:GLN:HB3	1.57	0.41
1:A:150:ARG:NH2	5:A:571:HOH:O	2.53	0.41
1:A:109:GLY:O	1:A:110:LEU:HD23	2.20	0.41
1:A:37:ASN:OD1	1:A:130:VAL:HB	2.21	0.41
1:A:84:ILE:HG22	1:A:85:SER:H	1.83	0.41
1:A:109:GLY:C	1:A:110:LEU:HD23	2.41	0.41
1:A:270:GLY:O	1:A:273:ASP:HB2	2.21	0.41
1:A:87:ASP:OD1	1:A:88:THR:N	2.50	0.41
1:A:99:GLN:OE1	1:A:136:PRO:HA	2.21	0.41
1:A:35:SER:OG	1:A:75:TYR:HE1	2.04	0.40
1:A:89:LEU:HD21	1:A:91:ILE:HD11	2.03	0.40
1:A:257:ASP:HB3	1:A:268:THR:CG2	2.51	0.40
1:A:18:ILE:O	1:A:18:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	327/329 (99%)	305 (93%)	19 (6%)	3 (1%)	17 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	TRP
1	A	159(C)	THR
1	A	161	ASN

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%)	219 (82%)	49 (18%)	1 2

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	20	LEU
1	A	26	ASN
1	A	27	PHE
1	A	30	ILE
1	A	35	SER
1	A	48	LEU
1	A	51	PHE
1	A	55	LYS
1	A	63	SER
1	A	74	GLN
1	A	79	SER
1	A	80	LEU
1	A	84	ILE
1	A	91	ILE
1	A	93	ASP
1	A	98	LYS
1	A	106	SER
1	A	111	THR
1	A	121	LEU
1	A	128	ILE
1	A	142	GLN
1	A	144	ASP
1	A	145	LEU
1	A	158	THR
1	A	159	SER
1	A	159(C)	THR
1	A	161	ASN
1	A	170	ILE
1	A	176	LYS

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	197	ILE
1	A	199	LEU
1	A	234	GLU
1	A	235	ILE
1	A	238	LYS
1	A	241	TRP
1	A	244	GLN
1	A	247	LEU
1	A	250	ASN
1	A	261	ASN
1	A	281	SER
1	A	293	GLU
1	A	294	PRO
1	A	298	LEU
1	A	300	ILE
1	A	315	ILE
1	A	320	VAL
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	86	GLN
1	A	139	ASN
1	A	161	ASN
1	A	232	ASN
1	A	244	GLN
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	1.41	2 (14%)	17,19,21	3.43	8 (47%)
2	NAG	B	2	2	14,14,15	1.38	2 (14%)	17,19,21	2.79	8 (47%)
2	BMA	B	3	2	11,11,12	1.73	3 (27%)	15,15,17	4.18	7 (46%)
2	BMA	B	4	2	11,11,12	1.89	5 (45%)	15,15,17	2.60	6 (40%)
2	MAN	B	5	2	11,11,12	1.58	1 (9%)	15,15,17	2.91	7 (46%)

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	-	3/6/23/26	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	MAN	B	5	2	3/3/4/5	2/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	MAN	O5-C1	3.83	1.49	1.43
2	B	3	BMA	O2-C2	3.34	1.50	1.43
2	B	4	BMA	O5-C1	3.11	1.48	1.43
2	B	2	NAG	O5-C5	3.06	1.49	1.43
2	B	1	NAG	C1-C2	2.83	1.56	1.52
2	B	4	BMA	O5-C5	2.77	1.49	1.43
2	B	1	NAG	C2-N2	2.65	1.50	1.46
2	B	3	BMA	C2-C3	2.52	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BMA	O3-C3	2.40	1.48	1.43
2	B	4	BMA	C2-C3	2.38	1.56	1.52
2	B	4	BMA	O2-C2	2.36	1.48	1.43
2	B	2	NAG	C2-N2	2.26	1.50	1.46
2	B	3	BMA	O4-C4	2.24	1.48	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BMA	O5-C5-C4	-11.01	84.04	110.83
2	B	3	BMA	C1-O5-C5	9.61	125.22	112.19
2	B	1	NAG	O5-C1-C2	-7.18	99.95	111.29
2	B	1	NAG	C2-N2-C7	-6.66	113.42	122.90
2	B	5	MAN	O5-C5-C4	-6.28	95.56	110.83
2	B	4	BMA	C1-O5-C5	-6.05	104.00	112.19
2	B	2	NAG	C1-O5-C5	5.95	120.25	112.19
2	B	1	NAG	O5-C5-C4	-5.37	97.77	110.83
2	B	4	BMA	O5-C1-C2	-4.83	103.31	110.77
2	B	1	NAG	O7-C7-C8	-4.72	113.28	122.06
2	B	2	NAG	C8-C7-N2	-4.47	108.53	116.10
2	B	5	MAN	O5-C1-C2	-4.41	103.97	110.77
2	B	2	NAG	O5-C5-C6	-4.39	100.33	107.20
2	B	3	BMA	O3-C3-C4	-4.19	100.66	110.35
2	B	2	NAG	C2-N2-C7	-4.18	116.95	122.90
2	B	5	MAN	O6-C6-C5	4.03	125.12	111.29
2	B	2	NAG	O7-C7-C8	4.02	129.51	122.06
2	B	4	BMA	O2-C2-C1	-3.90	101.17	109.15
2	B	5	MAN	C6-C5-C4	3.57	121.36	113.00
2	B	1	NAG	O5-C5-C6	-3.56	101.62	107.20
2	B	5	MAN	O2-C2-C3	3.56	117.27	110.14
2	B	5	MAN	O3-C3-C4	-3.28	102.76	110.35
2	B	1	NAG	C8-C7-N2	3.20	121.52	116.10
2	B	2	NAG	O4-C4-C3	2.91	117.08	110.35
2	B	3	BMA	C2-C3-C4	-2.85	105.96	110.89
2	B	5	MAN	C1-C2-C3	2.84	113.15	109.67
2	B	1	NAG	O6-C6-C5	-2.81	101.66	111.29
2	B	4	BMA	O5-C5-C6	-2.77	102.86	107.20
2	B	4	BMA	O3-C3-C4	-2.59	104.36	110.35
2	B	1	NAG	C1-C2-N2	-2.53	106.16	110.49
2	B	3	BMA	C1-C2-C3	-2.41	106.71	109.67
2	B	3	BMA	O2-C2-C1	-2.25	104.56	109.15
2	B	2	NAG	O3-C3-C2	-2.15	105.02	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	O4-C4-C5	2.15	114.62	109.30
2	B	3	BMA	O4-C4-C3	-2.13	105.42	110.35
2	B	4	BMA	O6-C6-C5	-2.04	104.30	111.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	5	MAN	C5
2	B	5	MAN	C2
2	B	5	MAN	C1

All (10) torsion outliers are listed below:

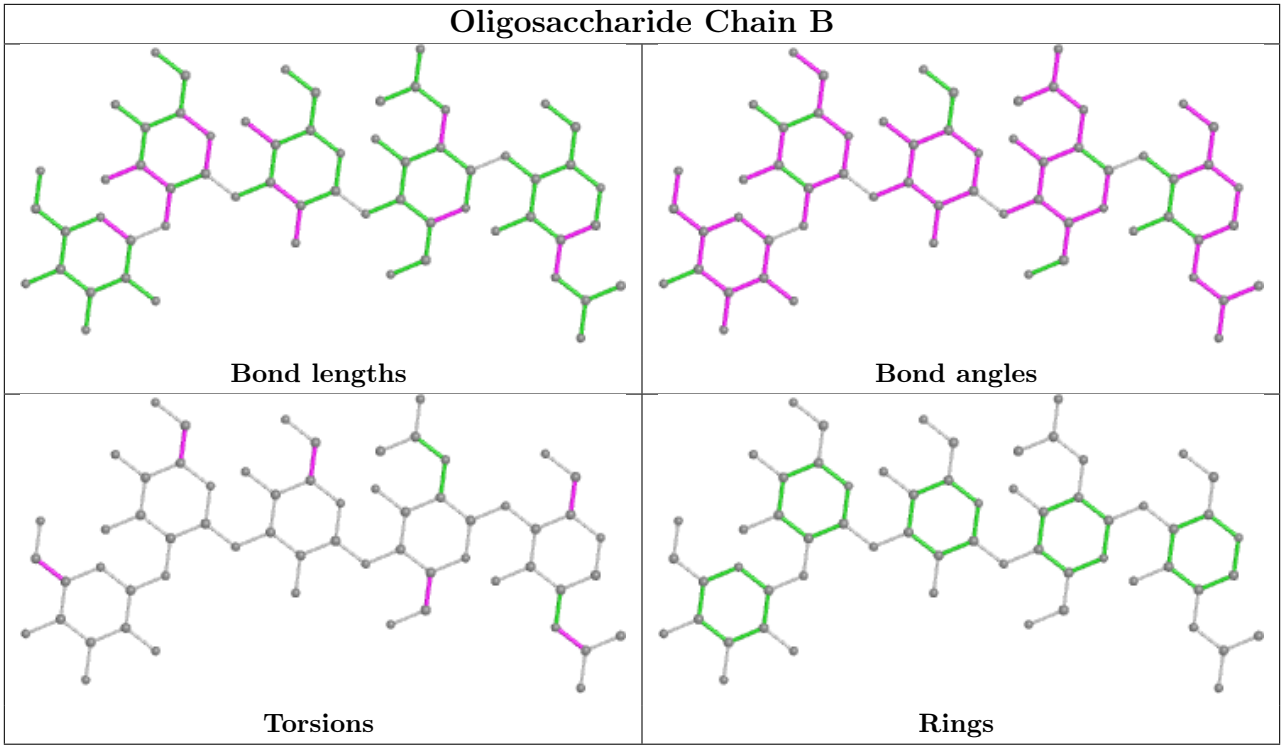
Mol	Chain	Res	Type	Atoms
2	B	5	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	5	MAN	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	BMA	3	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	$\#\|Z\| > 2$
4	NAG	A	337	1	14,14,15	1.47	3 (21%)	17,19,21	3.78	11 (64%)
3	2Z3	A	327	-	46,48,48	1.18	6 (13%)	55,66,66	2.33	21 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	337	1	2/2/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2Z3	A	327	-	-	5/50/75/75	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	337	NAG	C3-C2	-3.35	1.45	1.52
3	A	327	2Z3	O4-C7	2.95	1.28	1.22
3	A	327	2Z3	OH2-CH	2.49	1.42	1.40
3	A	327	2Z3	CD11-CG2	-2.28	1.46	1.52
3	A	327	2Z3	CE2-CD2	2.24	1.43	1.38
3	A	327	2Z3	OH1-CH	2.24	1.42	1.40
3	A	327	2Z3	CM-C7	-2.10	1.52	1.54
4	A	337	NAG	C2-N2	2.07	1.49	1.46
4	A	337	NAG	O5-C5	2.01	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	337	NAG	C2-N2-C7	-8.44	110.89	122.90
4	A	337	NAG	C1-O5-C5	7.07	121.77	112.19
4	A	337	NAG	C4-C3-C2	6.20	120.11	111.02
3	A	327	2Z3	C5-N4-C3	5.96	124.09	112.62
3	A	327	2Z3	CE2-CD2-CG	5.60	129.22	120.63
3	A	327	2Z3	CZ1-CE21-CD21	5.17	121.95	111.42
4	A	337	NAG	O5-C5-C6	-4.96	99.42	107.20
3	A	327	2Z3	CZ-CE2-CD2	-4.14	113.89	120.19
3	A	327	2Z3	CE11-CD11-CG2	4.06	119.83	112.15
3	A	327	2Z3	OH2-CH-CM	-3.86	97.00	107.44
4	A	337	NAG	O5-C5-C4	3.58	119.53	110.83
3	A	327	2Z3	CD21-CG2-CD11	3.49	117.85	109.33
3	A	327	2Z3	F2-CM-F1	-3.45	98.94	106.49
3	A	327	2Z3	CB2-CG2-CD11	3.27	118.84	111.73
3	A	327	2Z3	F2-CM-C7	-3.27	105.77	109.92
3	A	327	2Z3	F1-CM-C7	3.07	113.83	109.92
3	A	327	2Z3	O4-C7-N3	-2.89	118.81	122.79
4	A	337	NAG	O3-C3-C2	2.87	115.41	109.47
3	A	327	2Z3	CD2-CG-CD1	-2.81	113.75	118.17
4	A	337	NAG	C8-C7-N2	-2.73	111.47	116.10
4	A	337	NAG	C3-C4-C5	2.72	115.09	110.24
3	A	327	2Z3	CZ1-CE11-CD11	2.64	116.80	111.42
3	A	327	2Z3	CB2-CA2-N2	2.62	115.45	109.46
3	A	327	2Z3	C8-N3-C7	-2.54	118.19	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	327	2Z3	CZ-CE1-CD1	2.49	123.98	120.19
4	A	337	NAG	O5-C1-C2	2.38	115.05	111.29
3	A	327	2Z3	OH2-CH-OH1	2.36	117.75	110.89
4	A	337	NAG	O7-C7-C8	2.35	126.43	122.06
3	A	327	2Z3	O4-C7-CM	2.33	120.21	118.44
4	A	337	NAG	O6-C6-C5	-2.15	103.91	111.29
3	A	327	2Z3	C3-N4-C	-2.09	114.25	121.94
3	A	327	2Z3	O2-C1-CA	2.04	124.74	120.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	337	NAG	C2
4	A	337	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	337	NAG	C1-C2-N2-C7
4	A	337	NAG	C8-C7-N2-C2
4	A	337	NAG	O7-C7-N2-C2
4	A	337	NAG	O5-C5-C6-O6
3	A	327	2Z3	N3-C7-CM-F1
3	A	327	2Z3	CA2-CB2-CG2-CD21
3	A	327	2Z3	O3-C4-CA1-N1
3	A	327	2Z3	N2-CA2-CB2-CG2
3	A	327	2Z3	N2-C4-CA1-N1

There are no ring outliers.

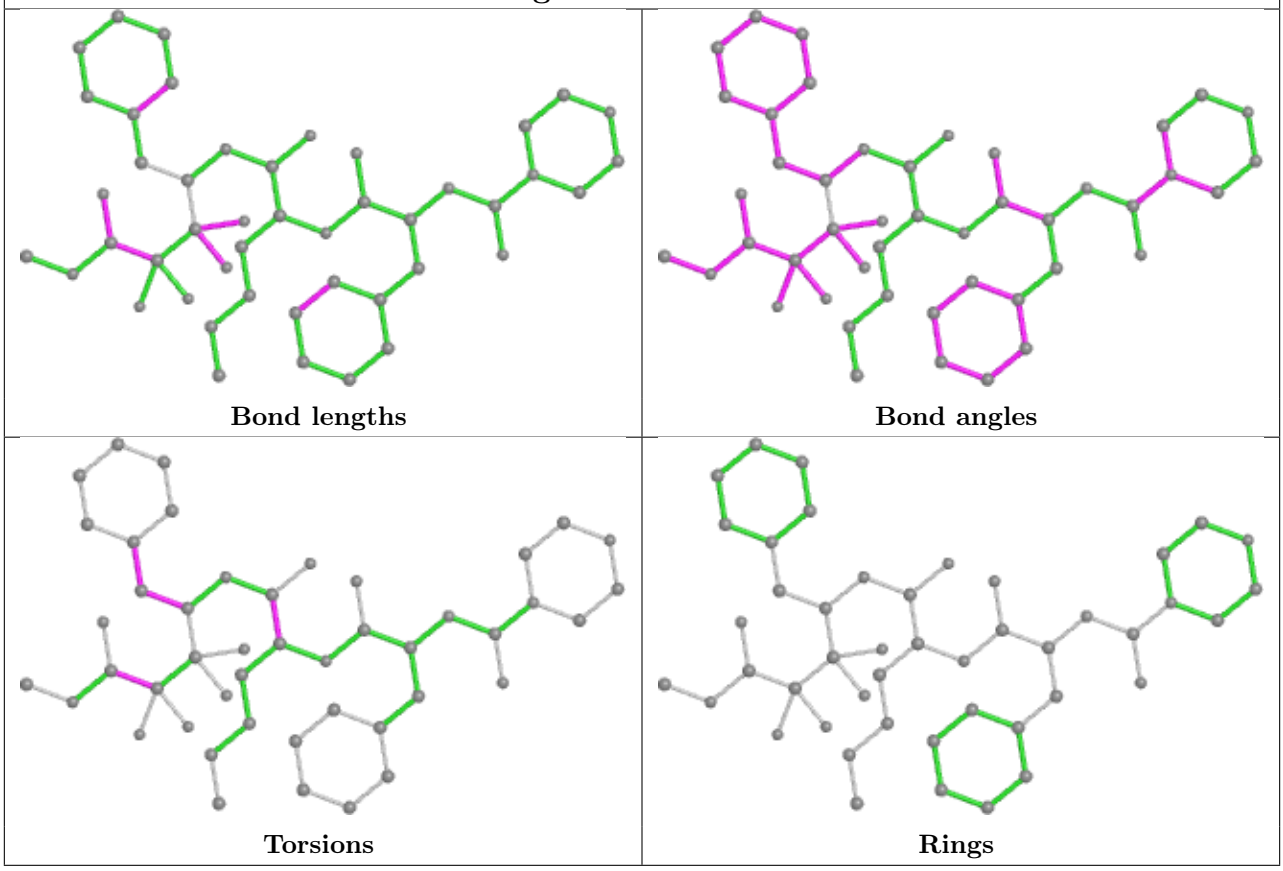
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	337	NAG	10	0
3	A	327	2Z3	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 then 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.

Ligand 2Z3 A 327



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.