



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:58 AM UTC

PDB ID : 1RPA / pdb_00001rpa
Title : THREE-DIMENSIONAL STRUCTURE OF RAT ACID PHOSPHATASE IN
COMPLEX WITH L(+) TARTRATE
Authors : Lindqvist, Y.; Schneider, G.
Deposited on : 1993-06-12
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

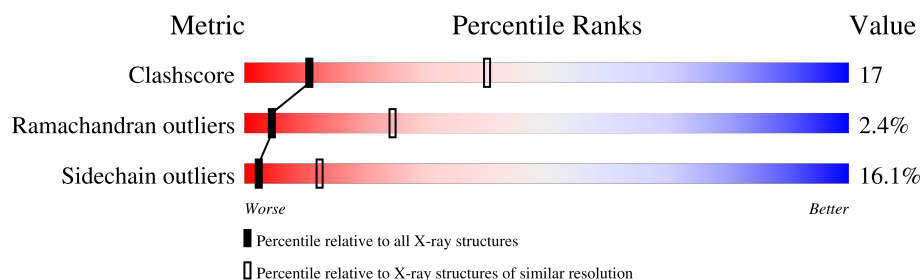
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	342	38% 41% 18% .
2	B	3	33% 67%

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
4	TAR	A	343	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2857 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.

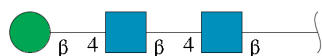
- Molecule 1 is a protein called PROSTATIC ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2794	1793	468	517	16	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	ILE	conflict	UNP P20646
A	191	LEU	PHE	conflict	UNP P20646
A	192	PRO	ARG	conflict	UNP P20646
A	257	HIS	TYR	conflict	UNP P20646
A	269	ASP	GLU	conflict	UNP P20646
A	270	VAL	LEU	conflict	UNP P20646
A	293	HIS	THR	conflict	UNP P20646

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



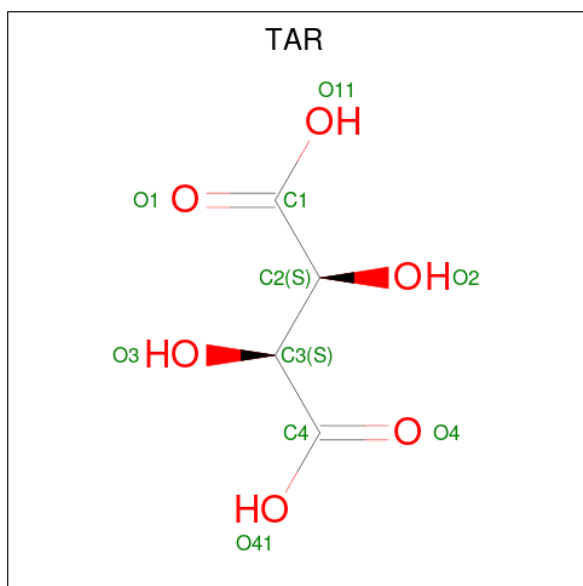
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



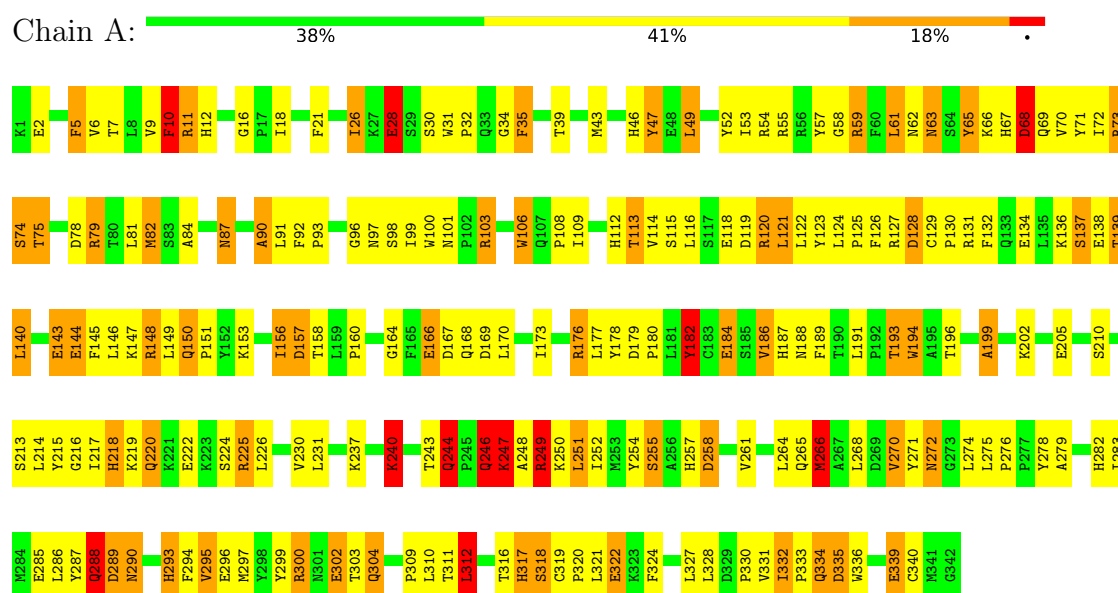
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: PROSTATIC ACID PHOSPHATASE



• Molecule 2: 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

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	89.40Å 89.40Å 152.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2857	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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, TAR

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	1.59	33/2873 (1.1%)	2.36	163/3898 (4.2%)

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	0	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	HIS	CD2-NE2	-7.82	1.29	1.37
1	A	252	ILE	CA-CB	-7.79	1.44	1.54
1	A	293	HIS	CD2-NE2	-7.54	1.29	1.37
1	A	282	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	12	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	317	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	257	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	309	PRO	CA-CB	-7.04	1.45	1.53
1	A	46	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	113	THR	CA-CB	-6.93	1.44	1.54
1	A	46	HIS	CG-ND1	-6.88	1.30	1.38
1	A	113	THR	CA-C	-6.66	1.45	1.53
1	A	18	ILE	CA-CB	-6.09	1.46	1.54
1	A	243	THR	CA-CB	6.05	1.63	1.53
1	A	12	HIS	CG-ND1	-5.94	1.31	1.38
1	A	218	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	299	TYR	CA-C	-5.88	1.46	1.52
1	A	257	HIS	CG-ND1	-5.83	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	VAL	CA-CB	-5.79	1.48	1.54
1	A	112	HIS	CG-ND1	-5.76	1.31	1.38
1	A	114	VAL	CA-CB	-5.66	1.47	1.55
1	A	282	HIS	CG-ND1	-5.58	1.32	1.38
1	A	266	MET	CA-CB	-5.48	1.43	1.53
1	A	74	SER	CA-CB	-5.38	1.45	1.53
1	A	47	TYR	CA-CB	-5.31	1.45	1.53
1	A	106	TRP	CG-CD2	-5.28	1.34	1.43
1	A	143	GLU	CA-CB	5.25	1.62	1.53
1	A	70	VAL	CA-CB	-5.16	1.48	1.54
1	A	187	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	7	THR	CA-CB	-5.12	1.45	1.53
1	A	309	PRO	N-CA	-5.07	1.41	1.47
1	A	320	PRO	CA-CB	-5.05	1.47	1.53
1	A	59	ARG	NE-CZ	5.03	1.38	1.33

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	GLN	N-CA-C	13.91	126.44	111.28
1	A	122	LEU	N-CA-C	12.28	127.52	112.54
1	A	179	ASP	CA-CB-CG	-12.07	100.53	112.60
1	A	68	ASP	CA-CB-CG	10.73	123.33	112.60
1	A	145	PHE	CA-CB-CG	-10.26	103.54	113.80
1	A	258	ASP	CA-CB-CG	10.19	122.79	112.60
1	A	244	GLN	CA-C-O	9.85	128.16	119.59
1	A	290	ASN	CA-CB-CG	9.81	122.41	112.60
1	A	87	ASN	OD1-CG-ND2	-9.40	113.20	122.60
1	A	139	THR	O-C-N	9.37	132.05	122.12
1	A	121	LEU	N-CA-C	-8.77	92.12	110.80
1	A	119	ASP	CA-CB-CG	-8.75	103.85	112.60
1	A	312	LEU	CA-C-O	-8.51	111.29	119.80
1	A	324	PHE	CA-CB-CG	8.40	122.20	113.80
1	A	62	ASN	CA-CB-CG	8.29	120.89	112.60
1	A	6	VAL	O-C-N	-8.27	112.23	122.57
1	A	247	LYS	CA-CB-CG	-8.18	97.75	114.10
1	A	46	HIS	CA-CB-CG	-8.13	105.67	113.80
1	A	10	PHE	N-CA-C	8.06	121.42	109.24
1	A	112	HIS	O-C-N	-7.99	113.89	123.16
1	A	319	CYS	O-C-N	-7.96	113.55	121.27
1	A	252	ILE	N-CA-C	-7.92	96.84	108.89
1	A	70	VAL	O-C-N	-7.80	114.37	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	PHE	CA-CB-CG	7.70	121.50	113.80
1	A	148	ARG	CA-CB-CG	-7.62	98.87	114.10
1	A	293	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	A	252	ILE	O-C-N	-7.52	115.16	122.98
1	A	31	TRP	N-CA-C	-7.46	97.70	109.04
1	A	288	GLN	N-CA-C	-7.32	97.80	109.59
1	A	290	ASN	CA-C-O	-7.29	110.09	120.51
1	A	264	LEU	N-CA-C	-7.25	102.99	111.03
1	A	58	GLY	O-C-N	7.24	129.13	122.18
1	A	157	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	339	GLU	CA-CB-CG	-7.18	99.74	114.10
1	A	250	LYS	N-CA-C	-7.03	95.84	110.80
1	A	249	ARG	CA-CB-CG	-7.02	100.07	114.10
1	A	187	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	222	GLU	N-CA-C	-6.97	103.30	111.03
1	A	68	ASP	N-CA-C	-6.96	102.91	111.40
1	A	92	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	43	MET	N-CA-C	-6.94	103.40	110.97
1	A	218	HIS	CB-CG-CD2	-6.93	122.19	131.20
1	A	143	GLU	CB-CG-CD	6.92	124.37	112.60
1	A	137	SER	CA-CB-OG	6.88	124.85	111.10
1	A	70	VAL	CA-C-O	-6.87	113.22	120.57
1	A	303	THR	CA-C-O	-6.86	113.22	120.63
1	A	128	ASP	CA-CB-CG	-6.86	105.74	112.60
1	A	335	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	272	ASN	CA-CB-CG	-6.82	105.78	112.60
1	A	213	SER	CA-CB-OG	-6.79	97.51	111.10
1	A	71	TYR	CA-C-O	-6.77	113.54	120.71
1	A	34	GLY	CA-C-O	6.76	126.61	122.22
1	A	317	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	A	72	ILE	O-C-N	-6.66	116.57	123.03
1	A	218	HIS	CA-C-O	6.66	127.49	120.36
1	A	250	LYS	O-C-N	-6.63	113.77	122.59
1	A	282	HIS	O-C-N	-6.60	114.29	122.68
1	A	335	ASP	CA-C-O	6.59	127.69	119.98
1	A	249	ARG	CA-C-O	6.57	128.00	119.98
1	A	215	TYR	N-CA-C	6.56	121.32	113.12
1	A	136	LYS	CG-CD-CE	6.53	126.32	111.30
1	A	322	GLU	CB-CG-CD	6.52	123.69	112.60
1	A	240	LYS	N-CA-C	-6.51	104.11	111.07
1	A	169	ASP	CA-CB-CG	-6.42	106.17	112.60
1	A	255	SER	N-CA-CB	6.39	120.90	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	SER	CB-CA-C	-6.36	99.59	110.22
1	A	103	ARG	O-C-N	-6.35	114.24	122.37
1	A	112	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	149	LEU	O-C-N	6.21	129.23	122.15
1	A	101	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	210	SER	CB-CA-C	-6.18	101.17	110.88
1	A	10	PHE	O-C-N	-6.16	115.72	123.17
1	A	289	ASP	O-C-N	6.16	130.50	123.48
1	A	97	ASN	N-CA-C	6.10	118.73	111.71
1	A	254	TYR	CA-C-O	-6.09	113.62	120.32
1	A	334	GLN	CG-CD-NE2	-6.06	107.31	116.40
1	A	300	ARG	CA-CB-CG	5.98	126.07	114.10
1	A	225	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	186	VAL	O-C-N	-5.96	114.33	122.26
1	A	282	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	148	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	A	28	GLU	CA-CB-CG	5.95	125.99	114.10
1	A	224	SER	N-CA-C	5.94	117.76	111.28
1	A	179	ASP	CA-C-O	-5.92	112.05	120.16
1	A	270	VAL	N-CA-CB	-5.91	101.48	111.23
1	A	189	PHE	N-CA-C	-5.89	102.05	110.59
1	A	39	THR	CA-C-O	-5.88	114.88	121.81
1	A	12	HIS	CA-CB-CG	5.86	119.66	113.80
1	A	312	LEU	CA-C-N	5.85	126.15	119.83
1	A	312	LEU	C-N-CA	5.85	126.15	119.83
1	A	332	ILE	CA-C-N	5.84	125.60	119.76
1	A	332	ILE	C-N-CA	5.84	125.60	119.76
1	A	156	ILE	N-CA-CB	-5.84	104.26	110.62
1	A	266	MET	CG-SD-CE	-5.83	88.06	100.90
1	A	282	HIS	CA-C-O	-5.83	114.86	120.92
1	A	246	GLN	CA-C-N	-5.80	113.12	121.42
1	A	246	GLN	C-N-CA	-5.80	113.12	121.42
1	A	293	HIS	CA-CB-CG	-5.79	108.01	113.80
1	A	87	ASN	CB-CG-ND2	5.79	125.09	116.40
1	A	138	GLU	CB-CA-C	-5.79	101.19	110.79
1	A	334	GLN	O-C-N	5.78	129.17	122.17
1	A	218	HIS	CB-CG-ND1	5.76	131.34	122.70
1	A	112	HIS	CA-C-O	-5.74	114.32	120.92
1	A	295	VAL	N-CA-CB	-5.73	104.50	111.21
1	A	317	HIS	CB-CA-C	-5.73	101.28	110.79
1	A	30	SER	CA-CB-OG	-5.72	99.66	111.10
1	A	178	TYR	CB-CG-CD2	-5.71	112.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	220	GLN	CA-C-O	-5.67	114.83	121.07
1	A	334	GLN	CA-CB-CG	-5.65	102.80	114.10
1	A	124	LEU	O-C-N	-5.63	115.34	121.53
1	A	164	GLY	N-CA-C	-5.63	107.22	115.72
1	A	99	ILE	N-CA-C	-5.62	100.59	108.12
1	A	115	SER	CA-C-O	-5.60	114.99	121.15
1	A	93	PRO	O-C-N	-5.58	114.88	121.46
1	A	283	ILE	CA-C-O	-5.55	114.16	120.65
1	A	73	ARG	CA-CB-CG	-5.54	103.01	114.10
1	A	194	TRP	CE2-CD2-CG	-5.51	100.58	107.20
1	A	31	TRP	CA-C-N	5.50	126.71	119.84
1	A	31	TRP	C-N-CA	5.50	126.71	119.84
1	A	304	GLN	CA-CB-CG	5.49	125.08	114.10
1	A	28	GLU	N-CA-CB	-5.49	101.47	110.14
1	A	275	LEU	CA-C-N	5.48	126.02	120.38
1	A	275	LEU	C-N-CA	5.48	126.02	120.38
1	A	318	SER	CA-CB-OG	5.46	122.02	111.10
1	A	246	GLN	N-CA-C	5.45	120.04	113.17
1	A	194	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	A	297	MET	O-C-N	-5.43	116.09	123.10
1	A	336	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	A	319	CYS	CA-C-N	5.43	125.19	119.76
1	A	319	CYS	C-N-CA	5.43	125.19	119.76
1	A	199	ALA	O-C-N	5.42	127.89	122.08
1	A	275	LEU	CA-C-O	-5.42	114.94	119.76
1	A	16	GLY	CA-C-N	5.40	125.38	120.03
1	A	16	GLY	C-N-CA	5.40	125.38	120.03
1	A	196	THR	CA-C-O	-5.39	115.58	121.89
1	A	254	TYR	O-C-N	-5.38	116.92	123.27
1	A	318	SER	N-CA-C	-5.38	101.47	109.11
1	A	336	TRP	CB-CG-CD1	-5.36	118.86	126.90
1	A	52	TYR	CA-C-O	-5.34	115.21	120.82
1	A	265	GLN	CA-CB-CG	-5.32	103.45	114.10
1	A	69	GLN	CA-CB-CG	-5.30	103.51	114.10
1	A	182	TYR	N-CA-C	-5.28	105.44	111.14
1	A	139	THR	CA-CB-OG1	-5.27	101.70	109.60
1	A	191	LEU	N-CA-C	5.27	117.42	110.36
1	A	188	ASN	N-CA-CB	-5.27	103.91	111.70
1	A	100	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	A	184	GLU	CA-CB-CG	5.23	124.57	114.10
1	A	237	LYS	CA-CB-CG	5.19	124.49	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ALA	N-CA-C	-5.19	107.60	114.04
1	A	167	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	100	TRP	CB-CG-CD1	-5.16	119.16	126.90
1	A	5	PHE	N-CA-CB	-5.16	103.26	111.62
1	A	82	MET	CB-CG-SD	-5.13	97.31	112.70
1	A	193	THR	CA-CB-OG1	-5.13	101.91	109.60
1	A	5	PHE	CA-C-O	-5.12	115.78	121.51
1	A	57	TYR	CA-CB-CG	-5.07	104.78	113.90
1	A	69	GLN	CA-C-O	-5.06	115.19	120.55
1	A	194	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	26	ILE	CA-CB-CG1	-5.05	101.81	110.40
1	A	28	GLU	CB-CG-CD	5.03	121.15	112.60
1	A	35	PHE	CA-C-O	5.02	126.87	121.55
1	A	166	GLU	CB-CG-CD	-5.00	104.09	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	TYR	Sidechain
1	A	244	GLN	Peptide
1	A	278	TYR	Sidechain
1	A	65	TYR	Sidechain

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	2794	0	2736	91	0
2	B	39	0	34	3	0
3	A	14	0	13	2	0
4	A	10	0	4	3	0
All	All	2857	0	2787	94	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 17.

All (94) 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:177:LEU:HD11	1:A:194:TRP:HH2	1.35	0.92
1:A:177:LEU:HD11	1:A:194:TRP:CH2	2.21	0.75
1:A:66:LYS:HE2	3:A:347:NAG:H81	1.68	0.74
1:A:180:PRO:O	1:A:184:GLU:HG2	1.89	0.73
1:A:218:HIS:CE1	1:A:219:LYS:HE3	2.29	0.68
1:A:302:GLU:HG3	1:A:304:GLN:NE2	2.10	0.66
1:A:126:PHE:HE2	1:A:230:VAL:HG21	1.61	0.65
1:A:79:ARG:NH1	4:A:343:TAR:H3	2.13	0.64
1:A:334:GLN:HA	1:A:334:GLN:OE1	1.98	0.64
1:A:266:MET:SD	1:A:271:TYR:HD2	2.21	0.63
1:A:247:LYS:HZ1	1:A:249:ARG:HB2	1.65	0.62
1:A:176:ARG:HG3	1:A:176:ARG:HH11	1.64	0.62
1:A:84:ALA:HB2	1:A:255:SER:OG	2.00	0.62
1:A:120:ARG:HA	1:A:126:PHE:CE1	2.35	0.61
1:A:258:ASP:HB2	1:A:276:PRO:HD2	1.84	0.60
1:A:28:GLU:HG2	1:A:35:PHE:CE2	2.38	0.58
1:A:54:ARG:NH1	1:A:63:ASN:HD22	2.02	0.58
1:A:137:SER:O	1:A:140:LEU:HB2	2.03	0.58
1:A:302:GLU:HG3	1:A:304:GLN:HE22	1.67	0.57
1:A:300:ARG:HH11	1:A:300:ARG:HG3	1.70	0.56
1:A:28:GLU:HG2	1:A:35:PHE:CD2	2.40	0.56
1:A:327:LEU:O	1:A:330:PRO:HD2	2.06	0.56
1:A:266:MET:SD	1:A:271:TYR:CD2	2.98	0.55
1:A:270:VAL:HG12	1:A:310:LEU:HD13	1.89	0.55
1:A:144:GLU:O	1:A:148:ARG:HB2	2.06	0.55
1:A:270:VAL:CG1	1:A:310:LEU:HB3	2.38	0.54
1:A:247:LYS:HZ3	1:A:248:ALA:C	2.15	0.54
1:A:10:PHE:CE1	1:A:255:SER:HA	2.42	0.53
1:A:289:ASP:HB3	1:A:294:PHE:CE2	2.44	0.53
1:A:285:GLU:HG3	1:A:287:TYR:HE1	1.72	0.53
1:A:218:HIS:HE1	1:A:219:LYS:HE3	1.75	0.51
1:A:139:THR:OG1	1:A:218:HIS:HB3	2.11	0.51
1:A:130:PRO:HD2	1:A:340:CYS:O	2.12	0.50
1:A:61:LEU:HD21	1:A:251:LEU:HD21	1.92	0.50
1:A:199:ALA:O	1:A:202:LYS:HB2	2.11	0.50
1:A:247:LYS:HG2	1:A:248:ALA:N	2.27	0.49
1:A:268:LEU:HD23	1:A:328:LEU:HD11	1.93	0.49
1:A:289:ASP:HB3	1:A:294:PHE:HE2	1.77	0.49
1:A:246:GLN:H	1:A:246:GLN:CD	2.21	0.49
1:A:225:ARG:NH2	1:A:334:GLN:H	2.10	0.49
1:A:11:ARG:CD	1:A:258:ASP:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:NH2	1:A:333:PRO:HA	2.28	0.48
1:A:156:ILE:O	1:A:160:PRO:HD3	2.12	0.48
2:B:2:NAG:O6	2:B:2:NAG:H2	2.14	0.48
1:A:225:ARG:HA	1:A:331:VAL:O	2.14	0.48
1:A:160:PRO:HB3	1:A:166:GLU:HA	1.96	0.47
1:A:131:ARG:O	1:A:134:GLU:HG2	2.13	0.47
1:A:268:LEU:O	1:A:312:LEU:HD12	2.14	0.47
1:A:168:GLN:HA	1:A:173:ILE:HD11	1.97	0.47
1:A:247:LYS:HE2	1:A:249:ARG:HD2	1.96	0.47
1:A:328:LEU:O	1:A:331:VAL:HG12	2.16	0.46
1:A:79:ARG:NH1	4:A:343:TAR:C3	2.79	0.46
1:A:125:PRO:HG3	1:A:214:LEU:HD21	1.97	0.46
1:A:139:THR:HA	1:A:218:HIS:HD2	1.79	0.46
1:A:176:ARG:HG3	1:A:176:ARG:NH1	2.30	0.46
1:A:116:LEU:HD22	1:A:123:TYR:CE2	2.51	0.46
1:A:311:THR:HG23	1:A:317:HIS:HA	1.97	0.46
1:A:11:ARG:O	1:A:279:ALA:HA	2.17	0.45
1:A:240:LYS:HE2	1:A:321:LEU:HD21	1.97	0.45
1:A:300:ARG:HH11	1:A:300:ARG:CG	2.28	0.45
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.79	0.45
1:A:270:VAL:HG11	1:A:310:LEU:HB3	1.98	0.45
1:A:288:GLN:HB2	1:A:293:HIS:HE2	1.82	0.45
1:A:129:CYS:HA	1:A:130:PRO:HD3	1.69	0.44
1:A:61:LEU:HD21	1:A:251:LEU:CD2	2.47	0.44
1:A:288:GLN:HB2	1:A:293:HIS:NE2	2.33	0.44
1:A:225:ARG:O	1:A:333:PRO:HB3	2.17	0.43
1:A:47:TYR:CE1	1:A:90:ALA:HB2	2.54	0.43
1:A:79:ARG:HH12	4:A:343:TAR:H3	1.84	0.43
1:A:332:ILE:HA	1:A:333:PRO:HD2	1.90	0.43
1:A:65:TYR:CG	1:A:109:ILE:HD13	2.54	0.43
1:A:21:PHE:CD1	1:A:177:LEU:HD12	2.53	0.42
1:A:10:PHE:CD1	1:A:255:SER:HA	2.54	0.42
1:A:186:VAL:HG12	1:A:186:VAL:O	2.19	0.42
1:A:272:ASN:HD21	1:A:274:LEU:HB2	1.85	0.42
1:A:5:PHE:HD1	1:A:249:ARG:O	2.02	0.42
1:A:49:LEU:CD1	1:A:53:ILE:HD11	2.49	0.42
1:A:78:ASP:O	1:A:82:MET:HG3	2.19	0.42
1:A:182:TYR:CE2	1:A:186:VAL:HG21	2.55	0.42
1:A:66:LYS:HE2	3:A:347:NAG:C8	2.45	0.42
2:B:2:NAG:O6	2:B:2:NAG:C2	2.68	0.41
1:A:106:TRP:CH2	1:A:108:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HA	1:A:126:PHE:HE1	1.83	0.41
1:A:74:SER:OG	1:A:75:THR:N	2.52	0.41
1:A:296:GLU:HG2	1:A:318:SER:HA	2.03	0.41
1:A:49:LEU:HD12	1:A:87:ASN:ND2	2.36	0.41
1:A:150:GLN:O	1:A:151:PRO:C	2.62	0.41
2:B:1:NAG:H62	2:B:2:NAG:C1	2.51	0.41
1:A:274:LEU:N	1:A:274:LEU:HD12	2.35	0.41
1:A:286:LEU:HD12	1:A:295:VAL:HG22	2.03	0.41
1:A:216:GLY:HA2	1:A:220:GLN:HG3	2.03	0.40
1:A:66:LYS:O	1:A:68:ASP:N	2.55	0.40
1:A:11:ARG:HD2	1:A:258:ASP:HB3	2.02	0.40
1:A:139:THR:HA	1:A:218:HIS:CD2	2.56	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	340/342 (99%)	305 (90%)	27 (8%)	8 (2%)	4	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ILE
1	A	290	ASN
1	A	67	HIS
1	A	96	GLY
1	A	128	ASP
1	A	143	GLU
1	A	63	ASN
1	A	32	PRO

5.3.2 Protein sidechains ⓘ

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	311/311 (100%)	261 (84%)	50 (16%)	2 12

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	VAL
1	A	10	PHE
1	A	11	ARG
1	A	26	ILE
1	A	28	GLU
1	A	49	LEU
1	A	55	ARG
1	A	59	ARG
1	A	61	LEU
1	A	68	ASP
1	A	73	ARG
1	A	75	THR
1	A	79	ARG
1	A	81	LEU
1	A	91	LEU
1	A	98	SER
1	A	103	ARG
1	A	113	THR
1	A	118	GLU
1	A	120	ARG
1	A	127	ARG
1	A	140	LEU
1	A	144	GLU
1	A	146	LEU
1	A	147	LYS
1	A	150	GLN
1	A	153	LYS
1	A	157	ASP
1	A	158	THR

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Mol	Chain	Res	Type
1	A	170	LEU
1	A	176	ARG
1	A	193	THR
1	A	205	GLU
1	A	226	LEU
1	A	231	LEU
1	A	240	LYS
1	A	244	GLN
1	A	246	GLN
1	A	247	LYS
1	A	249	ARG
1	A	251	LEU
1	A	266	MET
1	A	288	GLN
1	A	302	GLU
1	A	312	LEU
1	A	316	THR
1	A	322	GLU
1	A	335	ASP
1	A	339	GLU

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	33	GLN
1	A	46	HIS
1	A	63	ASN
1	A	87	ASN
1	A	133	GLN
1	A	265	GLN
1	A	290	ASN
1	A	304	GLN
1	A	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

3 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	1.09	1 (7%)	17,19,21	2.53	7 (41%)
2	NAG	B	2	2	14,14,15	1.18	1 (7%)	17,19,21	2.61	9 (52%)
2	BMA	B	3	2	11,11,12	2.16	2 (18%)	15,15,17	2.57	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	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C4-C3	5.77	1.67	1.52
2	B	3	BMA	C2-C3	2.92	1.57	1.52
2	B	2	NAG	C1-C2	-2.61	1.48	1.52
2	B	1	NAG	C4-C3	-2.07	1.47	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	5.99	120.21	112.19
2	B	3	BMA	C1-C2-C3	-5.70	101.34	109.64
2	B	2	NAG	C1-O5-C5	4.70	118.48	112.19
2	B	3	BMA	C3-C4-C5	4.40	118.21	110.23
2	B	2	NAG	C2-N2-C7	-4.34	117.08	122.90
2	B	2	NAG	C1-C2-N2	-4.16	103.88	110.43
2	B	1	NAG	C1-C2-N2	3.88	116.54	110.43
2	B	1	NAG	O5-C5-C6	-3.87	100.14	107.66
2	B	1	NAG	C6-C5-C4	-3.74	103.84	113.02
2	B	2	NAG	C4-C3-C2	3.73	116.48	111.02
2	B	3	BMA	O4-C4-C5	-3.42	100.90	109.32
2	B	1	NAG	C2-N2-C7	-3.06	118.81	122.90
2	B	3	BMA	C1-O5-C5	-3.02	108.14	112.19
2	B	3	BMA	O5-C5-C6	2.68	112.88	107.66
2	B	2	NAG	O7-C7-C8	2.67	126.80	122.05
2	B	2	NAG	C3-C4-C5	2.66	115.06	110.23
2	B	2	NAG	O5-C5-C6	2.60	112.71	107.66
2	B	1	NAG	O5-C5-C4	2.51	116.92	110.83
2	B	3	BMA	O2-C2-C3	2.43	115.19	110.15
2	B	1	NAG	C3-C4-C5	2.25	114.31	110.23
2	B	2	NAG	O3-C3-C2	-2.11	105.01	109.40
2	B	2	NAG	O3-C3-C4	-2.01	105.64	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

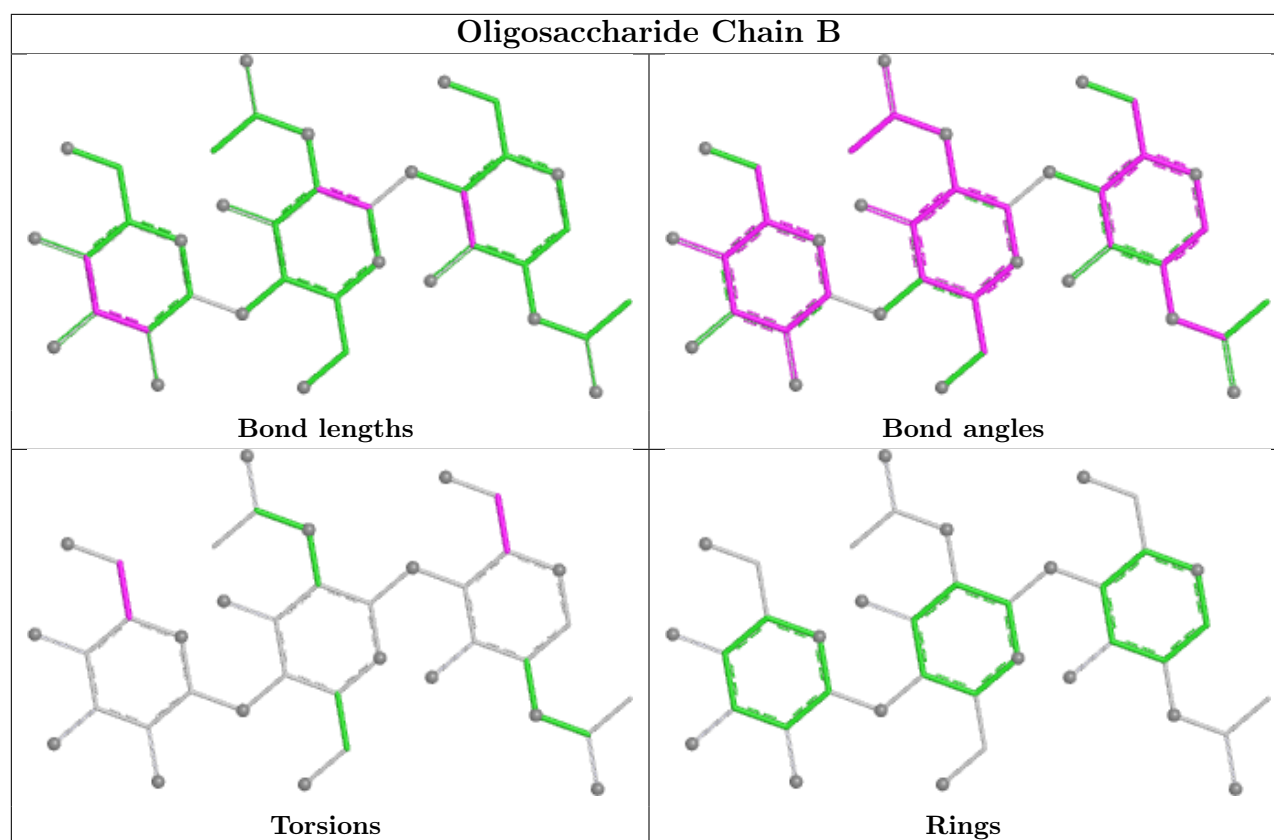
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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



5.6 Ligand geometry [i](#)

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	NAG	A	347	1	14,14,15	2.51	7 (50%)	17,19,21	2.93	6 (35%)
4	TAR	A	343	-	9,9,9	1.47	1 (11%)	12,12,12	2.65	5 (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	NAG	A	347	1	-	3/6/23/26	0/1/1/1
4	TAR	A	343	-	-	9/12/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	347	NAG	C4-C5	5.57	1.64	1.53
3	A	347	NAG	C4-C3	4.47	1.63	1.52
3	A	347	NAG	O5-C5	3.08	1.49	1.43
4	A	343	TAR	O11-C1	-2.88	1.21	1.30
3	A	347	NAG	C1-C2	2.59	1.55	1.52
3	A	347	NAG	C3-C2	2.55	1.57	1.52
3	A	347	NAG	C8-C7	2.22	1.55	1.50
3	A	347	NAG	C2-N2	2.12	1.49	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	347	NAG	C3-C4-C5	6.82	122.60	110.23
3	A	347	NAG	C1-O5-C5	-6.14	103.95	112.19
4	A	343	TAR	C3-C2-C1	4.98	120.86	109.82
3	A	347	NAG	C1-C2-N2	4.94	118.21	110.43
4	A	343	TAR	C2-C3-C4	4.64	120.11	109.82
4	A	343	TAR	O2-C2-C3	-4.61	100.79	110.17
3	A	347	NAG	O4-C4-C5	-3.58	100.50	109.32
4	A	343	TAR	O3-C3-C2	-2.34	105.40	110.17
3	A	347	NAG	C4-C3-C2	-2.31	107.64	111.02
3	A	347	NAG	O3-C3-C2	2.23	114.04	109.40
4	A	343	TAR	O41-C4-C3	2.04	118.99	113.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	347	NAG	C1-C2-N2-C7
4	A	343	TAR	O3-C3-C4-O4
4	A	343	TAR	O3-C3-C4-O41
4	A	343	TAR	C2-C3-C4-O4
4	A	343	TAR	C2-C3-C4-O41
3	A	347	NAG	O5-C5-C6-O6
4	A	343	TAR	O2-C2-C3-O3
4	A	343	TAR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	343	TAR	O11-C1-C2-C3
4	A	343	TAR	O1-C1-C2-C3
3	A	347	NAG	C4-C5-C6-O6
4	A	343	TAR	O11-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	347	NAG	2	0
4	A	343	TAR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.