Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 08:10 AM EDT

PDB ID	:	1RPA
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:

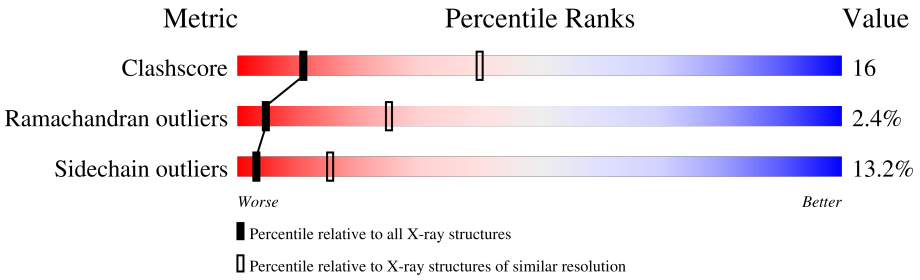
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	342	50% 35% 13%
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.

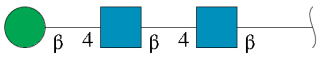
- Molecule 1 is a protein called PROSTATIC ACID PHOSPHATASE.

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

There are 7 discrepancies between the modelled and reference sequences:

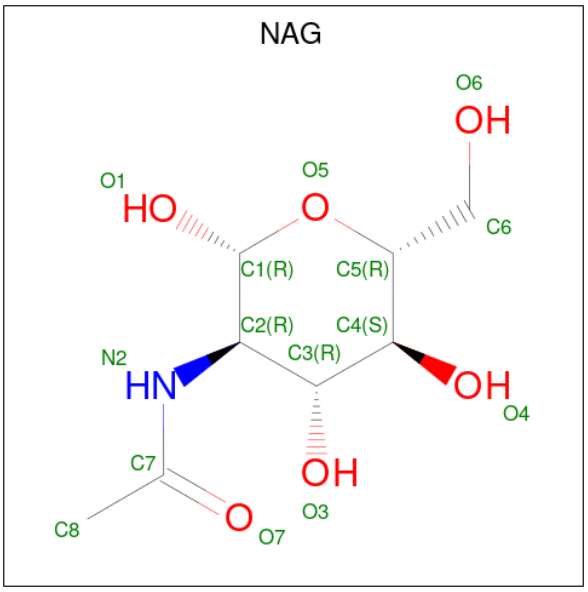
Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	ILE	conflict	UNP P20646
A	191	LEU	PHE	conflict	UNP P20646
A	192	PRO	ARG	conflict	UNP P20646
A	257	HIS	TYR	conflict	UNP P20646
A	269	ASP	GLU	conflict	UNP P20646
A	270	VAL	LEU	conflict	UNP P20646
A	293	HIS	THR	conflict	UNP P20646

- 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.



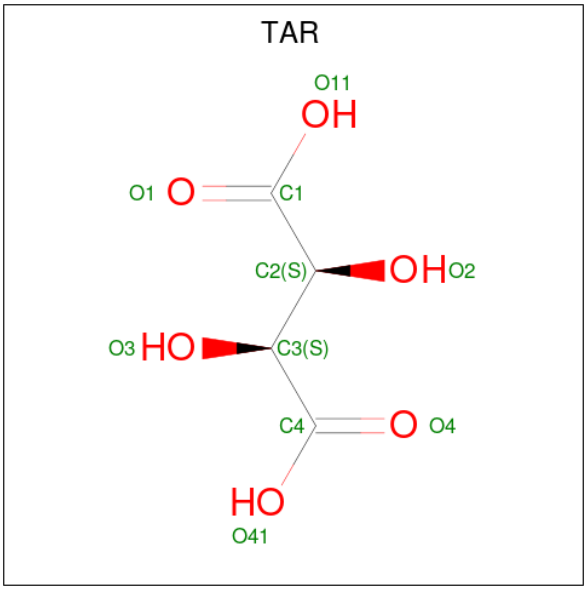
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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 (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

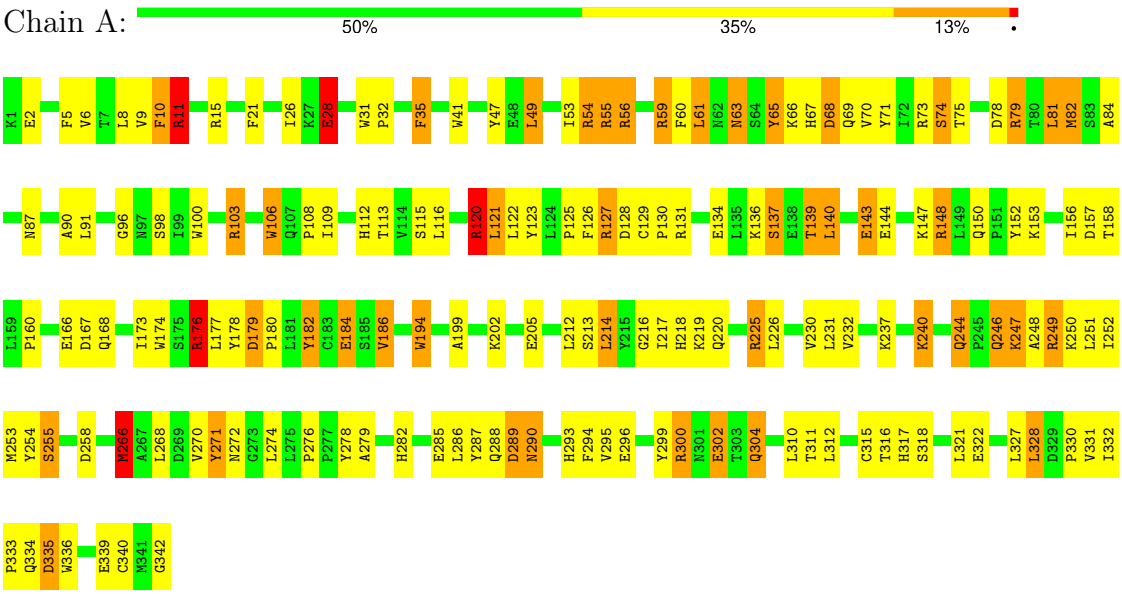
3 Residue-property plots (i)

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: PROSTATIC ACID PHOSPHATASE

Chain A:



• Molecule 2: 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	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TAR, BMA, 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	1.27	4/2873 (0.1%)	2.06	114/3898 (2.9%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CB-CG	6.00	1.63	1.52
1	A	106	TRP	CG-CD2	-5.53	1.34	1.43
1	A	143	GLU	CG-CD	5.51	1.60	1.51
1	A	74	SER	CA-CB	-5.06	1.45	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	TYR	CB-CG-CD2	-14.61	112.24	121.00
1	A	225	ARG	NE-CZ-NH1	14.33	127.47	120.30
1	A	71	TYR	CB-CG-CD1	-12.78	113.33	121.00
1	A	176	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	176	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	225	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	178	TYR	CB-CG-CD1	10.04	127.02	121.00
1	A	194	TRP	CD1-CG-CD2	9.64	114.01	106.30
1	A	56	ARG	NE-CZ-NH2	-9.07	115.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ASP	CB-CG-OD1	8.82	126.23	118.30
1	A	71	TYR	CB-CG-CD2	8.81	126.28	121.00
1	A	194	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	A	11	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	59	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	59	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	100	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	335	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	266	MET	CG-SD-CE	-7.59	88.06	100.20
1	A	100	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	290	ASN	CA-C-N	7.34	130.89	116.20
1	A	247	LYS	CA-CB-CG	-7.12	97.75	113.40
1	A	249	ARG	CA-C-N	-7.11	101.56	117.20
1	A	121	LEU	N-CA-C	-6.99	92.12	111.00
1	A	336	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	289	ASP	CA-C-N	-6.94	101.92	117.20
1	A	255	SER	N-CA-CB	6.93	120.90	110.50
1	A	70	VAL	CA-C-N	6.91	132.41	117.20
1	A	106	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	A	6	VAL	CA-C-N	6.75	132.06	117.20
1	A	8	LEU	CA-C-N	6.65	131.82	117.20
1	A	8	LEU	CA-CB-CG	6.62	130.54	115.30
1	A	112	HIS	CA-C-N	6.61	131.75	117.20
1	A	148	ARG	CA-CB-CG	-6.61	98.87	113.40
1	A	6	VAL	O-C-N	-6.54	112.23	122.70
1	A	6	VAL	CG1-CB-CG2	-6.50	100.49	110.90
1	A	127	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	31	TRP	CD1-CG-CD2	6.39	111.42	106.30
1	A	336	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	A	41	TRP	CD1-CG-CD2	6.38	111.40	106.30
1	A	54	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	194	TRP	CG-CD1-NE1	-6.26	103.84	110.10
1	A	336	TRP	CB-CG-CD1	-6.26	118.86	127.00
1	A	335	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	339	GLU	CA-CB-CG	-6.21	99.74	113.40
1	A	328	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	41	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	140	LEU	CB-CG-CD1	-6.17	100.52	111.00
1	A	122	LEU	N-CA-C	6.12	127.52	111.00
1	A	249	ARG	CA-CB-CG	-6.06	100.07	113.40
1	A	194	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	A	336	TRP	CG-CD2-CE3	6.04	139.33	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	TRP	CB-CG-CD1	-6.03	119.16	127.00
1	A	282	HIS	CA-C-N	6.03	130.47	117.20
1	A	174	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	A	55	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	103	ARG	CA-C-N	5.91	130.21	117.20
1	A	194	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	A	212	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	A	179	ASP	CA-CB-CG	-5.85	100.53	113.40
1	A	100	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	A	139	THR	O-C-N	5.84	132.05	122.70
1	A	174	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	A	106	TRP	CE2-CD2-CG	-5.79	102.66	107.30
1	A	250	LYS	CA-C-N	5.76	129.88	117.20
1	A	300	ARG	CA-CB-CG	5.76	126.07	113.40
1	A	28	GLU	CA-CB-CG	5.72	125.99	113.40
1	A	69	GLN	N-CA-C	5.72	126.44	111.00
1	A	8	LEU	O-C-N	-5.71	113.57	122.70
1	A	120	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	271	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	54	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	254	TYR	CB-CG-CD2	5.63	124.38	121.00
1	A	250	LYS	N-CA-C	-5.62	95.84	111.00
1	A	250	LYS	O-C-N	-5.58	113.77	122.70
1	A	254	TYR	CA-C-N	5.57	129.45	117.20
1	A	249	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	232	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	A	214	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	255	SER	CB-CA-C	-5.53	99.59	110.10
1	A	112	HIS	O-C-N	-5.50	113.89	122.70
1	A	31	TRP	CE2-CD2-CG	-5.49	102.91	107.30
1	A	11	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	152	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	299	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	82	MET	CG-SD-CE	5.38	108.81	100.20
1	A	148	ARG	CD-NE-CZ	-5.38	116.07	123.60
1	A	15	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	81	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	100	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	304	GLN	CA-CB-CG	5.31	125.08	113.40
1	A	148	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	103	ARG	O-C-N	-5.29	114.24	122.70
1	A	282	HIS	O-C-N	-5.25	114.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ILE	N-CA-C	-5.24	96.84	111.00
1	A	186	VAL	O-C-N	-5.23	114.33	122.70
1	A	253	MET	CA-CB-CG	5.22	122.17	113.30
1	A	315	CYS	CA-CB-SG	-5.22	104.61	114.00
1	A	342	GLY	N-CA-C	-5.21	100.07	113.10
1	A	70	VAL	O-C-N	-5.21	114.37	122.70
1	A	271	TYR	CB-CG-CD1	5.19	124.12	121.00
1	A	35	PHE	CA-C-N	-5.18	105.83	116.20
1	A	60	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	41	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	A	167	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	179	ASP	CA-C-N	5.10	131.37	117.10
1	A	59	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	184	GLU	CA-CB-CG	5.08	124.57	113.40
1	A	28	GLU	N-CA-CB	-5.07	101.47	110.60
1	A	213	SER	CA-CB-OG	-5.07	97.51	111.20
1	A	55	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	137	SER	CA-CB-OG	5.06	124.85	111.20
1	A	237	LYS	CA-CB-CG	5.04	124.49	113.40
1	A	82	MET	CB-CG-SD	-5.03	97.31	112.40
1	A	120	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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 (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	2794	0	2736	89	0
2	B	39	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	2	0
4	A	10	0	4	3	0
All	All	2857	0	2787	92	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 16.

All (92) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:247:LYS:HZ3	1:A:248:ALA:C	2.15	0.49
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:246:GLN:H	1:A:246:GLN:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:SER:OG	1:A:75:THR:N	2.52	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
1:A:120:ARG:HA	1:A:126:PHE:HE1	1.83	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
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%)	5 25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ILE

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Mol	Chain	Res	Type
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 (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	311/311 (100%)	270 (87%)	41 (13%)	3 15

All (41) 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	56	ARG
1	A	59	ARG
1	A	61	LEU
1	A	68	ASP
1	A	73	ARG
1	A	79	ARG
1	A	81	LEU
1	A	91	LEU
1	A	98	SER
1	A	103	ARG
1	A	113	THR

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Mol	Chain	Res	Type
1	A	115	SER
1	A	120	ARG
1	A	127	ARG
1	A	136	LYS
1	A	147	LYS
1	A	150	GLN
1	A	153	LYS
1	A	157	ASP
1	A	158	THR
1	A	176	ARG
1	A	179	ASP
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	266	MET
1	A	302	GLU
1	A	316	THR
1	A	322	GLU
1	A	335	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	63	ASN
1	A	87	ASN
1	A	265	GLN
1	A	304	GLN

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)

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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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:

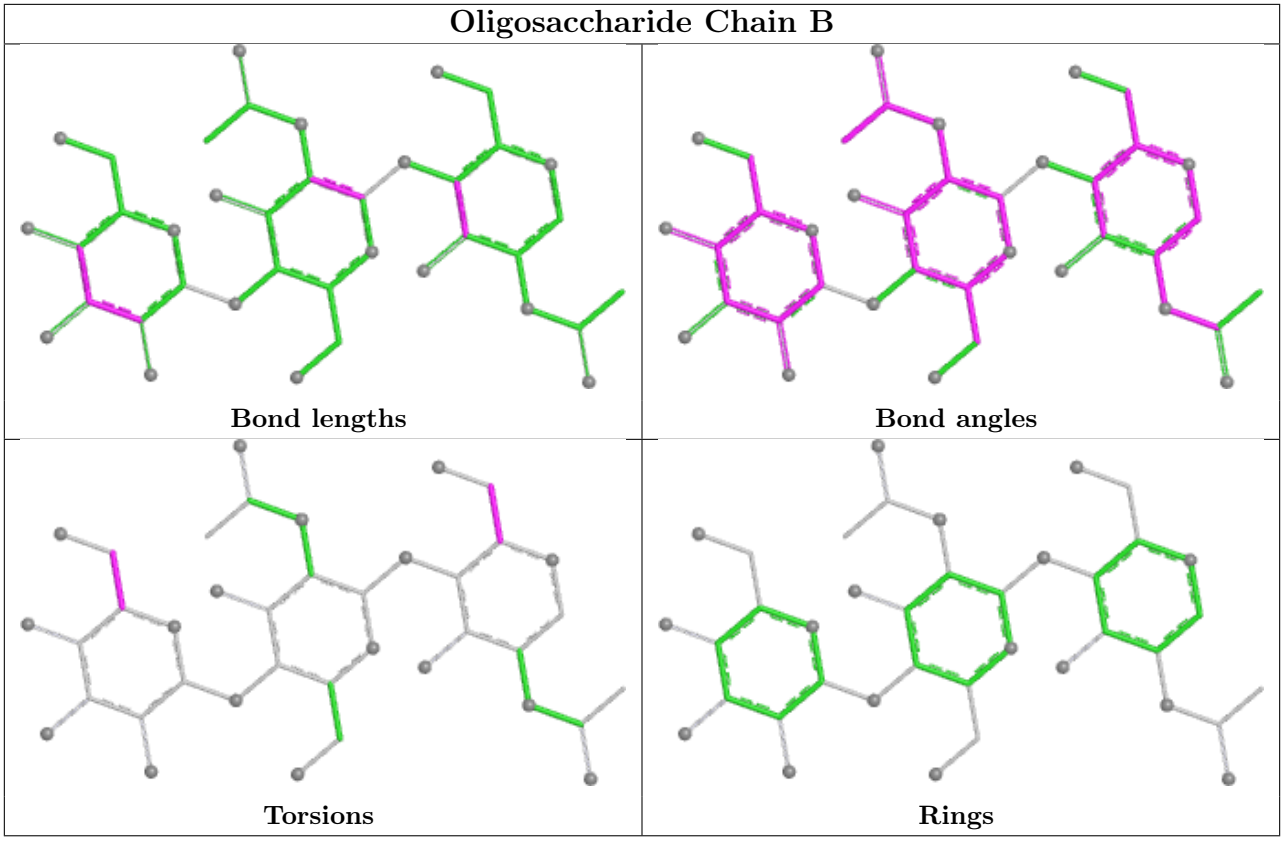
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

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(^{o})	Ideal(^{o})
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.