



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 PM UTC

PDB ID : 1RPT / pdb_00001rpt
Title : CRYSTAL STRUCTURES OF RAT ACID PHOSPHATASE COMPLEXED WITH THE TRANSITIONS STATE ANALOGS VANADATE AND MOLYBDATE: IMPLICATIONS FOR THE REACTION MECHANISM
Authors : Lindqvist, Y.; Schneider, G.
Deposited on : 1993-11-29
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

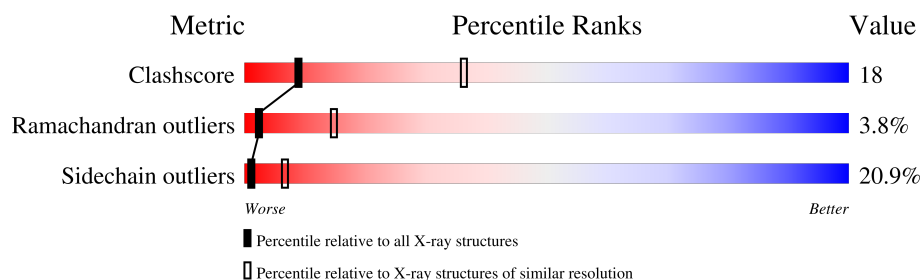
1 Overall quality at a glance

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	32% 37% 24% 7%
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	VO4	A	343	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2852 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.

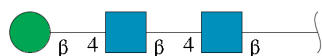
- Molecule 1 is a protein called PROSTATIC ACID PHOSPHATASE.

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.



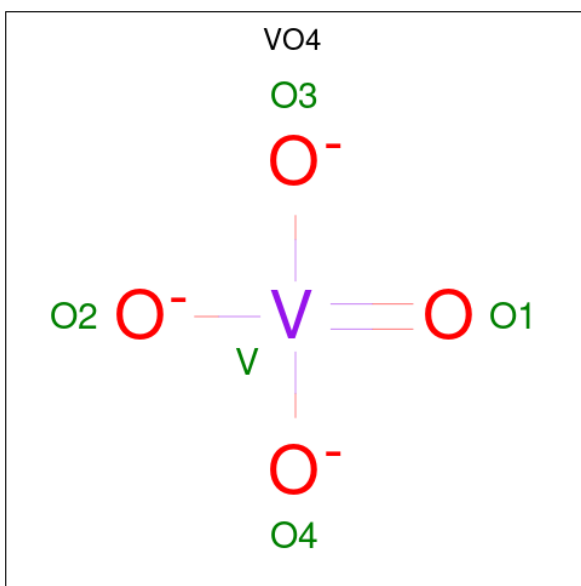
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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 VANADATE ION (CCD ID: VO4) (formula: O_4V).



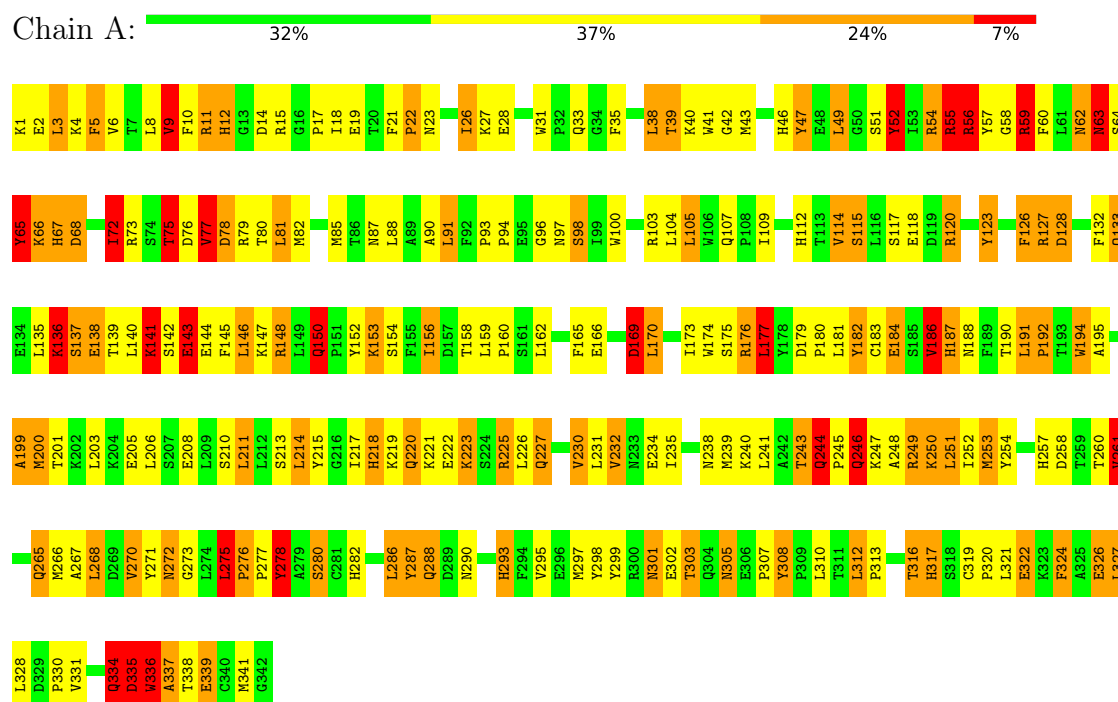
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		

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	2852	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: NAG, BMA, VO4

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	1.58	30/2873 (1.0%)	2.46	208/3898 (5.3%)

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	6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	HIS	CD2-NE2	-8.68	1.28	1.37
1	A	293	HIS	CD2-NE2	-8.19	1.28	1.37
1	A	12	HIS	CG-ND1	-7.41	1.30	1.38
1	A	12	HIS	CD2-NE2	-7.27	1.29	1.37
1	A	317	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	31	TRP	CA-CB	-6.99	1.44	1.53
1	A	257	HIS	CG-ND1	-6.84	1.30	1.38
1	A	127	ARG	NE-CZ	6.75	1.40	1.33
1	A	93	PRO	CA-C	6.71	1.56	1.52
1	A	282	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	22	PRO	CA-CB	-6.16	1.44	1.53
1	A	114	VAL	CA-CB	-6.11	1.46	1.55
1	A	244	GLN	CA-CB	5.78	1.61	1.53
1	A	103	ARG	CA-C	5.63	1.60	1.53
1	A	55	ARG	NE-CZ	5.61	1.39	1.33
1	A	46	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	187	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	73	ARG	CA-CB	-5.50	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	SER	CA-CB	-5.50	1.44	1.53
1	A	31	TRP	CG-CD2	-5.47	1.33	1.43
1	A	9	VAL	CA-CB	5.44	1.61	1.54
1	A	139	THR	CA-CB	5.42	1.61	1.53
1	A	43	MET	CA-C	-5.39	1.47	1.53
1	A	75	THR	CA-C	-5.35	1.45	1.52
1	A	59	ARG	CZ-NH1	5.32	1.40	1.32
1	A	218	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	59	ARG	NE-CZ	5.23	1.38	1.33
1	A	103	ARG	NE-CZ	5.13	1.38	1.33
1	A	145	PHE	N-CA	-5.10	1.40	1.46
1	A	287	TYR	CA-CB	-5.10	1.46	1.53

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	PHE	CA-CB-CG	-12.51	101.30	113.80
1	A	93	PRO	O-C-N	-11.47	115.76	121.15
1	A	305	ASN	CA-CB-CG	-11.28	101.32	112.60
1	A	46	HIS	CA-CB-CG	-10.97	102.83	113.80
1	A	126	PHE	CA-CB-CG	10.11	123.91	113.80
1	A	68	ASP	N-CA-C	-9.46	101.87	113.50
1	A	301	ASN	CA-C-O	-9.36	109.85	120.24
1	A	112	HIS	CA-C-O	-9.05	110.38	120.69
1	A	41	TRP	N-CA-C	-8.98	101.89	113.12
1	A	238	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	A	100	TRP	N-CA-C	-8.86	102.27	113.43
1	A	43	MET	N-CA-C	-8.80	97.40	111.04
1	A	87	ASN	OD1-CG-ND2	-8.54	114.06	122.60
1	A	41	TRP	CG-CD2-CE3	8.51	142.41	133.90
1	A	51	SER	CA-C-O	-8.49	111.81	120.90
1	A	8	LEU	CA-C-O	-8.39	111.33	120.30
1	A	150	GLN	CA-CB-CG	-8.24	97.61	114.10
1	A	97	ASN	CA-C-N	-8.09	109.71	122.65
1	A	97	ASN	C-N-CA	-8.09	109.71	122.65
1	A	293	HIS	CB-CG-CD2	-8.09	120.69	131.20
1	A	63	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	A	67	HIS	N-CA-C	8.05	127.94	110.80
1	A	176	ARG	CB-CG-CD	7.85	129.35	111.30
1	A	253	MET	N-CA-CB	-7.80	99.71	111.64
1	A	107	GLN	CA-C-O	-7.76	112.97	120.19
1	A	128	ASP	CA-CB-CG	-7.72	104.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LYS	CA-CB-CG	7.69	129.49	114.10
1	A	331	VAL	N-CA-C	-7.61	105.13	112.29
1	A	184	GLU	CA-CB-CG	7.59	129.28	114.10
1	A	272	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A	250	LYS	CB-CG-CD	-7.57	93.88	111.30
1	A	52	TYR	CA-C-O	-7.55	113.07	121.00
1	A	23	ASN	CB-CG-ND2	7.46	127.60	116.40
1	A	254	TYR	N-CA-C	7.46	121.49	110.30
1	A	23	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	A	65	TYR	O-C-N	-7.38	112.64	122.38
1	A	107	GLN	CA-CB-CG	7.32	128.74	114.10
1	A	238	ASN	CB-CG-ND2	7.30	127.35	116.40
1	A	317	HIS	CB-CG-CD2	-7.29	121.72	131.20
1	A	257	HIS	N-CA-C	7.26	121.40	110.14
1	A	170	LEU	N-CA-C	7.18	119.97	111.71
1	A	324	PHE	CA-CB-CG	7.13	120.93	113.80
1	A	21	PHE	CA-C-N	7.11	126.94	119.05
1	A	21	PHE	C-N-CA	7.11	126.94	119.05
1	A	63	ASN	CB-CG-ND2	7.08	127.03	116.40
1	A	75	THR	N-CA-C	-7.01	98.19	109.96
1	A	93	PRO	N-CA-CB	-7.01	99.58	103.22
1	A	199	ALA	O-C-N	6.99	129.30	122.03
1	A	28	GLU	N-CA-C	-6.99	103.66	111.28
1	A	293	HIS	CA-CB-CG	-6.92	106.88	113.80
1	A	166	GLU	CB-CG-CD	-6.91	100.85	112.60
1	A	87	ASN	CB-CG-ND2	6.90	126.75	116.40
1	A	141	LYS	CB-CG-CD	6.88	127.12	111.30
1	A	249	ARG	N-CA-C	-6.88	98.52	109.59
1	A	227	GLN	N-CA-C	6.79	118.90	108.30
1	A	93	PRO	CB-CA-C	6.76	117.53	111.17
1	A	138	GLU	CA-CB-CG	6.73	127.56	114.10
1	A	253	MET	N-CA-C	6.67	122.33	108.53
1	A	4	LYS	O-C-N	-6.65	113.45	122.36
1	A	213	SER	CA-C-O	-6.64	113.39	120.42
1	A	5	PHE	O-C-N	-6.60	115.18	123.17
1	A	39	THR	CB-CA-C	-6.57	97.33	111.78
1	A	127	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	194	TRP	CG-CD2-CE3	6.52	140.42	133.90
1	A	265	GLN	N-CA-C	-6.52	104.25	111.82
1	A	257	HIS	CB-CG-CD2	-6.51	122.74	131.20
1	A	192	PRO	N-CA-C	6.47	121.12	111.41
1	A	265	GLN	CG-CD-NE2	6.42	126.04	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	HIS	CA-C-O	-6.40	113.07	120.49
1	A	252	ILE	N-CA-C	-6.38	99.02	108.85
1	A	276	PRO	CA-C-N	6.36	126.32	120.03
1	A	276	PRO	C-N-CA	6.36	126.32	120.03
1	A	336	TRP	CG-CD2-CE3	6.33	140.23	133.90
1	A	41	TRP	CB-CG-CD1	-6.31	117.43	126.90
1	A	12	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	335	ASP	N-CA-C	-6.28	98.98	108.46
1	A	261	VAL	CB-CA-C	-6.27	103.95	111.97
1	A	268	LEU	N-CA-CB	-6.26	99.89	110.41
1	A	156	ILE	N-CA-CB	-6.26	104.05	110.62
1	A	137	SER	N-CA-C	-6.25	105.30	113.12
1	A	208	GLU	CA-CB-CG	6.25	126.61	114.10
1	A	22	PRO	N-CA-C	6.24	122.20	113.53
1	A	213	SER	N-CA-C	-6.21	104.59	111.36
1	A	154	SER	CB-CA-C	-6.18	101.44	110.96
1	A	334	GLN	CA-CB-CG	-6.18	101.74	114.10
1	A	303	THR	N-CA-C	-6.17	105.41	113.12
1	A	78	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	218	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	275	LEU	CA-C-N	6.13	126.70	120.38
1	A	275	LEU	C-N-CA	6.13	126.70	120.38
1	A	243	THR	CA-CB-OG1	6.12	118.78	109.60
1	A	104	LEU	CA-C-O	6.11	127.04	120.63
1	A	254	TYR	O-C-N	-6.09	114.72	123.07
1	A	230	VAL	CA-CB-CG1	-6.09	100.04	110.40
1	A	10	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	331	VAL	O-C-N	-6.06	116.64	122.09
1	A	49	LEU	CB-CA-C	-6.05	101.39	110.88
1	A	46	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	147	LYS	CB-CA-C	6.00	120.41	110.81
1	A	147	LYS	CA-CB-CG	6.00	126.10	114.10
1	A	194	TRP	CB-CG-CD1	-5.97	117.94	126.90
1	A	98	SER	N-CA-C	5.96	120.25	112.92
1	A	33	GLN	CB-CG-CD	5.95	122.72	112.60
1	A	31	TRP	CD1-CG-CD2	5.94	115.81	106.30
1	A	147	LYS	N-CA-C	-5.94	103.98	111.11
1	A	81	LEU	N-CA-C	-5.94	104.16	111.40
1	A	253	MET	CG-SD-CE	-5.92	87.88	100.90
1	A	337	ALA	N-CA-C	5.92	123.40	110.80
1	A	91	LEU	N-CA-C	-5.87	104.81	111.14
1	A	8	LEU	N-CA-C	-5.86	98.86	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	PHE	CA-C-O	-5.86	115.20	121.94
1	A	192	PRO	O-C-N	5.86	130.15	123.00
1	A	278	TYR	CA-CB-CG	5.83	124.40	113.90
1	A	248	ALA	CA-C-O	5.83	128.14	120.15
1	A	295	VAL	N-CA-CB	-5.83	104.11	111.46
1	A	225	ARG	CB-CG-CD	-5.82	97.93	111.30
1	A	322	GLU	CB-CG-CD	5.81	122.48	112.60
1	A	76	ASP	N-CA-CB	-5.80	100.78	110.42
1	A	6	VAL	CA-CB-CG2	-5.80	100.53	110.40
1	A	194	TRP	CE2-CD2-CG	-5.80	100.24	107.20
1	A	166	GLU	N-CA-C	5.80	120.22	113.20
1	A	223	LYS	N-CA-C	-5.80	104.16	111.11
1	A	147	LYS	N-CA-CB	-5.79	101.31	109.94
1	A	290	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	56	ARG	N-CA-C	-5.77	104.96	112.23
1	A	31	TRP	CG-CD1-NE1	-5.75	102.73	110.20
1	A	31	TRP	CE2-CD2-CG	-5.72	100.33	107.20
1	A	267	ALA	O-C-N	5.71	128.66	122.15
1	A	169	ASP	N-CA-C	5.70	118.27	110.24
1	A	26	ILE	CA-CB-CG1	-5.68	100.73	110.40
1	A	138	GLU	CA-C-N	5.65	127.78	120.44
1	A	138	GLU	C-N-CA	5.65	127.78	120.44
1	A	152	TYR	N-CA-CB	-5.64	101.87	110.33
1	A	278	TYR	CA-C-N	5.63	130.84	122.74
1	A	278	TYR	C-N-CA	5.63	130.84	122.74
1	A	248	ALA	N-CA-C	5.61	117.36	107.61
1	A	293	HIS	CA-C-O	-5.60	114.10	120.32
1	A	27	LYS	CA-CB-CG	-5.60	102.91	114.10
1	A	190	THR	CA-C-O	-5.59	114.55	120.92
1	A	174	TRP	CA-CB-CG	5.58	124.21	113.60
1	A	39	THR	N-CA-CB	5.58	119.02	110.49
1	A	109	ILE	O-C-N	-5.58	114.74	121.10
1	A	282	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	A	66	LYS	O-C-N	-5.55	116.04	122.87
1	A	6	VAL	O-C-N	-5.53	116.69	123.00
1	A	47	TYR	CB-CG-CD1	-5.53	112.51	120.80
1	A	132	PHE	CA-C-O	-5.52	115.02	120.82
1	A	62	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	55	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	12	HIS	CA-CB-CG	5.48	119.28	113.80
1	A	75	THR	N-CA-CB	5.48	119.10	110.23
1	A	5	PHE	N-CA-CB	-5.47	102.17	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	CB-CG-CD	-5.46	98.73	111.30
1	A	179	ASP	CA-C-O	-5.46	112.68	120.16
1	A	308	TYR	CA-C-N	5.45	126.65	119.84
1	A	308	TYR	C-N-CA	5.45	126.65	119.84
1	A	1	LYS	CA-CB-CG	5.44	124.98	114.10
1	A	226	LEU	N-CA-C	-5.41	105.41	112.23
1	A	235	ILE	N-CA-C	-5.41	105.10	110.62
1	A	67	HIS	O-C-N	-5.41	115.40	122.59
1	A	220	GLN	CA-C-O	-5.40	112.78	120.51
1	A	191	LEU	CA-C-N	5.36	125.33	120.03
1	A	191	LEU	C-N-CA	5.36	125.33	120.03
1	A	218	HIS	CA-CB-CG	5.33	119.13	113.80
1	A	100	TRP	CG-CD2-CE3	5.33	139.23	133.90
1	A	183	CYS	CA-C-O	-5.33	115.41	120.90
1	A	49	LEU	N-CA-CB	5.32	117.72	110.01
1	A	150	GLN	CA-C-O	-5.31	112.88	120.16
1	A	232	VAL	CB-CA-C	-5.30	105.19	111.97
1	A	288	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	194	TRP	CD1-CG-CD2	5.28	114.75	106.30
1	A	19	GLU	CA-C-O	-5.28	115.63	121.33
1	A	77	VAL	O-C-N	-5.27	116.99	123.00
1	A	280	SER	CA-CB-OG	5.23	121.56	111.10
1	A	72	ILE	CB-CG1-CD1	5.23	124.78	113.80
1	A	85	MET	N-CA-C	-5.23	105.50	111.14
1	A	218	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	154	SER	N-CA-CB	5.21	117.51	109.91
1	A	251	LEU	N-CA-C	-5.20	99.79	108.32
1	A	148	ARG	N-CA-C	5.18	117.83	111.82
1	A	105	LEU	N-CA-CB	-5.18	104.21	110.53
1	A	276	PRO	CA-C-O	-5.18	113.05	120.56
1	A	165	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	240	LYS	CG-CD-CE	5.17	123.18	111.30
1	A	186	VAL	CA-CB-CG1	5.15	119.16	110.40
1	A	94	PRO	N-CA-C	5.13	119.25	111.19
1	A	214	LEU	CB-CA-C	-5.12	102.29	110.79
1	A	270	VAL	O-C-N	-5.11	116.18	122.57
1	A	136	LYS	N-CA-C	5.11	119.38	113.20
1	A	2	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	31	TRP	CB-CG-CD2	-5.10	119.66	126.80
1	A	246	GLN	CA-CB-CG	5.10	124.30	114.10
1	A	123	TYR	CA-CB-CG	-5.09	104.73	113.90
1	A	179	ASP	CA-C-N	5.09	125.38	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASP	C-N-CA	5.09	125.38	119.47
1	A	177	LEU	CB-CA-C	-5.09	102.02	110.37
1	A	194	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	67	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	141	LYS	CG-CD-CE	5.08	123.00	111.30
1	A	195	ALA	CA-C-O	5.08	127.88	121.58
1	A	174	TRP	CD2-CE2-CZ2	-5.07	117.33	122.40
1	A	321	LEU	CA-C-O	-5.07	113.26	120.51
1	A	316	THR	O-C-N	-5.07	117.01	122.79
1	A	41	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	A	55	ARG	CA-CB-CG	5.01	124.12	114.10
1	A	179	ASP	O-C-N	-5.01	115.56	121.32
1	A	38	LEU	CD1-CG-CD2	-5.01	99.78	110.80
1	A	58	GLY	O-C-N	5.00	129.20	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	182	TYR	Sidechain
1	A	278	TYR	Sidechain
1	A	298	TYR	Sidechain
1	A	52	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	101	0
2	B	39	0	34	2	0
3	A	14	0	13	2	0
4	A	5	0	0	4	0
All	All	2852	0	2783	104	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 18.

All (104) 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:266:MET:SD	1:A:271:TYR:HD2	1.95	0.89
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.44	0.81
1:A:338:THR:HA	1:A:341:MET:SD	2.19	0.81
1:A:258:ASP:HB2	1:A:276:PRO:HG2	1.68	0.76
1:A:211:LEU:HD23	1:A:275:LEU:HD23	1.71	0.71
1:A:54:ARG:HH22	1:A:63:ASN:HB3	1.57	0.69
1:A:126:PHE:CE2	1:A:230:VAL:HG21	2.28	0.69
1:A:135:LEU:HD22	1:A:219:LYS:HD3	1.75	0.69
1:A:266:MET:SD	1:A:271:TYR:CD2	2.84	0.67
1:A:312:LEU:HD12	1:A:313:PRO:HD2	1.76	0.67
1:A:327:LEU:O	1:A:330:PRO:HD2	1.95	0.66
4:A:343:VO4:O2	4:A:343:VO4:V	1.53	0.66
1:A:181:LEU:HB3	1:A:200:MET:HE1	1.78	0.65
1:A:72:ILE:HG12	1:A:88:LEU:HD11	1.78	0.65
1:A:180:PRO:O	1:A:184:GLU:HG2	1.97	0.64
1:A:66:LYS:CE	3:A:347:NAG:H81	2.29	0.62
1:A:66:LYS:HE2	3:A:347:NAG:H81	1.80	0.62
1:A:239:MET:SD	1:A:286:LEU:HD13	2.40	0.62
1:A:322:GLU:O	1:A:326:GLU:HB2	2.01	0.61
1:A:203:LEU:HA	1:A:206:LEU:HD12	1.82	0.61
1:A:144:GLU:O	1:A:148:ARG:HB2	2.02	0.59
1:A:270:VAL:HG11	1:A:310:LEU:HB3	1.85	0.59
1:A:169:ASP:O	1:A:173:ILE:HG12	2.04	0.58
1:A:191:LEU:HB2	1:A:192:PRO:HD2	1.86	0.58
1:A:79:ARG:NH1	4:A:343:VO4:O2	2.36	0.57
1:A:334:GLN:HA	1:A:334:GLN:OE1	2.04	0.56
1:A:55:ARG:HG2	1:A:55:ARG:NH1	2.17	0.56
1:A:186:VAL:HG12	1:A:187:HIS:ND1	2.20	0.56
1:A:159:LEU:HA	1:A:162:LEU:HD12	1.87	0.56
1:A:218:HIS:NE2	1:A:219:LYS:HD2	2.22	0.55
1:A:126:PHE:HE2	1:A:230:VAL:HG21	1.72	0.54
1:A:214:LEU:O	1:A:223:LYS:HE2	2.07	0.54
1:A:144:GLU:HB3	1:A:148:ARG:HH21	1.72	0.54
1:A:243:THR:HG22	1:A:293:HIS:CD2	2.43	0.53
1:A:258:ASP:CB	1:A:276:PRO:HG2	2.36	0.53
1:A:17:PRO:HD2	1:A:35:PHE:CD1	2.44	0.53
1:A:244:GLN:HB2	1:A:245:PRO:HD2	1.90	0.53
1:A:215:TYR:HB2	1:A:266:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:HE2	1:A:239:MET:HG2	1.75	0.52
1:A:78:ASP:HB3	1:A:82:MET:HE2	1.91	0.52
1:A:335:ASP:O	1:A:339:GLU:HB2	2.09	0.52
1:A:319:CYS:SG	1:A:320:PRO:HD2	2.50	0.51
1:A:261:VAL:O	1:A:265:GLN:HG3	2.11	0.51
1:A:297:MET:HE2	1:A:324:PHE:CE2	2.45	0.51
1:A:133:GLN:HA	1:A:136:LYS:HG3	1.92	0.50
1:A:47:TYR:CE1	1:A:90:ALA:HB2	2.47	0.50
1:A:288:GLN:OE1	1:A:293:HIS:NE2	2.44	0.50
1:A:218:HIS:O	1:A:219:LYS:HB2	2.11	0.50
1:A:12:HIS:HE1	1:A:15:ARG:HE	1.60	0.50
1:A:191:LEU:H	1:A:191:LEU:HD23	1.77	0.50
1:A:14:ASP:H	1:A:42:GLY:HA2	1.76	0.50
1:A:225:ARG:NH2	1:A:334:GLN:H	2.10	0.50
2:B:2:NAG:O6	2:B:2:NAG:H2	2.12	0.50
1:A:170:LEU:HB3	1:A:210:SER:HB3	1.93	0.49
1:A:177:LEU:HD22	1:A:181:LEU:HD11	1.94	0.49
1:A:12:HIS:NE2	4:A:343:VO4:O2	2.46	0.48
1:A:297:MET:O	1:A:317:HIS:HE1	1.97	0.48
1:A:114:VAL:HG12	1:A:115:SER:N	2.29	0.48
1:A:54:ARG:HG3	1:A:54:ARG:NH1	2.27	0.48
1:A:14:ASP:HA	1:A:278:TYR:CD2	2.49	0.47
1:A:52:TYR:OH	1:A:307:PRO:HG3	2.14	0.47
1:A:251:LEU:CD2	1:A:253:MET:HB2	2.44	0.47
1:A:162:LEU:HD13	1:A:194:TRP:CE3	2.50	0.46
1:A:17:PRO:HD2	1:A:35:PHE:HD1	1.81	0.46
1:A:159:LEU:HD23	1:A:162:LEU:HD12	1.97	0.46
1:A:162:LEU:HD22	1:A:194:TRP:CG	2.51	0.46
1:A:126:PHE:HD2	1:A:336:TRP:CZ2	2.33	0.46
1:A:301:ASN:OD1	1:A:302:GLU:N	2.49	0.46
1:A:138:GLU:O	1:A:142:SER:HB3	2.17	0.45
1:A:146:LEU:O	1:A:150:GLN:NE2	2.50	0.45
1:A:312:LEU:HD21	1:A:327:LEU:HD12	1.97	0.45
1:A:66:LYS:O	1:A:68:ASP:N	2.48	0.45
1:A:299:TYR:N	1:A:308:TYR:O	2.50	0.45
1:A:137:SER:O	1:A:141:LYS:HE2	2.17	0.45
1:A:182:TYR:CD1	1:A:182:TYR:C	2.94	0.45
1:A:77:VAL:HG23	1:A:80:THR:OG1	2.17	0.44
1:A:156:ILE:O	1:A:160:PRO:HD3	2.17	0.44
4:A:343:VO4:O2	4:A:343:VO4:O3	2.36	0.44
1:A:181:LEU:CB	1:A:200:MET:HE1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:O	1:A:188:ASN:HB3	2.17	0.44
1:A:75:THR:HG21	1:A:123:TYR:HD1	1.83	0.44
1:A:65:TYR:O	1:A:65:TYR:CG	2.71	0.43
1:A:47:TYR:CZ	1:A:90:ALA:HB2	2.53	0.43
1:A:3:LEU:HA	1:A:287:TYR:HA	2.00	0.43
1:A:201:THR:O	1:A:205:GLU:HG3	2.18	0.42
1:A:56:ARG:HD3	1:A:57:TYR:CZ	2.54	0.42
1:A:277:PRO:HD2	1:A:280:SER:HB3	2.00	0.42
1:A:302:GLU:HG3	2:B:1:NAG:H82	2.02	0.42
1:A:186:VAL:HG12	1:A:187:HIS:CE1	2.54	0.42
1:A:227:GLN:O	1:A:230:VAL:HG23	2.20	0.42
1:A:11:ARG:NH1	1:A:278:TYR:HD1	2.18	0.41
1:A:143:GLU:OE1	1:A:144:GLU:HG2	2.20	0.41
1:A:162:LEU:HD22	1:A:194:TRP:CD1	2.55	0.41
1:A:177:LEU:HD22	1:A:181:LEU:CD1	2.51	0.41
1:A:232:VAL:HG22	1:A:268:LEU:HD13	2.01	0.41
1:A:246:GLN:NE2	1:A:247:LYS:H	2.19	0.41
1:A:9:VAL:O	1:A:9:VAL:HG22	2.20	0.41
1:A:14:ASP:HA	1:A:278:TYR:CE2	2.56	0.41
1:A:138:GLU:HB2	1:A:218:HIS:NE2	2.36	0.41
1:A:199:ALA:O	1:A:203:LEU:N	2.54	0.41
1:A:211:LEU:HD23	1:A:275:LEU:CD2	2.45	0.41
1:A:177:LEU:HD21	1:A:194:TRP:HH2	1.86	0.41
1:A:268:LEU:HG	1:A:297:MET:HE1	2.03	0.41
1:A:59:ARG:O	1:A:60:PHE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	283 (83%)	44 (13%)	13 (4%)	2 15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	127	ARG
1	A	337	ALA
1	A	62	ASN
1	A	143	GLU
1	A	217	ILE
1	A	220	GLN
1	A	272	ASN
1	A	153	LYS
1	A	96	GLY
1	A	221	LYS
1	A	336	TRP
1	A	273	GLY

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%)	246 (79%)	65 (21%)	1 7

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	VAL
1	A	11	ARG
1	A	18	ILE
1	A	22	PRO
1	A	26	ILE
1	A	38	LEU
1	A	39	THR
1	A	40	LYS
1	A	49	LEU
1	A	54	ARG
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	56	ARG
1	A	59	ARG
1	A	63	ASN
1	A	64	SER
1	A	72	ILE
1	A	75	THR
1	A	77	VAL
1	A	81	LEU
1	A	91	LEU
1	A	98	SER
1	A	105	LEU
1	A	115	SER
1	A	117	SER
1	A	118	GLU
1	A	120	ARG
1	A	133	GLN
1	A	136	LYS
1	A	140	LEU
1	A	141	LYS
1	A	143	GLU
1	A	146	LEU
1	A	150	GLN
1	A	153	LYS
1	A	158	THR
1	A	169	ASP
1	A	175	SER
1	A	176	ARG
1	A	177	LEU
1	A	186	VAL
1	A	200	MET
1	A	211	LEU
1	A	222	GLU
1	A	231	LEU
1	A	234	GLU
1	A	241	LEU
1	A	244	GLN
1	A	246	GLN
1	A	249	ARG
1	A	250	LYS
1	A	260	THR
1	A	261	VAL
1	A	275	LEU

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Mol	Chain	Res	Type
1	A	286	LEU
1	A	303	THR
1	A	305	ASN
1	A	312	LEU
1	A	316	THR
1	A	326	GLU
1	A	327	LEU
1	A	328	LEU
1	A	334	GLN
1	A	335	ASP
1	A	339	GLU

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	33	GLN
1	A	87	ASN
1	A	107	GLN
1	A	238	ASN
1	A	265	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	2,1	14,14,15	1.54	2 (14%)	17,19,21	1.12	2 (11%)
2	NAG	B	2	2	14,14,15	1.19	1 (7%)	17,19,21	2.49	4 (23%)
2	BMA	B	3	2	11,11,12	1.94	2 (18%)	15,15,17	2.77	8 (53%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C4-C5	4.79	1.63	1.53
2	B	1	NAG	C4-C5	-4.03	1.44	1.53
2	B	3	BMA	C2-C3	-3.18	1.47	1.52
2	B	2	NAG	O5-C1	2.78	1.48	1.43
2	B	1	NAG	O3-C3	-2.24	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-C2-C3	-6.88	99.63	109.64
2	B	2	NAG	C2-N2-C7	-6.26	114.51	122.90
2	B	2	NAG	C1-O5-C5	4.80	118.62	112.19
2	B	2	NAG	C3-C4-C5	3.99	117.47	110.23
2	B	3	BMA	C2-C3-C4	-3.60	104.53	110.86
2	B	3	BMA	O5-C5-C6	-3.29	101.26	107.66
2	B	3	BMA	O2-C2-C1	3.00	116.10	109.22
2	B	3	BMA	C3-C4-C5	2.74	115.20	110.23
2	B	2	NAG	C1-C2-N2	-2.74	106.12	110.43
2	B	3	BMA	O2-C2-C3	2.51	115.36	110.15
2	B	3	BMA	O5-C5-C4	2.33	116.49	110.83
2	B	1	NAG	O5-C5-C4	-2.29	105.25	110.83
2	B	1	NAG	C1-O5-C5	2.26	115.22	112.19
2	B	3	BMA	O4-C4-C3	-2.17	105.25	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

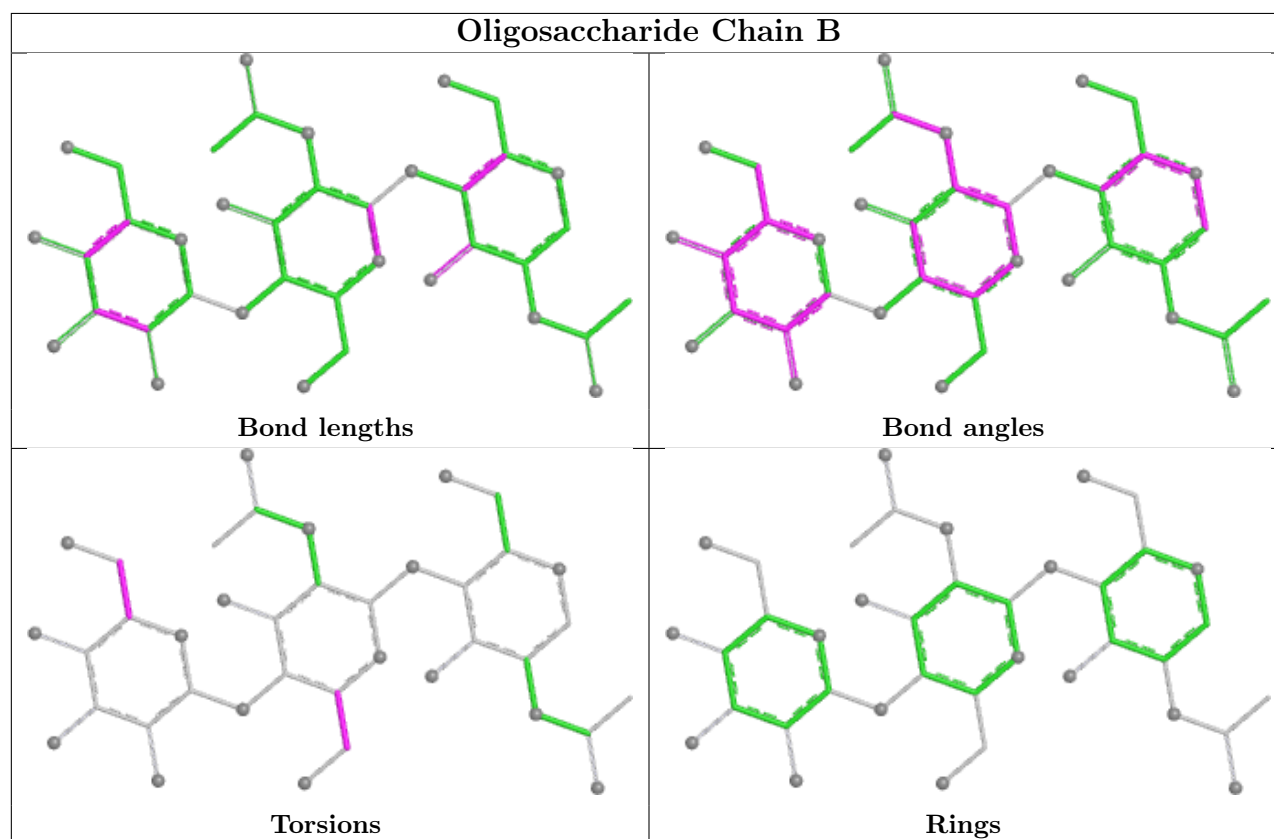
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	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 ⓘ

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	1.99	5 (35%)	17,19,21	1.86	3 (17%)
4	VO4	A	343	1	0,4,4	-	-	-		

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	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	347	NAG	C4-C3	4.18	1.63	1.52
3	A	347	NAG	C4-C5	3.57	1.60	1.53
3	A	347	NAG	O5-C5	2.47	1.48	1.43
3	A	347	NAG	C6-C5	2.38	1.59	1.51
3	A	347	NAG	C3-C2	2.09	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	347	NAG	C6-C5-C4	4.76	124.71	113.02
3	A	347	NAG	C1-O5-C5	-4.15	106.63	112.19
3	A	347	NAG	C8-C7-N2	-2.56	111.87	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	347	NAG	2	0
4	A	343	VO4	4	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.