



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 1ABE / pdb_00001abe
Title : NOVEL STEREOSPECIFICITY OF THE L-ARABINOSE-BINDING PROTEIN
Authors : Vyas, N.K.; Quijcho, F.A.
Deposited on : 1992-04-23
Resolution : 1.70 Å(reported)

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

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

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

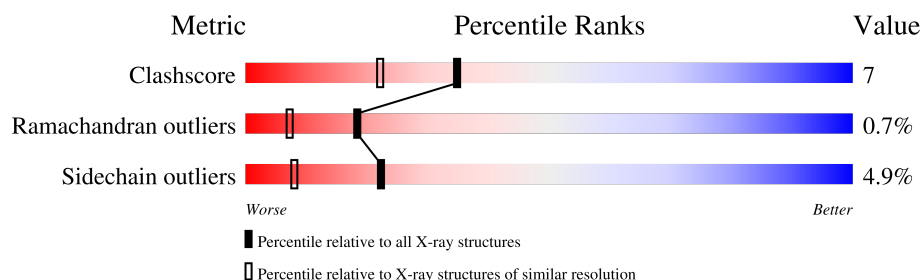
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	306	

2 Entry composition [i](#)

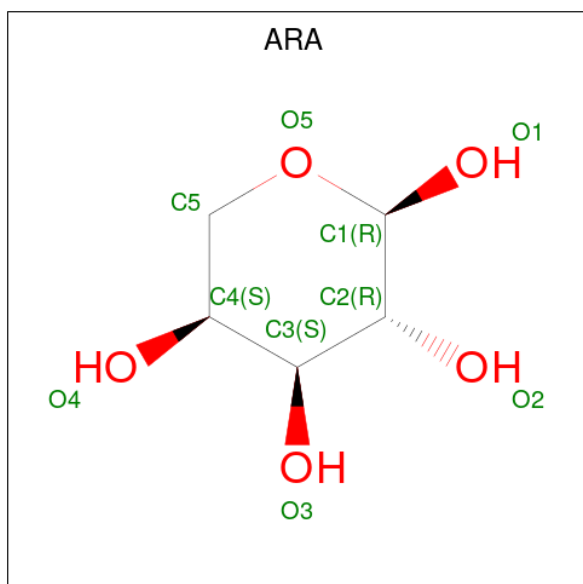
There are 4 unique types of molecules in this entry. The entry contains 2563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ARABINOSE-BINDING PROTEIN.

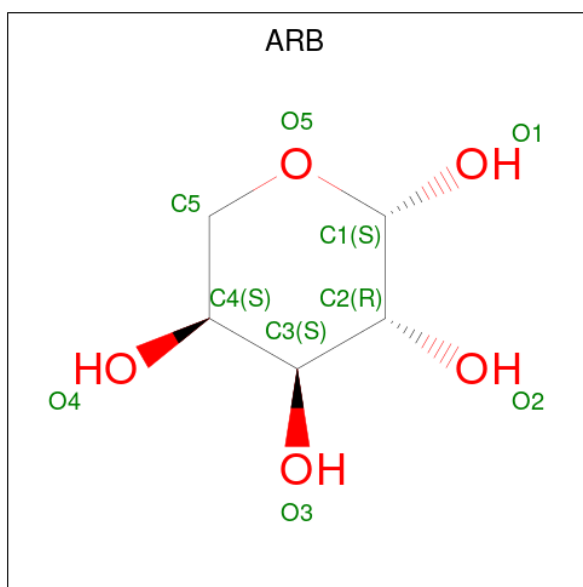
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2316	1473	389	443	11	0	0	0

- Molecule 2 is alpha-L-arabinopyranose (CCD ID: ARA) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	5	5	0	1

- Molecule 3 is beta-L-arabinopyranose (CCD ID: ARB) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		

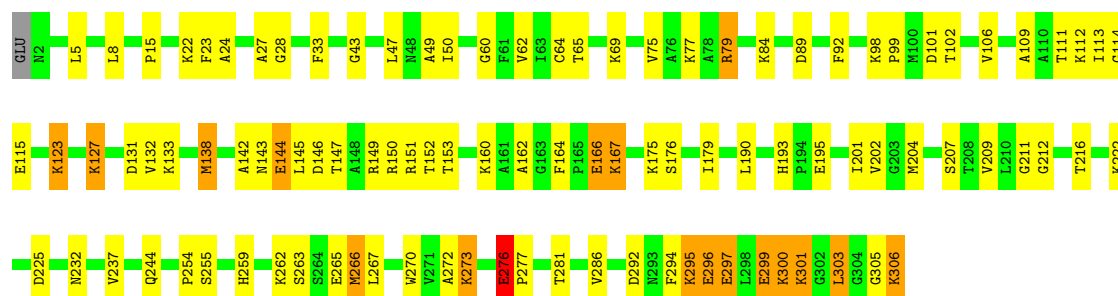
3 Residue-property plots

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: L-ARABINOSE-BINDING PROTEIN

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.46Å 71.82Å 77.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.137 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2563	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: ARB, ARA

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	5/2361 (0.2%)	2.22	97/3189 (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	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	LYS	CA-C	9.68	1.73	1.52
1	A	306	LYS	C-O	9.27	1.42	1.23
1	A	179	ILE	CA-CB	5.58	1.57	1.54
1	A	109	ALA	C-O	5.36	1.29	1.23
1	A	152	THR	N-CA	5.03	1.52	1.46

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	CD-NE-CZ	14.16	144.23	124.40
1	A	306	LYS	CA-C-O	-12.44	99.66	120.80
1	A	299	GLU	CB-CG-CD	9.93	129.48	112.60
1	A	79	ARG	CA-CB-CG	9.38	132.86	114.10
1	A	244	GLN	OE1-CD-NE2	9.03	131.63	122.60
1	A	143	ASN	OD1-CG-ND2	-8.56	114.04	122.60
1	A	144	GLU	CB-CG-CD	8.36	126.81	112.60
1	A	77	LYS	CA-CB-CG	7.80	129.71	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	VAL	CA-C-O	-7.61	112.79	120.85
1	A	131	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	263	SER	CA-C-O	-7.23	112.75	120.42
1	A	147	THR	CA-CB-OG1	-7.17	98.85	109.60
1	A	202	VAL	CA-C-O	-7.03	113.05	120.57
1	A	24	ALA	N-CA-C	-7.02	103.71	111.36
1	A	99	PRO	CA-C-O	-6.92	113.45	121.34
1	A	265	GLU	CA-C-O	6.73	127.89	120.82
1	A	259	HIS	CA-C-O	-6.65	113.84	120.82
1	A	299	GLU	CA-C-N	6.63	129.83	120.28
1	A	299	GLU	C-N-CA	6.63	129.83	120.28
1	A	15	PRO	CA-C-N	6.62	130.00	120.79
1	A	15	PRO	C-N-CA	6.62	130.00	120.79
1	A	5	LEU	CA-C-O	-6.54	113.46	121.11
1	A	98	LYS	N-CA-CB	6.50	119.06	110.29
1	A	64	CYS	N-CA-CB	6.49	121.42	110.46
1	A	27	ALA	CA-C-O	-6.46	113.70	120.55
1	A	23	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	276	GLU	CA-CB-CG	6.37	126.85	114.10
1	A	101	ASP	CA-CB-CG	-6.29	106.31	112.60
1	A	263	SER	CA-C-N	6.29	128.62	120.44
1	A	263	SER	C-N-CA	6.29	128.62	120.44
1	A	262	LYS	CA-C-O	-6.26	113.92	120.55
1	A	237	VAL	CA-C-O	-6.24	114.46	120.95
1	A	294	PHE	CA-C-O	-6.21	113.97	120.55
1	A	286	VAL	O-C-N	6.19	130.31	122.57
1	A	142	ALA	N-CA-C	-6.17	101.08	109.54
1	A	15	PRO	O-C-N	-6.11	115.22	122.24
1	A	8	LEU	CA-C-O	-6.10	113.78	120.43
1	A	106	VAL	CA-C-O	-6.07	114.08	120.39
1	A	33	PHE	CA-C-O	6.04	127.86	121.33
1	A	222	LYS	O-C-N	-5.97	116.04	122.85
1	A	75	VAL	O-C-N	5.96	127.65	121.87
1	A	297	GLU	CA-C-O	-5.93	114.26	120.55
1	A	150	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	A	149	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	89	ASP	CA-C-O	-5.87	112.12	120.51
1	A	102	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	162	ALA	CA-C-N	-5.86	112.90	122.40
1	A	162	ALA	C-N-CA	-5.86	112.90	122.40
1	A	281	THR	CA-C-N	-5.83	114.95	123.00
1	A	281	THR	C-N-CA	-5.83	114.95	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ALA	CA-C-O	-5.83	115.36	122.41
1	A	195	GLU	CA-C-N	-5.80	114.88	122.37
1	A	195	GLU	C-N-CA	-5.80	114.88	122.37
1	A	164	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	267	LEU	CA-C-O	5.71	126.82	120.82
1	A	62	VAL	CA-C-N	-5.71	114.49	122.71
1	A	62	VAL	C-N-CA	-5.71	114.49	122.71
1	A	49	ALA	CA-C-O	-5.69	113.42	119.97
1	A	211	GLY	CA-C-N	5.69	126.25	119.94
1	A	211	GLY	C-N-CA	5.69	126.25	119.94
1	A	255	SER	N-CA-C	5.63	118.84	108.94
1	A	114	GLY	N-CA-C	-5.59	105.62	112.77
1	A	109	ALA	CA-C-N	5.58	128.07	120.54
1	A	109	ALA	C-N-CA	5.58	128.07	120.54
1	A	144	GLU	CG-CD-OE1	5.50	131.06	118.40
1	A	131	ASP	CA-C-O	-5.49	114.12	120.49
1	A	295	LYS	O-C-N	5.49	127.72	122.07
1	A	299	GLU	CG-CD-OE1	5.47	130.99	118.40
1	A	294	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	296	GLU	CB-CA-C	-5.45	102.33	110.88
1	A	123	LYS	CB-CA-C	-5.44	102.34	110.88
1	A	244	GLN	N-CA-C	5.40	118.90	110.32
1	A	43	GLY	CA-C-O	5.39	126.30	120.75
1	A	150	ARG	CA-CB-CG	-5.36	103.37	114.10
1	A	299	GLU	N-CA-C	-5.36	105.44	111.28
1	A	176	SER	CA-C-O	-5.35	114.85	121.06
1	A	50	ILE	O-C-N	5.35	127.34	121.83
1	A	193	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	166	GLU	CG-CD-OE1	-5.22	106.39	118.40
1	A	149	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	292	ASP	N-CA-C	5.20	117.03	111.36
1	A	153	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	138	MET	CA-C-O	-5.19	114.91	120.46
1	A	113	ILE	CA-CB-CG1	-5.18	101.59	110.40
1	A	60	GLY	N-CA-C	-5.15	103.23	110.75
1	A	92	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	47	LEU	CA-C-O	-5.07	115.04	120.42
1	A	64	CYS	N-CA-C	-5.05	97.66	107.62
1	A	222	LYS	CA-C-N	5.05	127.30	120.38
1	A	222	LYS	C-N-CA	5.05	127.30	120.38
1	A	65	THR	N-CA-C	5.05	117.05	110.08
1	A	225	ASP	CA-CB-CG	-5.03	107.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLY	N-CA-C	-5.02	106.70	112.73
1	A	207	SER	O-C-N	5.02	127.44	122.12
1	A	266	MET	CA-C-N	5.02	126.97	120.44
1	A	266	MET	C-N-CA	5.02	126.97	120.44
1	A	145	LEU	CB-CA-C	5.00	118.78	110.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	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	2316	0	2326	35	0
2	A	10	0	10	0	0
3	A	10	0	10	0	0
4	A	227	0	0	11	0
All	All	2563	0	2346	35	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 7.

All (35) 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:146:ASP:HB2	4:A:497:HOH:O	1.54	1.07
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.56	0.86
1:A:115:GLU:OE1	4:A:487:HOH:O	1.99	0.81
1:A:22:LYS:HE3	4:A:479:HOH:O	1.80	0.80
1:A:167:LYS:HG3	4:A:506:HOH:O	1.86	0.74
1:A:305:GLY:O	1:A:306:LYS:C	2.31	0.73
1:A:295:LYS:HE3	1:A:306:LYS:CA	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:NZ	4:A:484:HOH:O	2.24	0.68
1:A:22:LYS:HZ3	1:A:22:LYS:HB2	1.59	0.68
1:A:22:LYS:HB2	1:A:22:LYS:NZ	1.94	0.68
1:A:296:GLU:CD	4:A:417:HOH:O	2.37	0.67
1:A:297:GLU:OE1	4:A:420:HOH:O	2.11	0.67
1:A:22:LYS:NZ	1:A:22:LYS:CB	2.55	0.65
1:A:295:LYS:CE	1:A:306:LYS:CA	2.76	0.64
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.37	0.59
1:A:123:LYS:NZ	4:A:486:HOH:O	2.36	0.58
1:A:266:MET:HE3	1:A:277:PRO:HB3	1.86	0.57
1:A:132:VAL:HG13	1:A:133:LYS:N	2.22	0.53
1:A:112:LYS:HE2	1:A:115:GLU:OE1	2.09	0.53
1:A:201:ILE:HD11	1:A:216:THR:HG21	1.90	0.52
1:A:272:ALA:C	1:A:273:LYS:HG3	2.31	0.51
1:A:22:LYS:CE	4:A:479:HOH:O	2.50	0.50
1:A:160:LYS:CD	1:A:166:GLU:HG2	2.36	0.50
1:A:132:VAL:CG1	1:A:133:LYS:N	2.76	0.48
1:A:22:LYS:HZ3	1:A:22:LYS:CB	2.21	0.47
1:A:301:LYS:HD3	1:A:303:LEU:HD11	1.97	0.46
1:A:127:LYS:NZ	1:A:127:LYS:HB2	2.19	0.45
1:A:212:GLY:O	1:A:216:THR:HG23	2.17	0.44
1:A:296:GLU:HG3	4:A:342:HOH:O	2.17	0.44
1:A:167:LYS:HD2	4:A:506:HOH:O	2.17	0.43
1:A:138:MET:HE1	1:A:190:LEU:HG	2.00	0.43
1:A:296:GLU:O	1:A:300:LYS:HB2	2.19	0.43
1:A:276:GLU:HA	1:A:276:GLU:OE1	2.19	0.41
1:A:111:THR:O	1:A:115:GLU:HG3	2.21	0.41
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.35	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	303/306 (99%)	295 (97%)	6 (2%)	2 (1%)	18 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	254	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	243/246 (99%)	231 (95%)	12 (5%)	22 8

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	127	LYS
1	A	144	GLU
1	A	167	LYS
1	A	175	LYS
1	A	204	MET
1	A	273	LYS
1	A	276	GLU
1	A	299	GLU
1	A	300	LYS
1	A	301	LYS
1	A	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	244	GLN

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 ⓘ

There are no oligosaccharides in this entry.

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	ARB	A	308[B]	-	10,10,10	1.06	2 (20%)	14,14,14	0.82	0
2	ARA	A	307[A]	-	10,10,10	0.90	1 (10%)	14,14,14	0.82	0

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	ARB	A	308[B]	-	-	-	0/1/1/1
2	ARA	A	307[A]	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	307[A]	ARA	O5-C5	2.47	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	ARB	O5-C1	2.26	1.46	1.43
3	A	308[B]	ARB	O5-C5	2.08	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.