



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:51 PM UTC

PDB ID : 3LIG / pdb_00003lig
Title : Crystal structure of fructosyltransferase (D191A) from *A. japonicus*
Authors : Chuankhayan, P.; Chen, C.J.; Chiang, C.M.
Deposited on : 2010-01-24
Resolution : 1.80 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

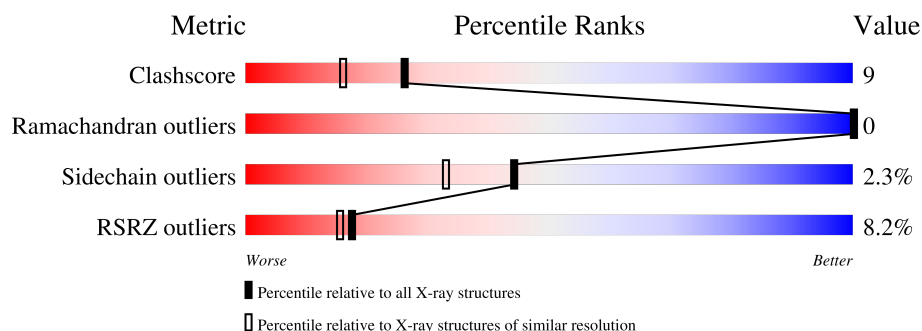
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	634	8% 79% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5207 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 Fructosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4883	3091	824	965	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	324	Total	O	0	0
			324	324		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Fructosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.41Å 110.78Å 66.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (20.00-1.80) 96.4 (20.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.244 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.48	7/5014 (0.1%)	1.02	36/6858 (0.5%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	THR	C-N	-9.44	1.23	1.33
1	A	476	LEU	C-N	7.88	1.44	1.33
1	A	284	ALA	C-N	7.34	1.44	1.33
1	A	344	GLY	C-N	6.95	1.43	1.33
1	A	283	TRP	C-N	-5.37	1.26	1.33
1	A	455	ASN	C-N	5.04	1.40	1.33
1	A	242	VAL	C-N	-5.01	1.26	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	THR	N-CA-C	-8.53	102.64	113.72
1	A	123	ILE	N-CA-C	-7.41	99.47	107.77
1	A	344	GLY	O-C-N	-7.17	113.38	122.70
1	A	495	VAL	N-CA-C	6.98	115.69	107.73
1	A	93	ALA	O-C-N	-6.80	114.22	122.25
1	A	583	GLY	N-CA-C	-6.61	106.61	115.21
1	A	650	TRP	CA-C-N	6.56	127.08	119.47
1	A	650	TRP	C-N-CA	6.56	127.08	119.47
1	A	376	LEU	CA-C-N	6.55	126.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	LEU	C-N-CA	6.55	126.59	119.90
1	A	61	PRO	N-CA-C	-6.46	101.75	111.57
1	A	226	GLU	N-CA-C	6.45	117.97	111.07
1	A	122	VAL	N-CA-C	6.31	117.57	108.48
1	A	528	GLU	N-CA-C	-6.18	99.64	109.59
1	A	548	LEU	N-CA-C	-6.11	99.28	109.24
1	A	619	TYR	N-CA-C	6.02	118.97	110.23
1	A	345	SER	CB-CA-C	-5.92	109.74	116.54
1	A	454	ASP	N-CA-C	-5.82	104.58	112.26
1	A	531	ALA	N-CA-C	5.79	118.98	109.72
1	A	115	VAL	N-CA-C	5.75	116.75	111.81
1	A	177	ILE	N-CA-C	-5.71	97.79	106.42
1	A	362	LEU	N-CA-C	-5.65	105.11	112.23
1	A	627	PHE	N-CA-C	-5.58	102.22	110.48
1	A	556	SER	N-CA-C	5.35	117.13	108.41
1	A	357	SER	N-CA-C	-5.33	107.44	114.31
1	A	210	VAL	N-CA-C	-5.31	105.95	111.58
1	A	421	LEU	N-CA-C	-5.28	102.24	110.42
1	A	236	SER	N-CA-C	5.24	118.61	110.17
1	A	335	LEU	N-CA-C	5.17	117.98	110.17
1	A	182	PHE	N-CA-C	5.16	118.04	110.30
1	A	279	ASP	N-CA-C	5.13	116.95	111.36
1	A	44	LEU	N-CA-C	5.10	117.23	111.11
1	A	190	ARG	N-CA-C	5.07	116.02	108.86
1	A	587	VAL	N-CA-C	-5.02	102.27	108.89
1	A	69	SER	N-CA-C	5.00	116.42	111.07
1	A	93	ALA	N-CA-C	-5.00	106.53	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	GLY	Mainchain

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	4883	0	4610	89	0
2	A	324	0	0	0	0
All	All	5207	0	4610	89	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 9.

All (89) 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:454:ASP:HB2	1:A:456:GLN:NE2	1.78	0.96
1:A:454:ASP:HB2	1:A:456:GLN:HE21	1.28	0.95
1:A:33:LEU:H	1:A:562:ASN:HD21	1.23	0.86
1:A:591:ASP:H	1:A:606:ASN:HD21	1.26	0.80
1:A:162:ARG:HG3	1:A:169:ASP:OD2	1.82	0.79
1:A:216:ALA:HA	1:A:219:GLN:OE1	1.85	0.77
1:A:454:ASP:CB	1:A:456:GLN:HE21	1.98	0.75
1:A:591:ASP:H	1:A:606:ASN:ND2	1.87	0.72
1:A:295:ASN:HD21	1:A:373:GLY:H	1.38	0.70
1:A:606:ASN:HD22	1:A:606:ASN:N	1.89	0.69
1:A:439:GLU:H	1:A:439:GLU:CD	2.01	0.69
1:A:295:ASN:ND2	1:A:373:GLY:H	1.93	0.67
1:A:200:LEU:HD21	1:A:341:VAL:HG11	1.78	0.65
1:A:523:LEU:C	1:A:523:LEU:HD23	2.22	0.64
1:A:523:LEU:HD23	1:A:524:GLN:N	2.13	0.64
1:A:456:GLN:CD	1:A:457:THR:H	2.05	0.63
1:A:57:GLN:HB2	1:A:418:THR:HB	1.80	0.63
1:A:606:ASN:HD22	1:A:606:ASN:H	1.48	0.61
1:A:454:ASP:CB	1:A:456:GLN:NE2	2.57	0.60
1:A:213:ASN:ND2	1:A:216:ALA:H	2.00	0.59
1:A:343:VAL:C	1:A:345:SER:H	2.12	0.57
1:A:299:LEU:N	1:A:299:LEU:HD12	2.19	0.57
1:A:379:SER:O	1:A:384:LYS:HE2	2.04	0.56
1:A:456:GLN:NE2	1:A:457:THR:H	2.02	0.56
1:A:57:GLN:CB	1:A:418:THR:HB	2.36	0.56
1:A:208:GLU:HG3	1:A:209:GLU:OE1	2.06	0.56
1:A:299:LEU:HD23	1:A:428:LYS:CA	2.36	0.55
1:A:210:VAL:C	1:A:212:ARG:H	2.15	0.54
1:A:296:VAL:C	1:A:297:LEU:HD12	2.32	0.54
1:A:33:LEU:H	1:A:562:ASN:ND2	1.98	0.54
1:A:45:TRP:HB3	1:A:599:ALA:CB	2.38	0.53
1:A:198:ALA:O	1:A:202:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HG21	1:A:341:VAL:HG23	1.91	0.53
1:A:295:ASN:HD21	1:A:373:GLY:N	2.06	0.53
1:A:200:LEU:CD2	1:A:341:VAL:HG11	2.38	0.53
1:A:536:ARG:HH11	1:A:536:ARG:HG3	1.73	0.53
1:A:513:GLU:OE1	1:A:638:ARG:HD2	2.08	0.53
1:A:199:ARG:NH1	1:A:217:VAL:HG11	2.24	0.52
1:A:215:THR:O	1:A:219:GLN:HG3	2.08	0.52
1:A:453:SER:HB2	1:A:458:ALA:HB2	1.91	0.52
1:A:439:GLU:CD	1:A:439:GLU:N	2.67	0.52
1:A:449:VAL:CG2	1:A:461:ARG:HB2	2.40	0.52
1:A:45:TRP:CE2	1:A:616:ARG:HB3	2.46	0.51
1:A:531:ALA:O	1:A:624:GLN:HB2	2.11	0.51
1:A:45:TRP:HB3	1:A:599:ALA:HB2	1.93	0.51
1:A:199:ARG:HH12	1:A:217:VAL:HG11	1.76	0.49
1:A:207:ASP:OD2	1:A:210:VAL:HG21	2.13	0.49
1:A:209:GLU:HA	1:A:212:ARG:HG2	1.95	0.48
1:A:175:PRO:HG2	1:A:178:ALA:HB2	1.94	0.48
1:A:315:LEU:N	1:A:315:LEU:HD23	2.29	0.48
1:A:154:GLU:OE2	1:A:190:ARG:HD3	2.13	0.47
1:A:299:LEU:HD23	1:A:428:LYS:HA	1.96	0.47
1:A:344:GLY:HA3	1:A:350:ALA:O	2.14	0.47
1:A:213:ASN:HD21	1:A:216:ALA:H	1.62	0.47
1:A:118:PHE:HB2	1:A:136:THR:HB	1.97	0.46
1:A:449:VAL:HG22	1:A:461:ARG:HB2	1.98	0.46
1:A:320:SER:HA	1:A:330:SER:OG	2.17	0.45
1:A:130:THR:OG1	1:A:160:VAL:HG13	2.17	0.44
1:A:297:LEU:CB	1:A:299:LEU:HD11	2.48	0.44
1:A:202:VAL:HG21	1:A:221:VAL:HG22	1.99	0.43
1:A:250:ARG:O	1:A:251:GLN:C	2.61	0.43
1:A:410:PHE:CG	1:A:411:PRO:HD2	2.52	0.43
1:A:89:THR:HB	1:A:95:TYR:CD1	2.54	0.42
1:A:454:ASP:C	1:A:456:GLN:H	2.26	0.42
1:A:209:GLU:HA	1:A:212:ARG:CG	2.50	0.42
1:A:432:VAL:HB	1:A:460:LEU:HB2	2.01	0.42
1:A:244:PRO:HB2	1:A:291:PHE:CD1	2.54	0.42
1:A:538:ALA:HB3	1:A:551:ASP:HB3	2.01	0.42
1:A:210:VAL:C	1:A:212:ARG:N	2.75	0.42
1:A:297:LEU:HD12	1:A:297:LEU:N	2.35	0.42
1:A:456:GLN:OE1	1:A:457:THR:HG23	2.19	0.42
1:A:299:LEU:HD13	1:A:312:PHE:CD2	2.54	0.42
1:A:536:ARG:HG3	1:A:536:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG21	1:A:44:LEU:HD13	2.02	0.41
1:A:539:ILE:HA	1:A:549:VAL:O	2.20	0.41
1:A:545:ASN:O	1:A:546:GLU:C	2.63	0.41
1:A:32:ASN:CG	1:A:35:THR:HG23	2.45	0.41
1:A:396:PHE:CE1	1:A:424:PRO:HG3	2.55	0.41
1:A:511:GLN:HA	1:A:590:LEU:O	2.20	0.41
1:A:364:TRP:HB2	1:A:611:LEU:HD13	2.03	0.41
1:A:312:PHE:CE1	1:A:338:ALA:HB2	2.55	0.41
1:A:298:PHE:CE1	1:A:311:VAL:HG22	2.56	0.41
1:A:251:GLN:OE1	1:A:256:ALA:HA	2.21	0.40
1:A:454:ASP:HB2	1:A:456:GLN:CD	2.41	0.40
1:A:340:GLU:N	1:A:340:GLU:CD	2.79	0.40
1:A:212:ARG:NH1	1:A:212:ARG:HG3	2.37	0.40
1:A:299:LEU:HD13	1:A:312:PHE:HB2	2.04	0.40
1:A:343:VAL:C	1:A:345:SER:N	2.79	0.40
1:A:521:SER:C	1:A:523:LEU:H	2.28	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	632/634 (100%)	591 (94%)	41 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	516/516 (100%)	504 (98%)	12 (2%)	44	33

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

Mol	Chain	Res	Type
1	A	52	LEU
1	A	57	GLN
1	A	119	ASP
1	A	208	GLU
1	A	297	LEU
1	A	326	PRO
1	A	347	GLN
1	A	427	LEU
1	A	456	GLN
1	A	460	LEU
1	A	606	ASN
1	A	652	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	57	GLN
1	A	156	GLN
1	A	213	ASN
1	A	295	ASN
1	A	434	ASN
1	A	456	GLN
1	A	511	GLN
1	A	524	GLN
1	A	554	GLN
1	A	562	ASN
1	A	606	ASN
1	A	621	ASN
1	A	639	ASN

5.3.3 RNA

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	634/634 (100%)	0.51	52 (8%)	17 15	8, 16, 39, 61	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	6.9
1	A	344	GLY	6.0
1	A	210	VAL	5.4
1	A	211	ALA	5.4
1	A	20	SER	5.2
1	A	346	GLU	5.1
1	A	206	LEU	4.8
1	A	347	GLN	4.8
1	A	207	ASP	4.7
1	A	21	TYR	4.0
1	A	213	ASN	4.0
1	A	456	GLN	3.8
1	A	343	VAL	3.7
1	A	228	ASN	3.7
1	A	212	ARG	3.6
1	A	452	GLU	3.5
1	A	220	ALA	3.5
1	A	217	VAL	3.4
1	A	279	ASP	3.4
1	A	208	GLU	3.2
1	A	216	ALA	3.2
1	A	348	GLU	3.2
1	A	349	GLY	3.1
1	A	214	GLU	3.0
1	A	219	GLN	2.9
1	A	215	THR	2.9
1	A	584	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	69	SER	2.7
1	A	225	THR	2.6
1	A	581	GLU	2.5
1	A	221	VAL	2.5
1	A	444	GLU	2.4
1	A	457	THR	2.4
1	A	480	SER	2.4
1	A	209	GLU	2.3
1	A	582	ASN	2.3
1	A	513	GLU	2.3
1	A	580	ILE	2.3
1	A	621	ASN	2.3
1	A	454	ASP	2.3
1	A	281	GLY	2.2
1	A	227	LYS	2.2
1	A	205	SER	2.2
1	A	518	ALA	2.2
1	A	453	SER	2.2
1	A	223	GLY	2.1
1	A	218	GLN	2.1
1	A	100	ASP	2.1
1	A	458	ALA	2.1
1	A	162	ARG	2.0
1	A	226	GLU	2.0
1	A	340	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.