



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 7K2P / pdb_00007k2p
Title : Kelch domain of human KEAP1 bound to Nrf2-based cyclic peptide, c[AVA-DPETGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.11 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) : 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

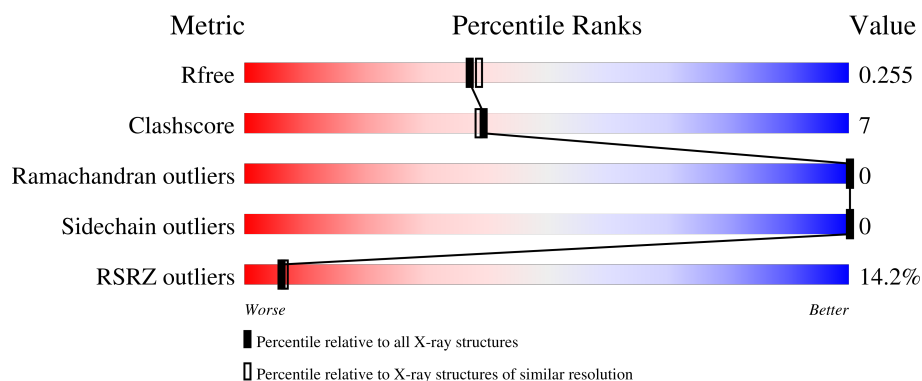
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	301	25% 77% 17% 6%
1	B	301	2% 87% 10% .
2	P	7	71% 29%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4514 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2152	1342	388	407	15			
1	B	290	Total	C	N	O	S	0	1	0
			2223	1382	403	422	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	SER	CYS	conflict	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145

- Molecule 2 is a protein called (DAV)DPETGE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			51	30	7	14			

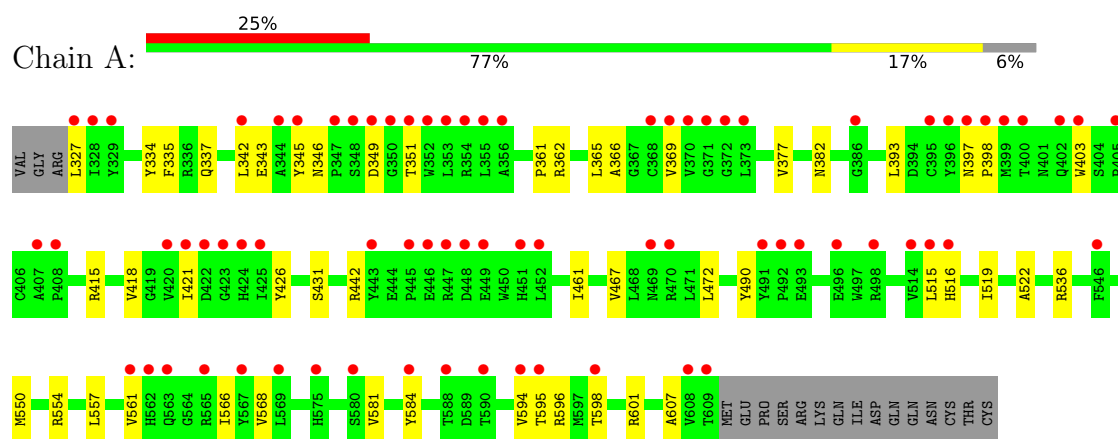
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	56	Total	O	0	0
			56	56		
3	P	3	Total	O	0	0
			3	3		

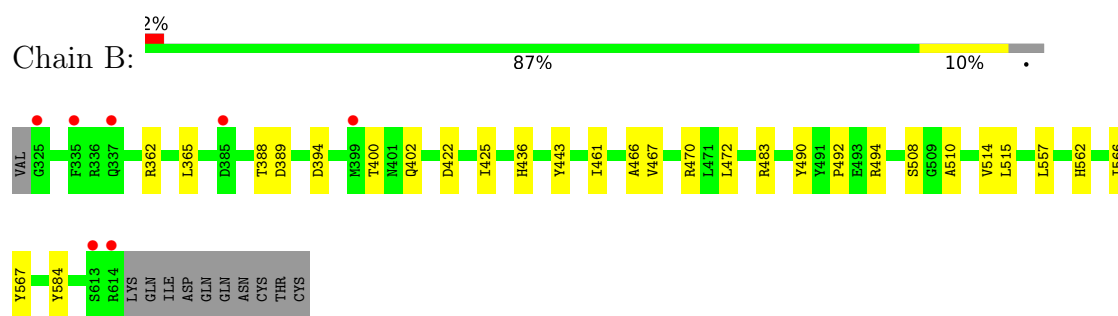
3 Residue-property plots

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.

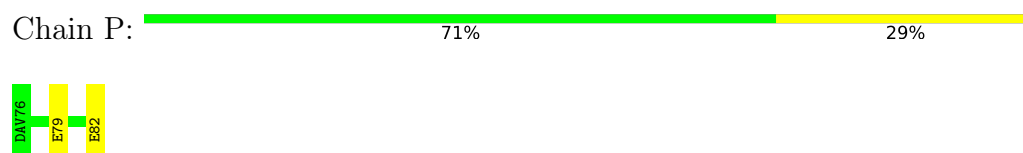
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 2: (DAV)DPETGE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.61Å 68.87Å 77.20Å 90.00° 117.79° 90.00°	Depositor
Resolution (Å)	29.38 – 2.11 29.38 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.38-2.11) 99.2 (29.38-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.243 0.224 , 0.255	Depositor DCC
R_{free} test set	1999 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4514	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAV

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	0.36	0/2204	0.61	0/3006
1	B	0.37	1/2279 (0.0%)	0.58	0/3104
2	P	0.36	0/44	0.43	0/59
All	All	0.37	1/4527 (0.0%)	0.60	0/6169

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	510	ALA	C-N	5.40	1.36	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2152	0	2032	41	0
1	B	2223	0	2107	19	0
2	P	51	0	35	3	0
3	A	29	0	0	2	0
3	B	56	0	0	0	0
3	P	3	0	0	0	0
All	All	4514	0	4174	58	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 (58) 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:415:ARG:NH2	2:P:79:GLU:OE2	1.98	0.97
1:A:536:ARG:HH12	1:B:494:ARG:HH21	1.17	0.90
1:A:467:VAL:O	3:A:701:HOH:O	1.94	0.86
1:A:515:LEU:HD13	1:A:561:VAL:HG11	1.62	0.81
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.72	0.72
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.73	0.70
1:A:550:MET:HE2	1:A:568:VAL:HG21	1.74	0.69
1:A:327:LEU:HD22	1:A:346:ASN:HA	1.76	0.68
1:A:536:ARG:HH12	1:B:494:ARG:NH2	1.94	0.61
1:A:598:THR:OG1	1:A:601:ARG:NH2	2.32	0.60
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.88	0.56
1:A:550:MET:CE	1:A:568:VAL:HG11	2.36	0.56
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.88	0.55
1:B:557:LEU:H	1:B:557:LEU:HD23	1.71	0.55
1:A:561:VAL:HG22	1:A:566:ILE:HG12	1.92	0.52
1:A:349:ASP:OD1	1:A:351:THR:N	2.37	0.52
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.93	0.50
1:A:581:VAL:HB	1:A:595:THR:HG23	1.94	0.49
1:A:415:ARG:HH22	2:P:79:GLU:CD	2.08	0.49
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.45	0.49
1:A:426:TYR:CZ	1:A:442:ARG:HD2	2.49	0.47
1:A:365:LEU:HD23	1:A:365:LEU:H	1.80	0.47
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.96	0.47
1:B:467:VAL:O	1:B:514:VAL:HG21	2.14	0.47
1:A:366:ALA:HB3	1:A:418:VAL:HG13	1.97	0.46
1:A:550:MET:HE2	1:A:568:VAL:HG11	1.97	0.46
1:A:557:LEU:HD23	1:A:557:LEU:H	1.80	0.46
1:B:483:ARG:HG2	1:B:508[B]:SER:HB2	1.98	0.45
1:A:342:LEU:HD22	1:A:403:TRP:CZ2	2.51	0.45
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.97	0.45
1:B:562:HIS:HB3	1:B:567:TYR:CE1	2.52	0.45
1:B:422:ASP:OD1	1:B:470:ARG:HD3	2.17	0.45
1:A:369:VAL:HG23	1:A:607:ALA:HB1	1.99	0.44
1:A:519:ILE:O	1:A:536:ARG:HA	2.17	0.44
1:A:345:TYR:OH	1:A:594:VAL:HG12	2.17	0.44
1:A:515:LEU:HD12	1:A:516:HIS:H	1.83	0.44
1:B:388:THR:HG22	1:B:389:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:THR:O	1:B:402:GLN:HG3	2.18	0.44
1:B:365:LEU:H	1:B:365:LEU:HD23	1.83	0.43
1:A:361:PRO:O	1:A:362:ARG:HG3	2.18	0.43
1:A:554:ARG:HG3	1:A:557:LEU:HD22	2.00	0.43
1:B:436:HIS:ND1	1:B:461:ILE:HD11	2.34	0.42
1:B:425:ILE:HB	1:B:443:TYR:HB3	2.02	0.42
1:A:335:PHE:C	1:A:337:GLN:H	2.27	0.42
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.02	0.42
1:A:334:TYR:CG	2:P:82:GLU:HG2	2.55	0.41
1:A:598:THR:HG1	1:A:601:ARG:HH22	1.65	0.41
1:B:490:TYR:CE2	1:B:492:PRO:HA	2.54	0.41
1:A:342:LEU:HD22	1:A:403:TRP:HZ2	1.85	0.41
1:B:436:HIS:HB3	1:B:461:ILE:HD11	2.02	0.41
1:B:472:LEU:HB3	1:B:490:TYR:HB3	2.01	0.41
1:A:343:GLU:OE1	1:A:598:THR:HG21	2.21	0.41
1:A:349:ASP:OD1	1:A:349:ASP:C	2.64	0.41
1:A:595:THR:OG1	1:A:596:ARG:N	2.53	0.41
1:A:327:LEU:HB3	1:A:345:TYR:O	2.21	0.41
1:A:382:ASN:ND2	3:A:704:HOH:O	2.54	0.41
1:A:397:ASN:HA	1:A:398:PRO:HD3	1.94	0.40
1:A:377:VAL:HG22	1:A:393:LEU:HD13	2.04	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	281/301 (93%)	270 (96%)	11 (4%)	0	100	100
1	B	289/301 (96%)	281 (97%)	8 (3%)	0	100	100
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	575/609 (94%)	556 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	223/247 (90%)	223 (100%)	0	100	100
1	B	233/247 (94%)	233 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	461/499 (92%)	461 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	402	GLN
1	A	414	ASN
1	A	469	ASN
1	A	516	HIS
1	B	402	GLN
1	B	432	HIS
1	B	469	ASN
1	B	517	ASN
1	B	552	HIS

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 [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	283/301 (94%)	1.22	75 (26%) 1 1	29, 63, 106, 132	0
1	B	290/301 (96%)	0.07	7 (2%) 59 62	22, 40, 63, 86	1 (0%)
2	P	6/7 (85%)	0.25	0 100 100	39, 47, 48, 51	0
All	All	579/609 (95%)	0.63	82 (14%) 6 7	22, 47, 99, 132	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	LEU	6.1
1	A	446	GLU	5.9
1	A	351	THR	5.3
1	A	399	MET	5.2
1	A	516	HIS	5.0
1	A	447	ARG	4.9
1	A	353	LEU	4.8
1	A	594	VAL	4.7
1	A	386	GLY	4.7
1	A	452	LEU	4.6
1	A	373	LEU	4.4
1	A	470	ARG	4.3
1	A	329	TYR	4.3
1	A	371	GLY	3.9
1	B	614	ARG	3.9
1	A	350	GLY	3.7
1	A	400	THR	3.5
1	A	369	VAL	3.5
1	A	349	ASP	3.4
1	A	407	ALA	3.4
1	A	562	HIS	3.2
1	A	395	CYS	3.2
1	A	348	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	609	THR	3.1
1	A	515	LEU	3.1
1	A	448	ASP	3.1
1	A	608	VAL	3.1
1	A	567	TYR	3.0
1	A	398	PRO	3.0
1	A	496	GLU	2.9
1	A	402	GLN	2.8
1	A	588	THR	2.8
1	A	590	THR	2.8
1	A	355	LEU	2.8
1	A	328	ILE	2.8
1	A	421	ILE	2.8
1	A	425	ILE	2.8
1	A	563	GLN	2.8
1	A	405	PRO	2.7
1	A	356	ALA	2.6
1	B	325	GLY	2.6
1	A	345	TYR	2.6
1	A	408	PRO	2.6
1	A	451	HIS	2.6
1	A	445	PRO	2.6
1	A	580	SER	2.6
1	A	420	VAL	2.5
1	A	423	GLY	2.5
1	A	443	TYR	2.5
1	B	399	MET	2.4
1	A	344	ALA	2.4
1	A	370	VAL	2.3
1	A	595	THR	2.3
1	A	368	CYS	2.3
1	A	372	GLY	2.3
1	A	514	VAL	2.3
1	A	569	LEU	2.3
1	A	347	PRO	2.3
1	A	584	TYR	2.2
1	A	424	HIS	2.2
1	A	354	ARG	2.2
1	A	469	ASN	2.2
1	A	575	HIS	2.2
1	A	498	ARG	2.2
1	A	491	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	2.1
1	A	396	TYR	2.1
1	A	598	THR	2.1
1	B	337	GLN	2.1
1	B	613	SER	2.1
1	A	493	GLU	2.1
1	A	492	PRO	2.1
1	A	403	TRP	2.1
1	B	385	ASP	2.1
1	A	546	PHE	2.1
1	A	352	TRP	2.1
1	A	397	ASN	2.0
1	A	422	ASP	2.0
1	A	449	GLU	2.0
1	A	561	VAL	2.0
1	B	335	PHE	2.0
1	A	565	ARG	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.