



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 12:07 PM EDT

PDB ID : 7K2P
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

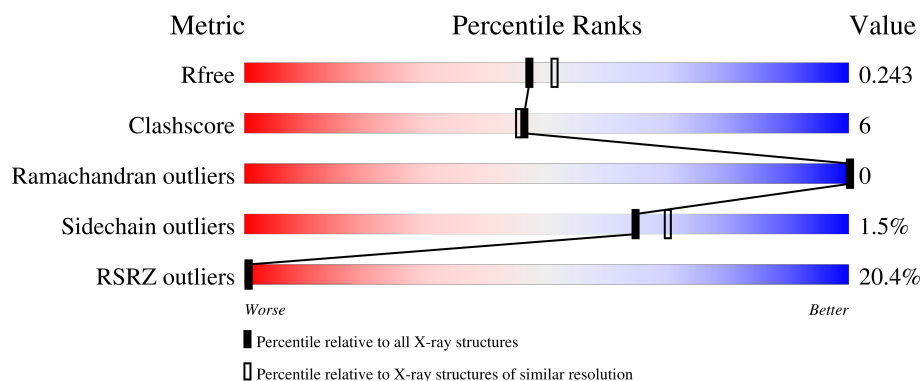
1 Overall quality at a glance

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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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	<div> <div>28%</div> <div>77%</div> <div>16%</div> <div>6%</div> </div>
1	B	301	<div> <div>11%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
2	P	7	<div> <div>71%</div> <div>29%</div> </div>

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			

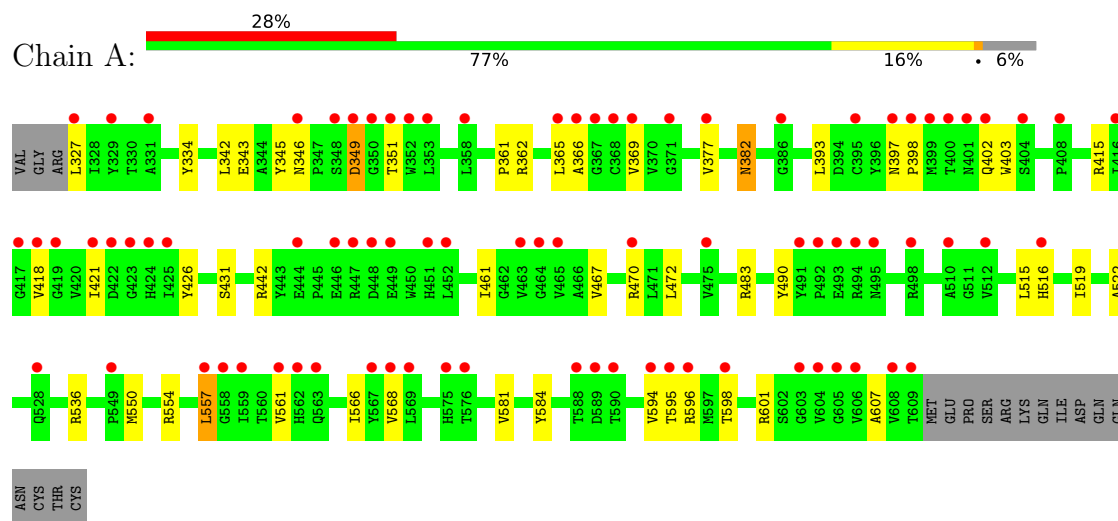
- Molecule 3 is water.

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		

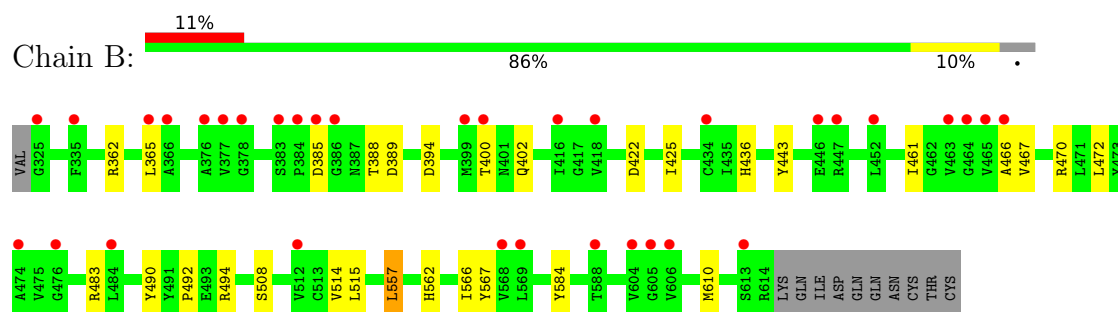
3 Residue-property plots

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.

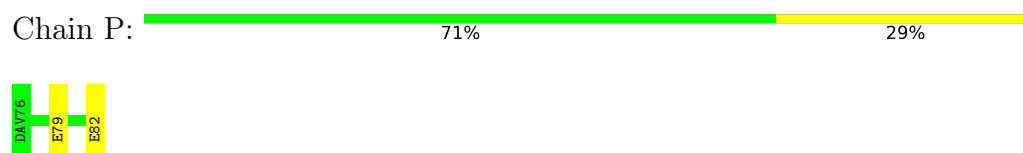
• Molecule 1: Kelch-like ECH-associated protein 1



• 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 0.209 , 0.243	Depositor DCC
R_{free} test set	1997 reflections (4.61%)	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)	0.35 , 43.4	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	0.41	0/2204	0.65	2/3006 (0.1%)
1	B	0.42	0/2279	0.62	0/3104
2	P	0.42	0/44	0.63	0/59
All	All	0.41	0/4527	0.63	2/6169 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	470	ARG	NE-CZ-NH2	-5.66	117.47	120.30

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	37	0
1	B	2223	0	2107	19	0
2	P	51	0	41	2	0
3	A	29	0	0	2	0
3	B	56	0	0	0	0
3	P	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4514	0	4180	54	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 6.

All (54) 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:B:466:ALA:HB1	1:B:514:VAL:HG23	1.73	0.70
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:522:ALA:HB1	1:A:550:MET:HE3	1.86	0.58
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.88	0.56
1:A:550:MET:HE1	1:A:568:VAL:HG21	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:550:MET:HE1	1:A:568:VAL:HG11	2.02	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: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 ⓘ

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	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%)	219 (98%)	4 (2%)	59	63
1	B	233/247 (94%)	230 (99%)	3 (1%)	69	74
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	461/499 (92%)	454 (98%)	7 (2%)	65	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	402	GLN
1	A	483	ARG
1	A	557	LEU
1	B	385	ASP
1	B	557	LEU
1	B	610	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	402	GLN
1	A	516	HIS
1	B	337	GLN
1	B	402	GLN
1	B	517	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 monosaccharides 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%)	1.45	84 (29%) 0 0	29, 63, 106, 132	0
1	B	290/301 (96%)	0.68	34 (11%) 4 5	28, 40, 63, 86	0
2	P	6/7 (85%)	0.21	0 100 100	39, 47, 48, 51	0
All	All	579/609 (95%)	1.05	118 (20%) 1 1	28, 47, 99, 132	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	8.6
1	A	452	LEU	6.6
1	A	349	ASP	6.4
1	A	400	THR	6.2
1	B	385	ASP	6.0
1	A	604	VAL	5.8
1	A	371	GLY	5.8
1	A	402	GLN	5.3
1	B	613	SER	5.2
1	A	351	THR	5.0
1	A	563	GLN	4.8
1	A	399	MET	4.7
1	A	401	ASN	4.6
1	B	365	LEU	4.5
1	A	365	LEU	4.5
1	A	348	SER	4.3
1	B	366	ALA	4.3
1	A	327	LEU	4.2
1	A	350	GLY	4.2
1	A	447	ARG	4.2
1	A	416	ILE	4.2
1	A	423	GLY	4.1
1	A	346	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	576	THR	4.1
1	A	557	LEU	4.0
1	A	367	GLY	4.0
1	A	421	ILE	3.9
1	A	575	HIS	3.9
1	A	408	PRO	3.8
1	B	399	MET	3.8
1	A	377	VAL	3.7
1	A	451	HIS	3.7
1	A	588	THR	3.7
1	A	608	VAL	3.6
1	A	512	VAL	3.5
1	A	470	ARG	3.5
1	B	606	VAL	3.5
1	A	510	ALA	3.5
1	A	567	TYR	3.5
1	A	559	ILE	3.4
1	B	465	VAL	3.4
1	A	562	HIS	3.3
1	B	512	VAL	3.3
1	A	352	TRP	3.3
1	A	368	CYS	3.3
1	B	447	ARG	3.2
1	A	449	GLU	3.2
1	A	329	TYR	3.2
1	B	416	ILE	3.2
1	A	366	ALA	3.2
1	A	569	LEU	3.2
1	A	494	ARG	3.2
1	A	422	ASP	3.2
1	A	418	VAL	3.1
1	A	605	GLY	3.1
1	A	493	GLU	3.1
1	B	384	PRO	3.1
1	A	590	THR	3.1
1	A	448	ASP	3.1
1	A	397	ASN	3.0
1	A	516	HIS	3.0
1	A	463	VAL	3.0
1	A	491	TYR	3.0
1	A	424	HIS	2.9
1	A	398	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	606	VAL	2.9
1	A	558	GLY	2.9
1	A	495	ASN	2.9
1	B	569	LEU	2.9
1	B	605	GLY	2.8
1	B	604	VAL	2.8
1	B	400	THR	2.7
1	A	596	ARG	2.7
1	A	386	GLY	2.7
1	B	588	THR	2.7
1	A	358	LEU	2.6
1	A	419	GLY	2.6
1	B	377	VAL	2.6
1	A	395	CYS	2.6
1	A	417	GLY	2.5
1	A	589	ASP	2.5
1	B	446	GLU	2.5
1	A	331	ALA	2.4
1	A	594	VAL	2.4
1	A	425	ILE	2.4
1	B	378	GLY	2.4
1	B	452	LEU	2.4
1	A	595	THR	2.4
1	A	561	VAL	2.3
1	A	498	ARG	2.3
1	A	404	SER	2.3
1	B	418	VAL	2.3
1	B	434	CYS	2.3
1	B	476	GLY	2.3
1	A	369	VAL	2.3
1	B	474	ALA	2.3
1	A	598	THR	2.3
1	A	444	GLU	2.3
1	A	475	VAL	2.3
1	B	383	SER	2.2
1	B	466	ALA	2.2
1	A	609	THR	2.2
1	A	464	GLY	2.2
1	B	464	GLY	2.2
1	A	549	PRO	2.2
1	A	568	VAL	2.2
1	B	463	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	325	GLY	2.2
1	B	386	GLY	2.2
1	B	484	LEU	2.2
1	B	335	PHE	2.2
1	A	465	VAL	2.1
1	A	528	GLN	2.1
1	A	492	PRO	2.1
1	B	376	ALA	2.1
1	B	568	VAL	2.1
1	A	446	GLU	2.1
1	A	603	GLY	2.1

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 monosaccharides 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.