



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 12:09 PM EDT

PDB ID : 7K2E
Title : Kelch domain of human KEAP1 bound to Nrf2-based cyclic peptide, c[GDEETGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.03 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
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

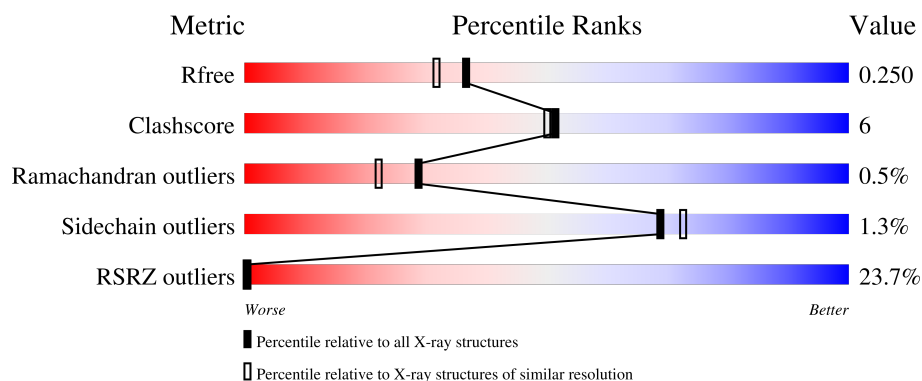
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 $\leq 5\%$. 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>39%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	B	301	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>• •</div> </div> </div>
2	P	7	<div> <div></div> <div> <div>71%</div> <div>29%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4490 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	282	Total	C	N	O	S	0	0	0
			2094	1305	378	396	15			
1	B	290	Total	C	N	O	S	0	1	0
			2223	1382	402	423	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	ALA	GLU	conflict	UNP Q14145
A	542	ALA	GLU	conflict	UNP Q14145
A	613	SER	CYS	conflict	UNP Q14145
B	540	ALA	GLU	conflict	UNP Q14145
B	542	ALA	GLU	conflict	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145

- Molecule 2 is a protein called GLY-ASP-GLU-GLU-THR-GLY-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			50	27	7	16			

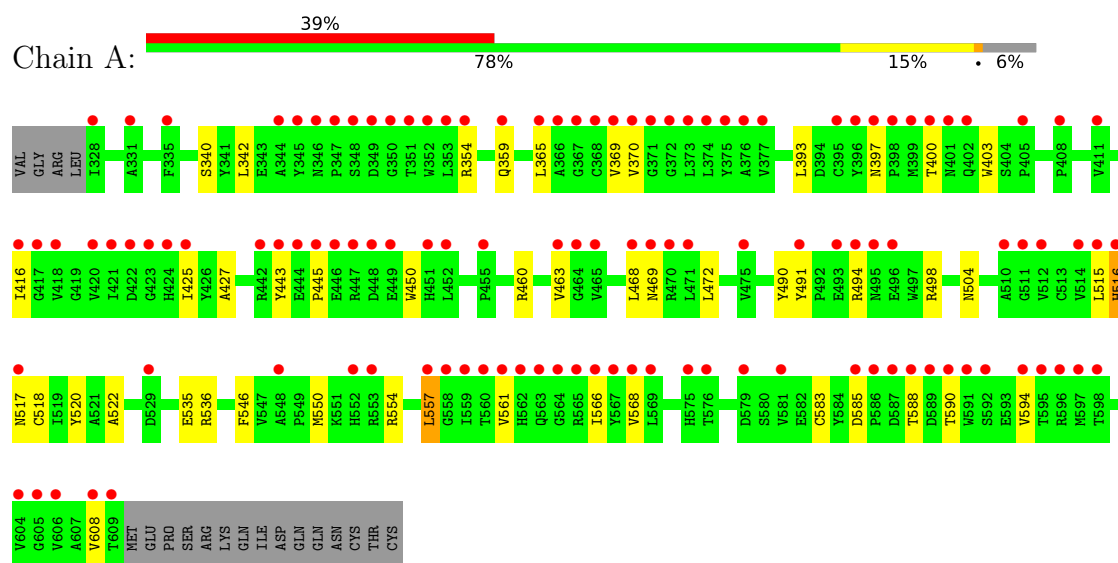
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	95	Total	O	0	0
			95	95		
3	P	3	Total	O	0	0
			3	3		

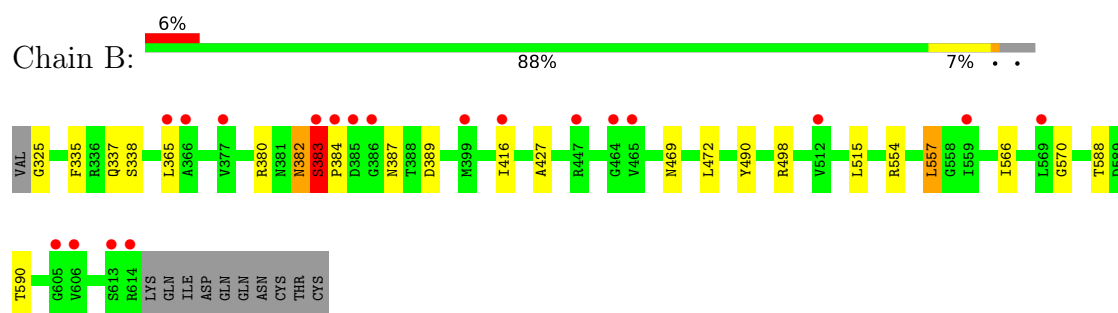
3 Residue-property plots [i](#)

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.

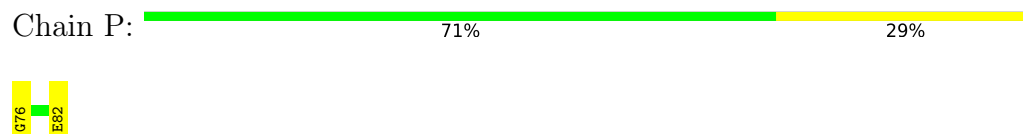
- Molecule 1: Kelch-like ECH-associated protein 1



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



- Molecule 2: GLY-ASP-GLU-GLU-THR-GLY-GLU



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.15Å 68.87Å 77.37Å 90.00° 117.48° 90.00°	Depositor
Resolution (Å)	29.31 – 2.03 29.31 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.31-2.03) 99.0 (29.31-2.03)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.215 , 0.250 0.215 , 0.250	Depositor DCC
R_{free} test set	1992 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.1	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	4490	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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](#)

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	0.35	0/2144	0.57	0/2926
1	B	0.46	0/2280	0.62	1/3105 (0.0%)
2	P	0.41	0/49	0.62	0/64
All	All	0.41	0/4473	0.60	1/6095 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ASN	C-N-CA	5.18	134.64	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	383	SER	Peptide

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	2094	0	1940	32	0
1	B	2223	0	2116	15	0
2	P	50	0	34	1	0
3	A	25	0	0	0	0
3	B	95	0	0	3	0
3	P	3	0	0	0	0
All	All	4490	0	4090	47	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 (47) 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:B:498:ARG:NH1	3:B:701:HOH:O	2.03	0.92
1:A:583:CYS:HB2	1:A:594:VAL:HG21	1.54	0.89
1:A:425:ILE:HB	1:A:443:TYR:HB3	1.62	0.80
1:B:325:GLY:N	3:B:702:HOH:O	2.23	0.71
1:A:561:VAL:HG12	1:A:566:ILE:HG12	1.73	0.70
1:A:583:CYS:HB2	1:A:594:VAL:CG2	2.25	0.67
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.77	0.67
1:A:491:TYR:HB3	1:A:494:ARG:NH2	2.16	0.61
1:A:554:ARG:HD2	1:A:557:LEU:HD13	1.86	0.57
1:B:325:GLY:N	3:B:703:HOH:O	2.38	0.56
1:A:585:ASP:OD2	1:A:588:THR:HG22	2.06	0.56
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.90	0.54
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.88	0.54
1:B:557:LEU:H	1:B:557:LEU:HD23	1.73	0.52
1:A:397:ASN:HB3	1:A:400:THR:OG1	2.10	0.52
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.91	0.51
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.92	0.51
1:A:393:LEU:HD22	1:A:450:TRP:CZ2	2.46	0.50
1:A:550:MET:CE	1:A:568:VAL:HG11	2.41	0.50
1:A:469:ASN:ND2	1:B:469:ASN:OD1	2.44	0.49
1:A:370:VAL:HG11	1:A:445:PRO:HG2	1.94	0.49
1:A:393:LEU:HD22	1:A:450:TRP:HZ2	1.78	0.48
1:A:369:VAL:HG11	1:A:608:VAL:O	2.14	0.48
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.48	0.48
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.94	0.48
1:B:335:PHE:C	1:B:337:GLN:H	2.17	0.48
1:B:380:ARG:NH1	1:B:389:ASP:OD1	2.37	0.47
1:A:518:CYS:HB3	1:A:536:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.96	0.47
2:P:76:GLY:N	2:P:82:GLU:C	2.68	0.47
1:A:515:LEU:HB2	1:A:566:ILE:HD11	1.97	0.46
1:B:365:LEU:H	1:B:365:LEU:HD23	1.79	0.46
1:A:342:LEU:HD22	1:A:403:TRP:CZ2	2.50	0.45
1:A:535:GLU:HB3	1:A:546:PHE:CD1	2.52	0.45
1:B:338:SER:OG	1:B:382:ASN:HB2	2.17	0.45
1:A:557:LEU:HD23	1:A:557:LEU:H	1.81	0.44
1:A:365:LEU:HD23	1:A:365:LEU:H	1.83	0.43
1:A:468:LEU:HD12	1:A:469:ASN:H	1.82	0.43
1:A:504:ASN:HB2	1:A:546:PHE:CZ	2.54	0.43
1:A:588:THR:HG23	1:A:590:THR:OG1	2.19	0.42
1:A:550:MET:HE1	1:A:568:VAL:HG21	2.02	0.42
1:A:516:HIS:CE1	1:A:517:ASN:HD22	2.37	0.42
1:A:342:LEU:HD22	1:A:403:TRP:HZ2	1.86	0.41
1:A:460:ARG:HB3	1:A:463:VAL:HB	2.02	0.41
1:B:383:SER:N	1:B:387:ASN:OD1	2.43	0.41
1:B:588:THR:O	1:B:590:THR:HG23	2.22	0.40
1:B:554:ARG:HD3	1:B:570:GLY:O	2.21	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	280/301 (93%)	267 (95%)	12 (4%)	1 (0%)	34	28
1	B	289/301 (96%)	280 (97%)	7 (2%)	2 (1%)	22	15
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	574/609 (94%)	552 (96%)	19 (3%)	3 (0%)	29	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	383	SER
1	B	384	PRO
1	A	516	HIS

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	208/245 (85%)	203 (98%)	5 (2%)	49	49
1	B	234/245 (96%)	233 (100%)	1 (0%)	91	93
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	447/495 (90%)	441 (99%)	6 (1%)	69	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	SER
1	A	354	ARG
1	A	359	GLN
1	A	498	ARG
1	A	557	LEU
1	B	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	HIS

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	282/301 (93%)	2.03	118 (41%) 0 0	30, 75, 135, 186	0
1	B	290/301 (96%)	0.41	19 (6%) 18 17	25, 34, 63, 114	0
2	P	7/7 (100%)	0.47	0 100 100	34, 41, 51, 62	0
All	All	579/609 (95%)	1.20	137 (23%) 0 0	25, 47, 127, 186	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	CYS	11.4
1	B	383	SER	10.6
1	A	351	THR	8.4
1	A	446	GLU	8.4
1	A	562	HIS	8.2
1	A	421	ILE	7.3
1	B	385	ASP	7.3
1	A	348	SER	7.2
1	A	347	PRO	7.2
1	A	371	GLY	7.0
1	A	563	GLN	7.0
1	A	399	MET	7.0
1	A	491	TYR	7.0
1	A	423	GLY	6.7
1	A	328	ILE	6.6
1	A	561	VAL	6.5
1	A	449	GLU	6.2
1	A	352	TRP	6.2
1	A	346	ASN	6.1
1	A	608	VAL	5.7
1	A	373	LEU	5.7
1	B	384	PRO	5.6
1	A	353	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	5.5
1	A	494	ARG	5.4
1	A	557	LEU	5.3
1	A	422	ASP	5.3
1	A	359	GLN	5.2
1	A	595	THR	5.1
1	A	401	ASN	5.1
1	A	447	ARG	5.0
1	A	590	THR	5.0
1	A	397	ASN	4.9
1	A	349	ASP	4.8
1	A	424	HIS	4.8
1	A	596	ARG	4.8
1	A	588	THR	4.7
1	A	398	PRO	4.7
1	A	448	ASP	4.6
1	A	350	GLY	4.5
1	A	416	ILE	4.5
1	A	567	TYR	4.4
1	A	564	GLY	4.3
1	A	366	ALA	4.3
1	B	386	GLY	4.3
1	A	445	PRO	4.3
1	A	587	ASP	4.3
1	A	365	LEU	4.2
1	A	402	GLN	4.2
1	A	569	LEU	4.2
1	A	591	TRP	4.1
1	A	495	ASN	4.1
1	A	395	CYS	4.1
1	A	594	VAL	4.1
1	A	604	VAL	4.1
1	A	400	THR	4.0
1	A	377	VAL	4.0
1	A	592	SER	3.9
1	A	372	GLY	3.9
1	A	575	HIS	3.7
1	B	366	ALA	3.6
1	A	425	ILE	3.6
1	B	613	SER	3.6
1	A	559	ILE	3.6
1	A	345	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	420	VAL	3.6
1	A	418	VAL	3.6
1	A	375	TYR	3.5
1	A	452	LEU	3.5
1	A	606	VAL	3.5
1	B	614	ARG	3.5
1	A	576	THR	3.4
1	A	515	LEU	3.4
1	A	493	GLU	3.4
1	A	455	PRO	3.4
1	A	548	ALA	3.3
1	A	367	GLY	3.3
1	B	416	ILE	3.3
1	A	405	PRO	3.3
1	A	552	HIS	3.2
1	A	510	ALA	3.2
1	A	609	THR	3.2
1	A	344	ALA	3.1
1	A	463	VAL	3.1
1	A	586	PRO	3.1
1	B	365	LEU	3.1
1	B	605	GLY	3.0
1	A	568	VAL	3.0
1	A	465	VAL	3.0
1	A	565	ARG	3.0
1	A	605	GLY	3.0
1	A	469	ASN	3.0
1	A	442	ARG	2.9
1	A	470	ARG	2.9
1	A	408	PRO	2.9
1	B	464	GLY	2.9
1	A	444	GLU	2.9
1	A	597	MET	2.9
1	B	465	VAL	2.8
1	A	566	ILE	2.8
1	A	443	TYR	2.8
1	A	512	VAL	2.7
1	B	606	VAL	2.7
1	A	589	ASP	2.7
1	A	376	ALA	2.7
1	A	374	LEU	2.6
1	A	496	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	512	VAL	2.6
1	A	471	LEU	2.5
1	B	447	ARG	2.5
1	A	585	ASP	2.5
1	A	396	TYR	2.5
1	A	411	VAL	2.5
1	A	464	GLY	2.4
1	A	331	ALA	2.4
1	B	569	LEU	2.4
1	B	399	MET	2.3
1	A	516	HIS	2.3
1	A	514	VAL	2.3
1	A	517	ASN	2.3
1	A	475	VAL	2.2
1	A	560	THR	2.2
1	A	529	ASP	2.2
1	A	581	VAL	2.2
1	A	579	ASP	2.2
1	B	377	VAL	2.1
1	A	369	VAL	2.1
1	A	354	ARG	2.1
1	A	511	GLY	2.1
1	A	558	GLY	2.1
1	A	335	PHE	2.1
1	A	417	GLY	2.1
1	A	553	ARG	2.0
1	B	559	ILE	2.0
1	A	451	HIS	2.0
1	A	598	THR	2.0
1	A	468	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.