



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:49 PM UTC

PDB ID : 7K2E / pdb_00007k2e
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 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

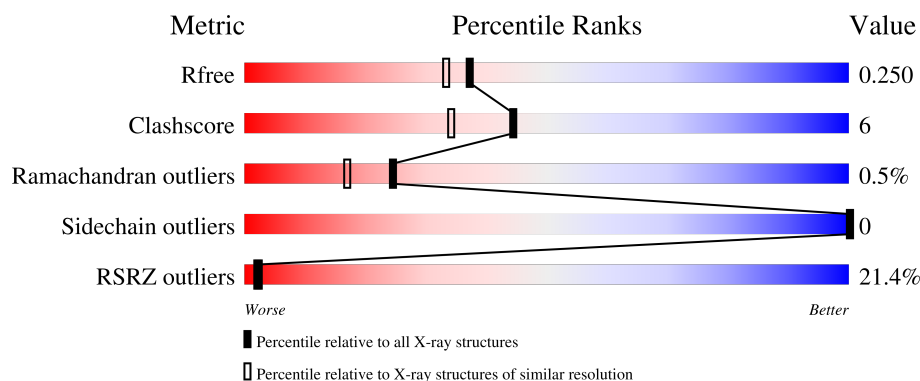
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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	38% 78%15%6%
1	B	301	4% 87%8%.
2	P	7	71%29%

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			

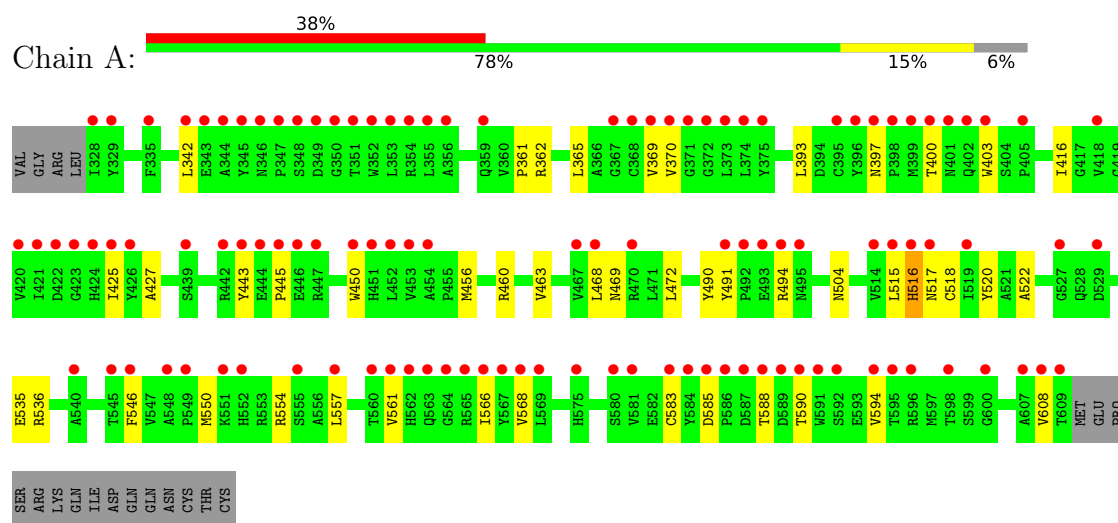
- Molecule 3 is water.

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		

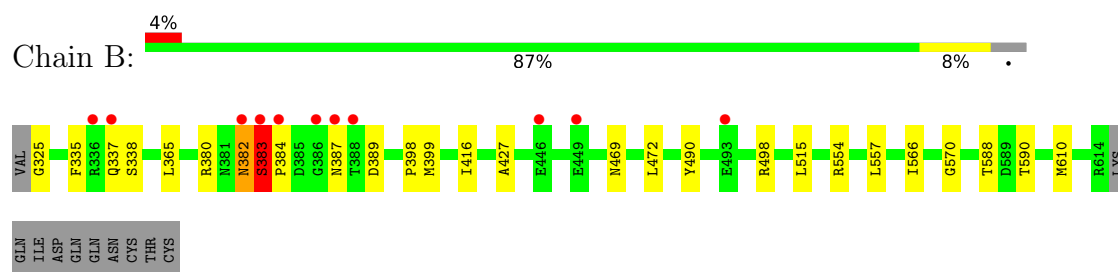
3 Residue-property plots

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.

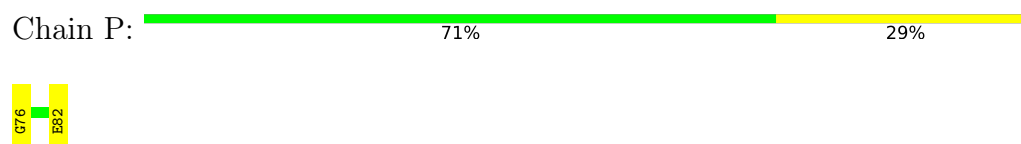
• Molecule 1: Kelch-like ECH-associated protein 1



• 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) 98.9 (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 0.216 , 0.250	Depositor DCC
R_{free} test set	1992 reflections (4.07%)	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)	0.38 , 56.6	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	0.94	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	0.29	0/2144	0.56	0/2926
1	B	0.38	0/2280	0.59	2/3105 (0.1%)
2	P	0.32	0/49	0.43	0/64
All	All	0.34	0/4473	0.57	2/6095 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ASN	CA-C-N	5.26	134.64	121.80
1	B	382	ASN	C-N-CA	5.26	134.64	121.80

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	34	0
1	B	2223	0	2116	17	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	51	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 (51) 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:550:MET:HE2	1:A:568:VAL:HG21	1.77	0.66
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:A:522:ALA:HB1	1:A:550:MET:HE3	1.89	0.53
1:B:335:PHE:C	1:B:337:GLN:H	2.17	0.52
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
2:P:76:GLY:N	2:P:82:GLU:C	2.68	0.52
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.91	0.51
1:B:399:MET:HG3	1:B:610:MET:HE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.96	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:456:MET:HE1	1:A:460:ARG:HB2	2.01	0.43
1:A:588:THR:HG23	1:A:590:THR:OG1	2.19	0.42
1:B:398:PRO:HB2	1:B:610:MET:HE3	2.02	0.42
1:A:516:HIS:CE1	1:A:517:ASN:HD22	2.37	0.42
1:A:361:PRO:C	1:A:362:ARG:HG3	2.45	0.41
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

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	280/301 (93%)	267 (95%)	12 (4%)	1 (0%)	30 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	289/301 (96%)	280 (97%)	7 (2%)	2 (1%)	18	10
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	574/609 (94%)	552 (96%)	19 (3%)	3 (0%)	24	17

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%)	208 (100%)	0	100	100
1	B	234/245 (96%)	234 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	447/495 (90%)	447 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	414	ASN
1	A	495	ASN
1	B	414	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	282/301 (93%)	1.90	113 (40%) 0 1	30, 75, 135, 186	0
1	B	290/301 (96%)	0.04	11 (3%) 44 43	19, 34, 63, 114	1 (0%)
2	P	7/7 (100%)	0.51	0 100 100	34, 41, 51, 62	0
All	All	579/609 (95%)	0.95	124 (21%) 2 2	19, 47, 127, 186	1 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	590	THR	8.5
1	A	368	CYS	7.8
1	A	328	ILE	7.2
1	A	373	LEU	6.6
1	A	353	LEU	6.3
1	A	344	ALA	6.1
1	A	349	ASP	5.6
1	A	446	GLU	5.6
1	A	347	PRO	5.4
1	A	346	ASN	5.4
1	A	369	VAL	5.3
1	A	371	GLY	5.3
1	A	395	CYS	5.2
1	B	383	SER	5.1
1	A	561	VAL	5.0
1	A	584	TYR	5.0
1	A	583	CYS	4.9
1	A	420	VAL	4.9
1	A	351	THR	4.8
1	A	591	TRP	4.7
1	A	374	LEU	4.6
1	A	359	GLN	4.6
1	A	515	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	367	GLY	4.4
1	A	588	THR	4.4
1	A	423	GLY	4.4
1	A	562	HIS	4.4
1	A	516	HIS	4.3
1	A	422	ASP	4.3
1	B	386	GLY	4.2
1	A	564	GLY	4.1
1	A	356	ALA	4.1
1	A	399	MET	4.0
1	A	563	GLN	4.0
1	A	348	SER	4.0
1	A	375	TYR	4.0
1	B	384	PRO	3.9
1	B	382	ASN	3.9
1	A	493	GLU	3.9
1	A	445	PRO	3.9
1	A	424	HIS	3.8
1	A	595	THR	3.8
1	A	345	TYR	3.8
1	A	592	SER	3.8
1	A	398	PRO	3.7
1	A	352	TRP	3.7
1	A	608	VAL	3.7
1	A	421	ILE	3.6
1	A	566	ILE	3.6
1	A	567	TYR	3.6
1	A	565	ARG	3.6
1	A	514	VAL	3.6
1	A	517	ASN	3.6
1	A	335	PHE	3.6
1	A	402	GLN	3.5
1	A	355	LEU	3.4
1	A	329	TYR	3.4
1	A	350	GLY	3.4
1	A	425	ILE	3.4
1	A	444	GLU	3.3
1	A	609	THR	3.3
1	B	387	ASN	3.3
1	A	585	ASP	3.3
1	A	581	VAL	3.2
1	A	400	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	546	PHE	3.2
1	A	495	ASN	3.2
1	A	540	ALA	3.2
1	A	470	ARG	3.1
1	A	491	TYR	3.1
1	A	586	PRO	3.1
1	A	594	VAL	3.1
1	A	397	ASN	3.1
1	A	468	LEU	3.0
1	A	467	VAL	2.9
1	A	557	LEU	2.9
1	A	370	VAL	2.9
1	A	560	THR	2.9
1	A	492	PRO	2.9
1	A	548	ALA	2.9
1	A	452	LEU	2.8
1	A	587	ASP	2.8
1	B	493	GLU	2.8
1	A	453	VAL	2.8
1	A	396	TYR	2.8
1	A	598	THR	2.8
1	A	494	ARG	2.7
1	A	372	GLY	2.7
1	A	552	HIS	2.6
1	A	549	PRO	2.6
1	A	568	VAL	2.6
1	A	451	HIS	2.6
1	A	342	LEU	2.6
1	A	405	PRO	2.6
1	A	596	ARG	2.5
1	B	388	THR	2.5
1	A	600	GLY	2.5
1	A	569	LEU	2.5
1	A	527	GLY	2.5
1	A	443	TYR	2.5
1	A	545	THR	2.5
1	A	450	TRP	2.5
1	A	403	TRP	2.4
1	A	447	ARG	2.4
1	A	519	ILE	2.3
1	B	337	GLN	2.2
1	A	551	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	454	ALA	2.2
1	A	439	SER	2.2
1	A	580	SER	2.2
1	A	529	ASP	2.2
1	B	446	GLU	2.1
1	A	442	ARG	2.1
1	A	426	TYR	2.1
1	A	555	SER	2.1
1	A	589	ASP	2.1
1	A	354	ARG	2.1
1	A	418	VAL	2.1
1	A	401	ASN	2.1
1	A	343	GLU	2.0
1	A	607	ALA	2.1
1	B	449	GLU	2.0
1	B	336	ARG	2.0
1	A	575	HIS	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.