



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:08 PM UTC

PDB ID : 7K2O / pdb_00007k2o
Title : Kelch domain of human KEAP1 bound to Nrf2-based cyclic peptide, c[GABA-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

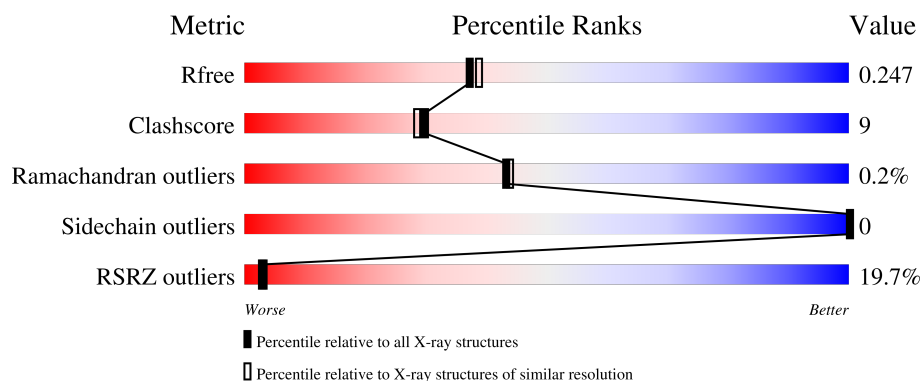
1 Overall quality at a glance

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	34% 74% 20% 6%
1	B	301	4% 83% 13% .
2	P	7	29% 57% 14%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4575 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
			2170	1351	392	412	15			
1	B	290	Total	C	N	O	S	0	1	0
			2229	1385	405	423	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 (ABU)DPETGE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			50	29	7	14			

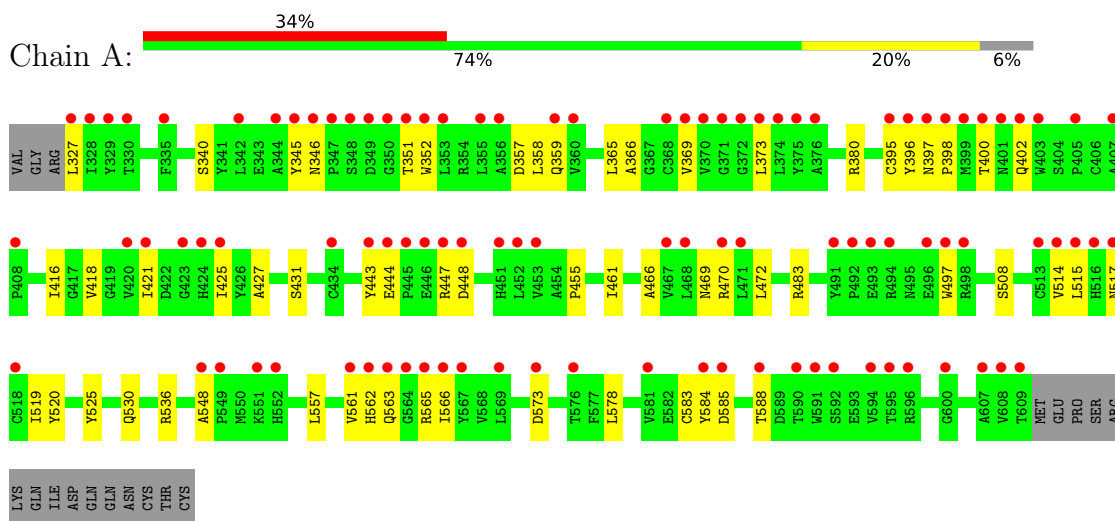
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	86	Total	O	0	0
			86	86		
3	P	3	Total	O	0	0
			3	3		

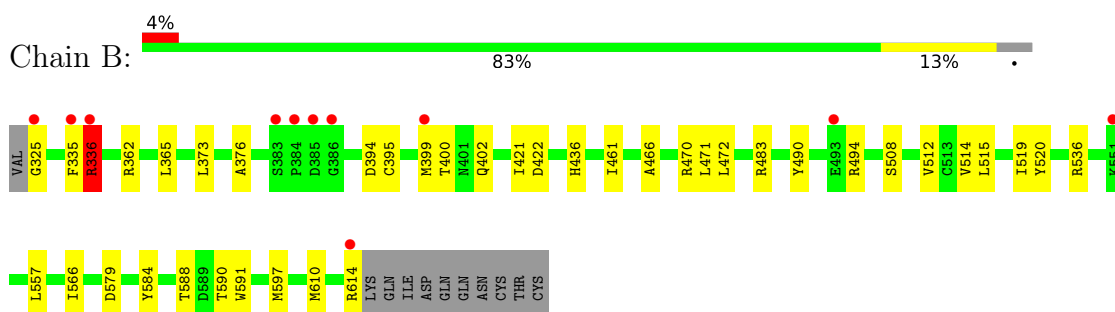
3 Residue-property plots

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: (ABU)DPETGE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.29Å 68.80Å 77.10Å 90.00° 117.59° 90.00°	Depositor
Resolution (Å)	29.33 – 2.11 29.33 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.33-2.11) 99.5 (29.33-2.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.208 , 0.246 0.211 , 0.247	Depositor DCC
R_{free} test set	2005 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: ABU

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	0/2223	0.64	2/3029 (0.1%)
1	B	0.41	1/2286 (0.0%)	0.66	4/3112 (0.1%)
2	P	1.18	1/45 (2.2%)	4.48	1/61 (1.6%)
All	All	0.40	2/4554 (0.0%)	0.79	7/6202 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	76	ABU	C-N	6.93	1.43	1.33
1	B	336	ARG	CB-CG	-5.54	1.35	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	76	ABU	O-C-N	-34.56	67.70	123.00
1	A	358	LEU	CA-C-N	-7.66	110.39	122.65
1	A	358	LEU	C-N-CA	-7.66	110.39	122.65
1	B	336	ARG	CB-CG-CD	-6.94	95.34	111.30
1	B	336	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	B	336	ARG	NH1-CZ-NH2	5.52	126.48	119.30
1	B	336	ARG	CG-CD-NE	-5.24	100.47	112.00

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	2170	0	2060	43	0
1	B	2229	0	2121	32	0
2	P	50	0	33	5	0
3	A	37	0	0	3	0
3	B	86	0	0	1	0
3	P	3	0	0	0	0
All	All	4575	0	4214	74	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 (74) 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:470:ARG:NH2	3:A:701:HOH:O	2.03	0.90
1:B:335:PHE:O	1:B:336:ARG:HB2	1.81	0.78
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.70	0.72
1:A:359:GLN:O	1:A:359:GLN:HG2	1.93	0.68
1:A:517:ASN:ND2	1:B:471:LEU:HD11	2.09	0.67
1:A:470:ARG:CZ	3:A:701:HOH:O	2.39	0.65
1:A:444:GLU:HG2	1:A:447:ARG:HB2	1.77	0.65
1:A:530:GLN:NE2	2:P:78:PRO:O	2.30	0.64
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.81	0.63
1:A:565:ARG:HD2	1:A:583:CYS:SG	2.40	0.62
1:B:325:GLY:N	3:B:701:HOH:O	2.32	0.61
1:A:397:ASN:HB3	1:A:400:THR:HB	1.83	0.60
1:A:469:ASN:N	3:A:701:HOH:O	2.36	0.59
1:A:561:VAL:HG22	1:A:566:ILE:HG12	1.86	0.57
1:A:562:HIS:CD2	1:A:563:GLN:HG3	2.40	0.57
1:A:536:ARG:HH12	1:B:494:ARG:NH2	2.03	0.56
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.87	0.56
1:A:365:LEU:HD23	1:A:365:LEU:H	1.70	0.56
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.87	0.56
1:B:335:PHE:O	1:B:336:ARG:CB	2.53	0.55
1:B:557:LEU:H	1:B:557:LEU:HD23	1.71	0.54
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.89	0.54
1:B:614:ARG:NH1	1:B:614:ARG:HA	2.23	0.54
1:A:525:TYR:CZ	2:P:78:PRO:HB2	2.44	0.53
1:A:483:ARG:HG2	1:A:508:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:HG2	1:B:508[B]:SER:HB2	1.91	0.52
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.92	0.52
1:A:425:ILE:HB	1:A:443:TYR:HB3	1.92	0.51
1:A:517:ASN:CG	1:B:471:LEU:HD11	2.35	0.51
1:A:573:ASP:OD2	1:A:578:LEU:HD21	2.10	0.51
1:A:557:LEU:HD23	1:A:557:LEU:H	1.76	0.49
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.94	0.49
1:B:470:ARG:C	1:B:471:LEU:HD12	2.38	0.48
1:B:436:HIS:HB3	1:B:461:ILE:HD11	1.96	0.48
1:A:340:SER:HB3	1:A:357:ASP:HB3	1.96	0.47
1:B:579:ASP:HA	1:B:597:MET:HE3	1.97	0.47
1:B:471:LEU:HD12	1:B:471:LEU:N	2.30	0.47
1:B:373:LEU:HB3	1:B:395:CYS:SG	2.56	0.46
1:A:351:THR:HG22	1:A:352:TRP:H	1.80	0.46
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.98	0.46
2:P:80:THR:OG1	2:P:82:GLU:HB3	2.15	0.46
1:B:365:LEU:H	1:B:365:LEU:HD23	1.80	0.46
1:B:399:MET:HE3	1:B:610:MET:SD	2.56	0.46
1:A:345:TYR:HB2	1:A:352:TRP:CZ3	2.51	0.45
1:B:588:THR:O	1:B:590:THR:HG23	2.17	0.44
1:A:519:ILE:O	1:A:536:ARG:HA	2.16	0.44
1:B:365:LEU:HD12	1:B:376:ALA:HB1	2.00	0.44
1:A:515:LEU:HD22	1:A:566:ILE:HG13	2.00	0.44
1:A:565:ARG:HG2	1:A:584:TYR:O	2.18	0.44
1:A:366:ALA:HB3	1:A:418:VAL:HG13	2.00	0.43
1:B:400:THR:O	1:B:402:GLN:HG3	2.18	0.43
1:A:548:ALA:HB3	1:A:584:TYR:HE1	1.83	0.43
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.99	0.43
1:B:436:HIS:ND1	1:B:461:ILE:HD11	2.33	0.43
1:B:519:ILE:O	1:B:536:ARG:HA	2.18	0.43
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.01	0.43
1:A:585:ASP:HB3	1:A:588:THR:OG1	2.19	0.43
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.54	0.43
1:A:373:LEU:HB3	1:A:395:CYS:SG	2.59	0.43
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.51	0.42
1:B:422:ASP:OD1	1:B:470:ARG:HD3	2.19	0.42
2:P:76:ABU:CD	2:P:77:ASP:H	2.32	0.42
1:A:396:TYR:CE1	1:A:398:PRO:HA	2.53	0.42
1:B:614:ARG:HA	1:B:614:ARG:CZ	2.50	0.42
1:B:584:TYR:HB2	1:B:591:TRP:CZ3	2.56	0.41
1:A:327:LEU:HD22	1:A:346:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLU:O	1:A:448:ASP:N	2.52	0.41
1:B:512:VAL:HA	1:B:520:TYR:O	2.21	0.41
1:A:380:ARG:HH11	2:P:82:GLU:HG2	1.86	0.40
1:A:400:THR:HG22	1:A:402:GLN:CB	2.51	0.40
1:A:455:PRO:O	1:A:497:TRP:CD1	2.75	0.40
1:B:494:ARG:HE	1:B:494:ARG:HB2	1.63	0.40
1:A:369:VAL:HA	1:A:373:LEU:O	2.21	0.40
1:A:400:THR:HG22	1:A:402:GLN:HB2	2.03	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%)	266 (95%)	15 (5%)	0	100	100
1	B	289/301 (96%)	280 (97%)	8 (3%)	1 (0%)	36	36
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	575/609 (94%)	551 (96%)	23 (4%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	ARG

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	228/247 (92%)	228 (100%)	0	100	100
1	B	235/247 (95%)	235 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	468/499 (94%)	468 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	A	424	HIS
1	A	469	ASN
1	A	562	HIS
1	B	469	ASN

5.3.3 RNA [i](#)

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 ⓘ

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%)	1.54	101 (35%) ⓘ ⓘ	30, 64, 117, 157	0
1	B	290/301 (96%)	0.14	11 (3%) 44 47	21, 39, 65, 103	1 (0%)
2	P	6/7 (85%)	1.28	2 (33%) ⓘ ⓘ	40, 48, 52, 69	0
All	All	579/609 (95%)	0.84	114 (19%) ⓘ ⓘ	21, 47, 109, 157	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	HIS	6.7
1	A	329	TYR	6.3
1	A	373	LEU	5.9
1	A	327	LEU	5.7
1	A	351	THR	5.2
1	A	399	MET	5.0
1	A	515	LEU	4.8
1	A	446	GLU	4.7
1	A	353	LEU	4.6
1	A	371	GLY	4.5
1	A	447	ARG	4.4
1	A	370	VAL	4.2
1	A	561	VAL	4.2
1	A	400	THR	4.1
1	A	369	VAL	4.1
1	A	594	VAL	4.1
1	A	355	LEU	4.0
1	A	398	PRO	3.9
1	A	470	ARG	3.9
1	A	360	VAL	3.8
1	A	567	TYR	3.8
1	A	445	PRO	3.6
1	A	350	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	493	GLU	3.6
1	A	609	THR	3.6
1	A	349	ASP	3.6
1	A	397	ASN	3.6
1	A	420	VAL	3.5
1	B	614	ARG	3.5
1	A	452	LEU	3.4
1	A	514	VAL	3.4
1	A	356	ALA	3.4
1	A	395	CYS	3.4
1	A	590	THR	3.4
1	B	335	PHE	3.4
1	A	588	THR	3.3
1	A	595	THR	3.3
1	A	344	ALA	3.3
1	A	443	TYR	3.3
1	A	372	GLY	3.2
1	A	347	PRO	3.2
1	A	368	CYS	3.2
1	A	375	TYR	3.1
1	A	548	ALA	3.1
1	A	374	LEU	3.1
1	A	359	GLN	3.1
1	A	423	GLY	3.0
1	A	401	ASN	3.0
1	A	405	PRO	3.0
1	A	345	TYR	3.0
1	A	424	HIS	3.0
1	A	467	VAL	2.9
1	A	608	VAL	2.9
1	B	385	ASP	2.9
1	A	451	HIS	2.9
1	A	453	VAL	2.9
1	A	335	PHE	2.9
1	A	352	TRP	2.9
1	A	448	ASP	2.8
1	A	342	LEU	2.8
1	A	492	PRO	2.8
1	A	549	PRO	2.8
1	B	493	GLU	2.8
1	A	591	TRP	2.8
1	A	402	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	564	GLY	2.7
1	A	517	ASN	2.7
1	A	376	ALA	2.7
1	A	396	TYR	2.7
1	B	384	PRO	2.7
1	A	403	TRP	2.7
1	A	425	ILE	2.6
1	A	584	TYR	2.6
1	A	562	HIS	2.6
1	A	346	ASN	2.6
1	A	607	ALA	2.6
1	A	592	SER	2.6
1	A	328	ILE	2.5
1	A	551	LYS	2.5
1	A	576	THR	2.5
2	P	77	ASP	2.5
1	A	566	ILE	2.5
1	A	565	ARG	2.5
1	A	585	ASP	2.5
1	B	336	ARG	2.5
1	A	468	LEU	2.5
1	A	569	LEU	2.5
1	A	348	SER	2.4
1	A	497	TRP	2.4
1	A	581	VAL	2.4
1	A	518	CYS	2.4
1	B	386	GLY	2.3
1	A	498	ARG	2.3
1	A	444	GLU	2.3
1	A	563	GLN	2.3
1	A	421	ILE	2.3
1	B	383	SER	2.2
1	B	551	LYS	2.2
1	A	330	THR	2.2
1	A	434	CYS	2.2
2	P	82	GLU	2.1
1	A	600	GLY	2.1
1	A	407	ALA	2.1
1	A	471	LEU	2.1
1	A	596	ARG	2.1
1	B	399	MET	2.1
1	A	496	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	573	ASP	2.1
1	B	325	GLY	2.1
1	A	408	PRO	2.1
1	A	494	ARG	2.1
1	A	513	CYS	2.0
1	A	552	HIS	2.0
1	A	491	TYR	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.