



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:42 AM UTC

PDB ID : 7K2D / pdb_00007k2d
Title : Kelch domain of human KEAP1 bound to Nrf2 linear peptide, Ac-GDEETGE-NH2
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.21 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

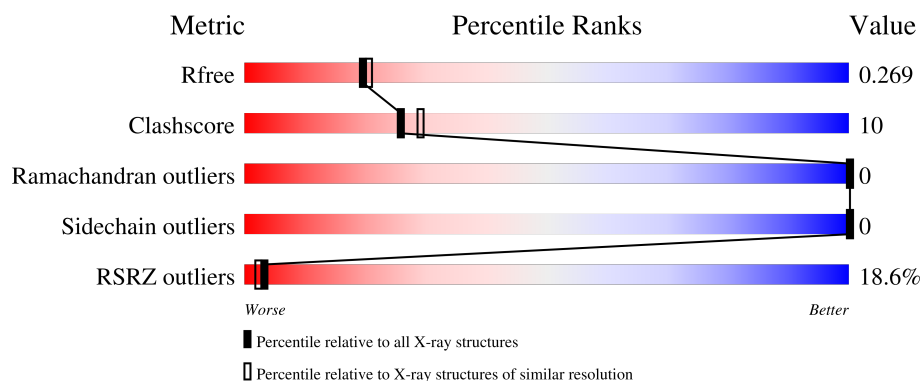
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	82% 12% 6%
1	B	301	35% 71% 22% 7%
2	P	9	78% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4521 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	280	Total	C	N	O	S	0	0	0
			2142	1330	389	408	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	SER	CYS	conflict	UNP Q14145
A	622	SER	CYS	conflict	UNP Q14145
A	624	SER	-	expression tag	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145
B	622	SER	CYS	conflict	UNP Q14145
B	624	SER	-	expression tag	UNP Q14145

- Molecule 2 is a protein called Nrf2 linear peptide, Ace-GDEETGE-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	0	0	1
			54	29	8	17			

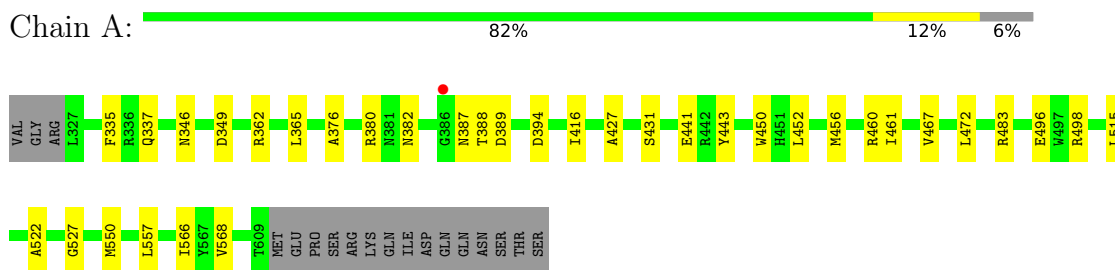
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	35	Total	O	0	0
			35	35		
3	P	2	Total	O	0	0
			2	2		

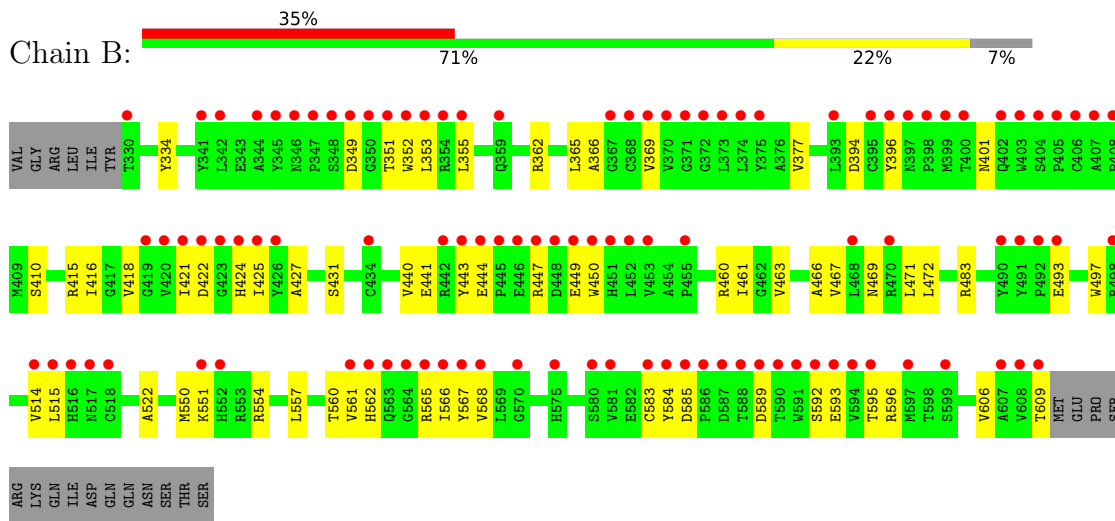
3 Residue-property plots

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.

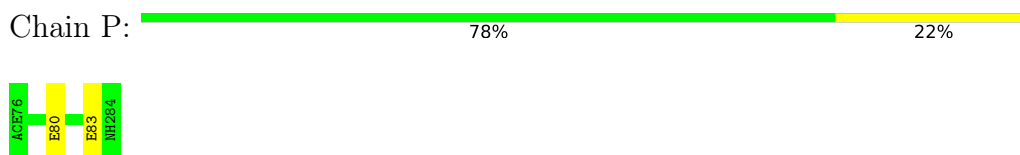
• Molecule 1: Kelch-like ECH-associated protein 1



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



• Molecule 2: Nrf2 linear peptide, Ace-GDEETGE-NH2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 68.85Å 143.91Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	27.47 – 2.21 27.47 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.47-2.21) 98.8 (27.47-2.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.223 , 0.267 0.224 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4521	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: ACE, NH2

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	0.42	0/2223	0.62	2/3029 (0.1%)
1	B	0.30	0/2194	0.56	0/2989
2	P	0.36	0/50	0.50	0/66
All	All	0.36	0/4467	0.59	2/6084 (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	498	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	498	ARG	NE-CZ-NH1	-5.32	116.18	121.50

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	20	0
1	B	2142	0	2029	61	0
2	P	54	0	38	3	0
3	A	118	0	0	2	0
3	B	35	0	0	0	0
3	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4521	0	4127	81	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 10.

All (81) 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:377:VAL:HG11	1:B:418:VAL:HG11	1.53	0.90
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.54	0.89
1:B:415:ARG:NH2	2:P:80:GLU:OE1	2.12	0.82
1:B:444:GLU:OE1	1:B:447:ARG:HD2	1.83	0.76
1:B:561:VAL:HG12	1:B:566:ILE:HG12	1.71	0.73
1:B:425:ILE:HB	1:B:443:TYR:HB3	1.73	0.70
1:B:551:LYS:HZ1	1:B:592:SER:HA	1.58	0.69
1:A:550:MET:HE2	1:A:568:VAL:HG11	1.77	0.67
1:B:425:ILE:HG13	1:B:443:TYR:HD2	1.61	0.65
1:A:496:GLU:OE2	3:A:701:HOH:O	2.14	0.65
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.80	0.64
1:B:550:MET:HE2	1:B:568:VAL:HG21	1.81	0.62
1:B:515:LEU:HB2	1:B:566:ILE:HD11	1.82	0.61
1:A:550:MET:CE	1:A:568:VAL:HG11	2.31	0.59
1:B:349:ASP:OD1	1:B:351:THR:OG1	2.21	0.59
1:B:444:GLU:HG3	1:B:447:ARG:HB2	1.86	0.58
1:B:522:ALA:HB1	1:B:550:MET:HE3	1.85	0.57
1:B:424:HIS:CE1	1:B:444:GLU:HB3	2.39	0.57
1:B:562:HIS:HB3	1:B:567:TYR:CE2	2.40	0.57
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.86	0.57
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.89	0.55
1:A:382:ASN:HA	1:A:387:ASN:HD22	1.72	0.55
1:B:362:ARG:HG3	1:B:365:LEU:HD13	1.89	0.55
1:B:444:GLU:OE1	1:B:447:ARG:CD	2.55	0.53
1:B:565:ARG:CG	1:B:583:CYS:SG	2.97	0.53
1:B:355:LEU:HD23	1:B:396:TYR:OH	2.08	0.53
1:B:377:VAL:CG1	1:B:418:VAL:HG11	2.32	0.52
1:B:369:VAL:HG21	1:B:609:THR:HB	1.92	0.52
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.43	0.52
1:B:565:ARG:HG3	1:B:583:CYS:SG	2.50	0.52
1:B:565:ARG:NH1	1:B:585:ASP:HB2	2.25	0.51
3:A:721:HOH:O	1:B:483:ARG:HG3	2.11	0.51
1:A:380:ARG:NH2	1:A:387:ASN:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:HE1	1:B:401:ASN:HD22	1.59	0.51
1:A:346:ASN:CG	1:A:349:ASP:HB2	2.36	0.50
1:B:551:LYS:NZ	1:B:593:GLU:H	2.08	0.50
1:A:388:THR:HG22	1:A:389:ASP:O	2.11	0.49
1:B:353:LEU:HD23	1:B:355:LEU:HD11	1.94	0.49
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.95	0.49
1:B:365:LEU:H	1:B:365:LEU:HD23	1.78	0.48
1:B:550:MET:CE	1:B:568:VAL:HG11	2.43	0.48
1:B:551:LYS:HD2	1:B:593:GLU:HG3	1.96	0.48
1:B:551:LYS:HZ2	1:B:593:GLU:H	1.60	0.48
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.48	0.48
1:B:469:ASN:O	1:B:471:LEU:HD22	2.13	0.48
1:B:334:TYR:CG	2:P:83:GLU:HG2	2.48	0.47
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.97	0.46
1:B:366:ALA:HB1	1:B:418:VAL:HG22	1.97	0.46
1:B:444:GLU:HB2	1:B:447:ARG:NH2	2.30	0.46
1:B:560:THR:HB	1:B:606:VAL:HG12	1.97	0.46
1:A:456:MET:HE1	1:A:460:ARG:HD2	1.97	0.46
1:B:467:VAL:O	1:B:514:VAL:HG21	2.16	0.45
1:A:467:VAL:HG22	1:A:472:LEU:HD12	1.99	0.45
1:A:483:ARG:HD3	1:A:527:GLY:N	2.31	0.45
1:B:595:THR:HG22	1:B:596:ARG:N	2.32	0.45
1:B:443:TYR:HB2	1:B:450:TRP:CD2	2.52	0.44
1:B:554:ARG:HG3	1:B:557:LEU:HD22	1.99	0.44
1:B:443:TYR:HA	1:B:449:GLU:O	2.17	0.44
1:A:441:GLU:HB3	1:A:452:LEU:HD23	2.00	0.44
1:B:421:ILE:HG22	1:B:422:ASP:OD2	2.17	0.44
1:B:421:ILE:O	1:B:424:HIS:HB2	2.18	0.44
1:B:425:ILE:HG13	1:B:443:TYR:CD2	2.47	0.44
1:B:410:SER:OG	1:B:441:GLU:OE2	2.33	0.44
1:A:365:LEU:HD12	1:A:376:ALA:HB1	2.00	0.43
1:A:416:ILE:HD11	1:A:427:ALA:HB1	2.00	0.43
1:B:493:GLU:N	1:B:493:GLU:OE2	2.52	0.43
1:B:584:TYR:OH	1:B:589:ASP:OD2	2.29	0.43
1:B:440:VAL:HG21	1:B:497:TRP:HZ2	1.83	0.43
1:B:444:GLU:OE1	1:B:447:ARG:HB2	2.18	0.43
1:A:362:ARG:NH1	1:A:394:ASP:OD1	2.51	0.43
1:A:557:LEU:HD23	1:A:557:LEU:H	1.84	0.43
1:B:352:TRP:HE1	1:B:595:THR:CG2	2.31	0.42
1:B:352:TRP:HE1	1:B:595:THR:HG21	1.84	0.42
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:H	1:B:557:LEU:HD23	1.85	0.42
1:B:424:HIS:HE1	1:B:444:GLU:HB3	1.83	0.42
1:B:415:ARG:HH22	2:P:80:GLU:CD	2.15	0.41
1:A:443:TYR:HB2	1:A:450:TRP:CD2	2.56	0.41
1:B:431:SER:HB3	1:B:461:ILE:HG21	2.03	0.41
1:A:335:PHE:C	1:A:337:GLN:H	2.29	0.40
1:B:421:ILE:HD13	1:B:421:ILE:HG21	1.89	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%)	271 (96%)	10 (4%)	0	100	100
1	B	278/301 (92%)	265 (95%)	13 (5%)	0	100	100
2	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	566/611 (93%)	542 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	225/247 (91%)	225 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	458/499 (92%)	458 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	469	ASN
1	B	401	ASN
1	B	414	ASN
1	B	424	HIS
1	B	517	ASN
1	B	575	HIS

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%)	-0.22	1 (0%) 88 87	19, 26, 47, 76	0
1	B	280/301 (93%)	1.54	105 (37%) 1 0	23, 49, 92, 116	0
2	P	7/9 (77%)	0.03	0 100 100	33, 34, 47, 50	0
All	All	570/611 (93%)	0.65	106 (18%) 3 2	19, 34, 83, 116	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	ALA	5.4
1	B	423	GLY	5.3
1	B	351	THR	5.2
1	B	424	HIS	5.1
1	B	561	VAL	5.0
1	B	353	LEU	4.8
1	B	352	TRP	4.8
1	B	590	THR	4.7
1	B	399	MET	4.7
1	B	588	THR	4.6
1	B	395	CYS	4.6
1	B	350	GLY	4.4
1	B	346	ASN	4.4
1	B	345	TYR	4.4
1	B	421	ILE	4.4
1	B	373	LEU	4.4
1	B	564	GLY	4.2
1	B	594	VAL	4.2
1	B	609	THR	4.2
1	B	445	PRO	4.0
1	B	591	TRP	4.0
1	B	567	TYR	4.0
1	B	447	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	608	VAL	3.9
1	B	562	HIS	3.8
1	B	425	ILE	3.8
1	B	374	LEU	3.8
1	B	491	TYR	3.7
1	B	347	PRO	3.7
1	B	371	GLY	3.7
1	B	583	CYS	3.6
1	B	349	ASP	3.6
1	B	566	ILE	3.6
1	B	516	HIS	3.6
1	B	369	VAL	3.6
1	B	370	VAL	3.5
1	B	348	SER	3.5
1	B	422	ASP	3.5
1	B	451	HIS	3.5
1	B	359	GLN	3.5
1	B	595	THR	3.4
1	B	581	VAL	3.4
1	B	575	HIS	3.4
1	B	517	ASN	3.4
1	B	398	PRO	3.4
1	B	420	VAL	3.4
1	B	607	ALA	3.4
1	B	515	LEU	3.4
1	B	452	LEU	3.3
1	B	446	GLU	3.3
1	B	585	ASP	3.3
1	B	514	VAL	3.3
1	B	442	ARG	3.2
1	B	400	THR	3.2
1	B	397	ASN	3.2
1	B	355	LEU	3.1
1	B	565	ARG	3.1
1	B	375	TYR	3.1
1	B	453	VAL	3.1
1	B	498	ARG	3.1
1	B	444	GLU	3.1
1	B	396	TYR	3.0
1	B	592	SER	3.0
1	B	563	GLN	3.0
1	B	372	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	552	HIS	2.9
1	B	407	ALA	2.9
1	B	584	TYR	2.9
1	B	586	PRO	2.9
1	B	450	TRP	2.9
1	B	408	PRO	2.8
1	B	342	LEU	2.8
1	B	404	SER	2.8
1	B	443	TYR	2.8
1	B	455	PRO	2.7
1	A	386	GLY	2.7
1	B	367	GLY	2.7
1	B	449	GLU	2.7
1	B	593	GLU	2.7
1	B	580	SER	2.6
1	B	470	ARG	2.6
1	B	419	GLY	2.5
1	B	492	PRO	2.5
1	B	403	TRP	2.5
1	B	490	TYR	2.4
1	B	368	CYS	2.4
1	B	468	LEU	2.4
1	B	330	THR	2.3
1	B	568	VAL	2.3
1	B	597	MET	2.3
1	B	354	ARG	2.2
1	B	493	GLU	2.2
1	B	448	ASP	2.2
1	B	587	ASP	2.2
1	B	405	PRO	2.2
1	B	406	CYS	2.2
1	B	434	CYS	2.2
1	B	341	TYR	2.1
1	B	518	CYS	2.1
1	B	393	LEU	2.1
1	B	589	ASP	2.1
1	B	426	TYR	2.1
1	B	570	GLY	2.1
1	B	599	SER	2.0
1	B	402	GLN	2.0
1	B	551	LYS	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.