Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:27 AM UTC

PDB ID	:	7K2M / pdb_00007k2m
Title	:	Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[GEPETGE]
Authors	:	Muellers, S.N.; Allen, K.N.
Deposited on	:	2020-09-08
Resolution	:	2.02 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:

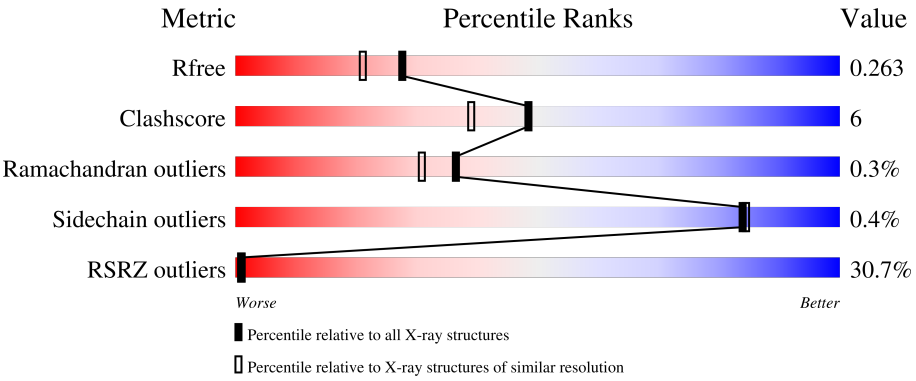
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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 <=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	289	55% 85% 13%
1	B	289	6% 91% 9%
2	P	7	86% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4511 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	B	289	Total	C	N	O	S	0	1	0
			2225	1383	404	421	17			
1	A	284	Total	C	N	O	S	0	1	0
			2101	1313	376	397	15			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Nrf2 cyclic peptide,c[GEPETGE].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			49	28	7	14			

- Molecule 3 is water.

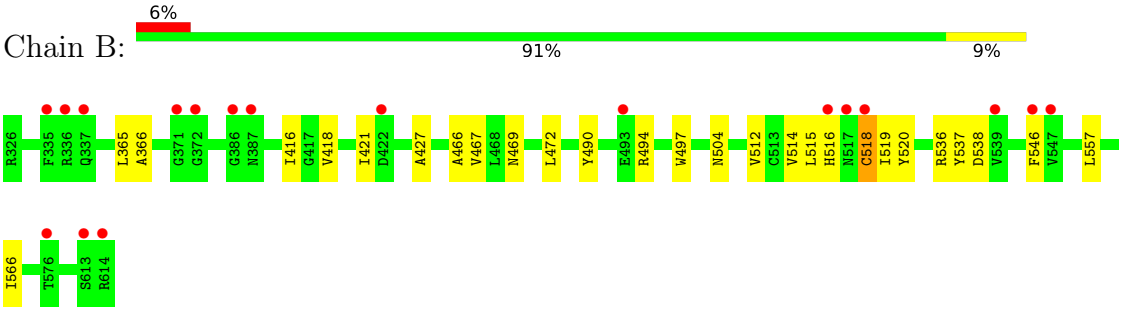
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	110	Total	O	0	0
			110	110		
3	A	25	Total	O	0	0
			25	25		
3	P	1	Total	O	0	0
			1	1		

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.

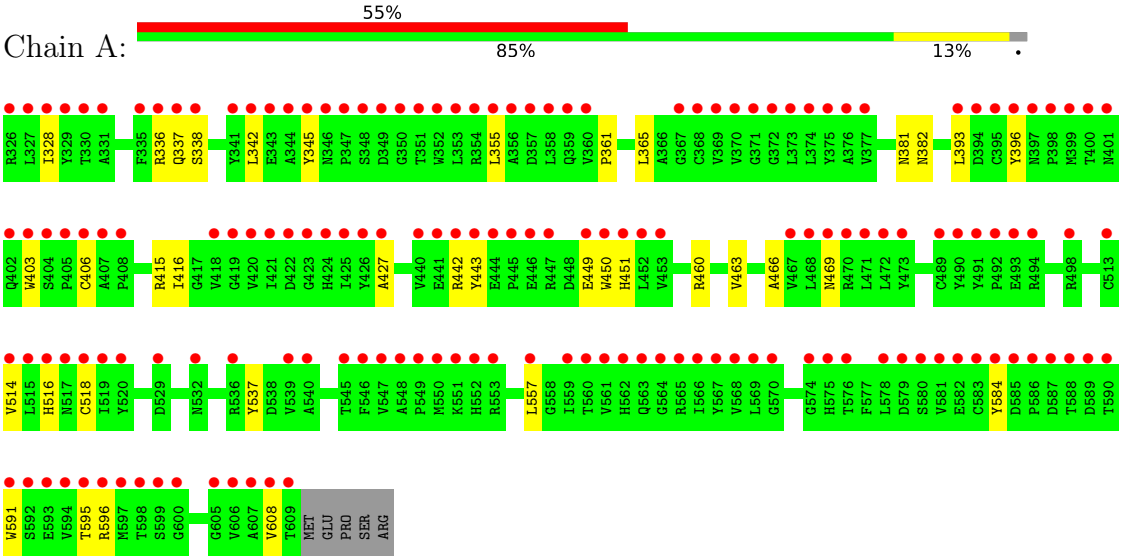
• Molecule 1: Kelch-like ECH-associated protein 1

Chain B:



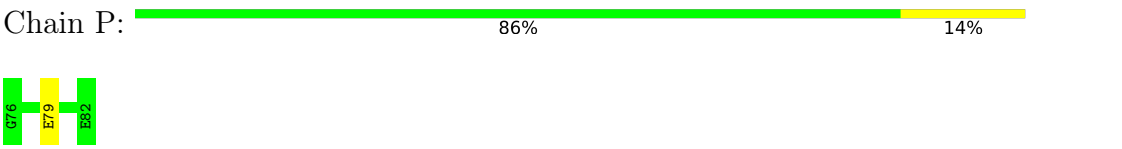
• Molecule 1: Kelch-like ECH-associated protein 1

Chain A:



• Molecule 2: Nrf2 cyclic peptide,c[GEPETGE]

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.76Å 68.86Å 77.39Å 90.00° 117.90° 90.00°	Depositor
Resolution (Å)	29.55 – 2.02 29.55 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.55-2.02) 97.9 (29.55-2.02)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.261 0.238 , 0.263	Depositor DCC
R_{free} test set	1995 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4511	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.18	0/2153	0.51	0/2941
1	B	0.22	0/2282	0.53	0/3107
2	P	0.14	0/49	0.81	0/65
All	All	0.20	0/4484	0.52	0/6113

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2101	0	1960	27	0
1	B	2225	0	2124	22	0
2	P	49	0	37	1	0
3	A	25	0	0	0	0
3	B	110	0	0	0	0
3	P	1	0	0	0	0
All	All	4511	0	4121	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:A:466:ALA:HB1	1:A:514:VAL:HG23	1.51	0.92
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.58	0.83
1:B:518:CYS:SG	1:B:537:TYR:O	2.38	0.81
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.71	0.73
1:A:415:ARG:NH2	2:P:79:GLU:OE2	2.22	0.71
1:A:514:VAL:HG12	1:A:514:VAL:O	2.00	0.61
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.82	0.60
1:B:518:CYS:HG	1:B:537:TYR:C	2.08	0.59
1:B:515:LEU:HB3	1:B:520:TYR:CE1	2.37	0.59
1:A:393:LEU:HD13	1:A:450:TRP:HZ2	1.70	0.57
1:B:518:CYS:HG	1:B:538:ASP:HA	1.70	0.56
1:A:338:SER:OG	1:A:381:ASN:HA	2.05	0.56
1:A:337:GLN:HA	1:A:382:ASN:O	2.05	0.55
1:A:338:SER:HB2	1:A:381:ASN:OD1	2.07	0.55
1:B:515:LEU:HD22	1:B:566:ILE:CG1	2.33	0.54
1:A:518:CYS:HB3	1:A:537:TYR:O	2.08	0.53
1:A:355:LEU:HD23	1:A:396:TYR:OH	2.09	0.53
1:B:518:CYS:SG	1:B:538:ASP:HA	2.49	0.53
1:A:328:ILE:HG12	1:A:608:VAL:HG22	1.90	0.53
1:A:443:TYR:HB2	1:A:450:TRP:CE2	2.46	0.51
1:A:557:LEU:HD23	1:A:557:LEU:H	1.78	0.48
1:A:595:THR:HG22	1:A:596:ARG:H	1.79	0.48
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.96	0.47
1:B:557:LEU:H	1:B:557:LEU:HD23	1.80	0.47
1:B:494:ARG:NH1	1:A:518:CYS:SG	2.88	0.46
1:A:393:LEU:HD23	1:A:406:CYS:HB2	1.98	0.46
1:B:519:ILE:O	1:B:536:ARG:HA	2.16	0.45
1:A:342:LEU:HD22	1:A:403:TRP:CZ2	2.52	0.45
1:A:460:ARG:HB3	1:A:463:VAL:HB	1.99	0.44
1:B:365:LEU:H	1:B:365:LEU:HD23	1.82	0.44
1:A:442:ARG:NH2	1:A:451:HIS:HB2	2.33	0.44
1:B:518:CYS:SG	1:B:537:TYR:C	2.98	0.44
1:B:467:VAL:O	1:B:514:VAL:HG21	2.19	0.43
1:A:345:TYR:CE1	1:A:595:THR:HG21	2.53	0.43
1:A:338:SER:O	1:A:361:PRO:HB3	2.19	0.43
1:B:512:VAL:HA	1:B:520:TYR:O	2.19	0.42
1:A:443:TYR:HB2	1:A:450:TRP:CD2	2.55	0.42
1:B:504:ASN:CB	1:B:546:PHE:CE2	3.02	0.42
1:B:366:ALA:HB1	1:B:418:VAL:HG22	2.01	0.42
1:A:365:LEU:HD23	1:A:365:LEU:H	1.84	0.42
1:A:443:TYR:HA	1:A:449:GLU:O	2.19	0.42
1:A:584:TYR:HB2	1:A:591:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASN:HB2	1:B:546:PHE:CZ	2.55	0.41
1:B:490:TYR:HB2	1:B:497:TRP:CE2	2.56	0.41
1:B:469:ASN:OD1	1:A:469:ASN:ND2	2.54	0.41
1:B:421:ILE:HD11	1:B:472:LEU:HB2	2.03	0.41
1:A:584:TYR:HB2	1:A:591:TRP:CH2	2.55	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	283/289 (98%)	271 (96%)	11 (4%)	1 (0%)	30	22
1	B	288/289 (100%)	276 (96%)	11 (4%)	1 (0%)	36	31
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	576/585 (98%)	552 (96%)	22 (4%)	2 (0%)	36	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	516	HIS
1	A	516	HIS

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	210/234 (90%)	209 (100%)	1 (0%)	81 81
1	B	235/234 (100%)	234 (100%)	1 (0%)	84 84
2	P	5/5 (100%)	5 (100%)	0	100 100
All	All	450/473 (95%)	448 (100%)	2 (0%)	84 84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	518	CYS
1	A	336	ARG

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

Mol	Chain	Res	Type
1	B	337	GLN
1	B	552	HIS
1	A	397	ASN
1	A	451	HIS
1	A	469	ASN
1	A	482	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 (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, 95^{th} 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	284/289 (98%)	2.66	160 (56%) 0 0	25, 57, 103, 126	1 (0%)
1	B	289/289 (100%)	0.27	18 (6%) 26 25	24, 30, 51, 74	1 (0%)
2	P	7/7 (100%)	0.38	0 100 100	37, 39, 40, 43	0
All	All	580/585 (99%)	1.44	178 (30%) 1 1	24, 38, 95, 126	2 (0%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ILE	7.2
1	A	344	ALA	7.2
1	A	353	LEU	7.1
1	A	369	VAL	6.9
1	A	421	ILE	6.8
1	A	518	CYS	6.8
1	A	373	LEU	6.6
1	A	516	HIS	6.6
1	A	590	THR	6.6
1	A	608	VAL	6.5
1	B	518	CYS	6.4
1	A	352	TRP	6.2
1	A	591	TRP	6.2
1	A	327	LEU	6.2
1	A	345	TYR	6.2
1	A	346	ASN	6.2
1	A	329	TYR	6.2
1	A	515	LEU	6.1
1	A	335	PHE	6.1
1	A	347	PRO	6.1
1	A	371	GLY	6.1
1	A	609	THR	6.1
1	A	586	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	581	VAL	5.9
1	A	395	CYS	5.8
1	A	355	LEU	5.8
1	A	349	ASP	5.8
1	A	566	ILE	5.8
1	A	445	PRO	5.8
1	A	338	SER	5.7
1	A	420	VAL	5.7
1	A	594	VAL	5.6
1	A	563	GLN	5.6
1	A	374	LEU	5.5
1	A	596	ARG	5.5
1	A	372	GLY	5.5
1	A	403	TRP	5.4
1	A	584	TYR	5.4
1	A	567	TYR	5.4
1	A	398	PRO	5.3
1	A	356	ALA	5.3
1	A	423	GLY	5.3
1	B	335	PHE	5.3
1	A	351	THR	5.3
1	A	491	TYR	5.3
1	A	348	SER	5.3
1	A	564	GLY	5.3
1	A	517	ASN	5.2
1	A	446	GLU	5.2
1	A	399	MET	5.2
1	A	585	ASP	5.2
1	A	593	GLU	5.2
1	A	595	THR	5.1
1	A	592	SER	5.1
1	A	396	TYR	5.0
1	A	367	GLY	5.0
1	A	375	TYR	5.0
1	A	370	VAL	4.9
1	A	447	ARG	4.8
1	A	562	HIS	4.8
1	A	565	ARG	4.7
1	A	514	VAL	4.6
1	A	425	ILE	4.6
1	A	350	GLY	4.6
1	A	442	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	598	THR	4.5
1	A	342	LEU	4.5
1	A	400	THR	4.5
1	A	561	VAL	4.4
1	A	568	VAL	4.4
1	A	583	CYS	4.4
1	A	580	SER	4.4
1	A	443	TYR	4.4
1	A	444	GLU	4.4
1	A	397	ASN	4.3
1	A	607	ALA	4.3
1	B	517	ASN	4.3
1	A	588	THR	4.2
1	A	368	CYS	4.1
1	A	549	PRO	4.1
1	A	552	HIS	4.1
1	A	407	ALA	4.1
1	A	422	ASP	4.1
1	A	406	CYS	4.1
1	A	419	GLY	4.0
1	A	547	VAL	4.0
1	A	587	ASP	3.9
1	A	493	GLU	3.9
1	A	451	HIS	3.8
1	A	597	MET	3.8
1	A	548	ALA	3.8
1	A	354	ARG	3.6
1	A	401	ASN	3.6
1	A	402	GLN	3.6
1	A	326	ARG	3.5
1	A	600	GLY	3.5
1	A	426	TYR	3.5
1	A	343	GLU	3.5
1	B	516	HIS	3.5
1	A	424	HIS	3.5
1	A	576	THR	3.5
1	A	492	PRO	3.5
1	A	579	ASP	3.4
1	A	468	LEU	3.4
1	B	387	ASN	3.3
1	A	519	ILE	3.3
1	A	337	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	490	TYR	3.3
1	A	453	VAL	3.2
1	B	546	PHE	3.2
1	A	599	SER	3.2
1	A	551	LYS	3.2
1	A	452	LEU	3.2
1	A	546	PHE	3.2
1	A	394	ASP	3.2
1	A	550	MET	3.1
1	A	470	ARG	3.1
1	A	589	ASP	3.1
1	A	336	ARG	3.1
1	A	450	TRP	3.0
1	B	493	GLU	3.0
1	A	498	ARG	3.0
1	A	606	VAL	3.0
1	B	336	ARG	3.0
1	A	605	GLY	3.0
1	A	393	LEU	2.9
1	A	408	PRO	2.9
1	A	520	TYR	2.9
1	A	582	GLU	2.9
1	A	404	SER	2.9
1	A	575	HIS	2.9
1	A	569	LEU	2.8
1	A	471	LEU	2.8
1	A	560	THR	2.8
1	A	330	THR	2.8
1	A	360	VAL	2.7
1	B	337	GLN	2.7
1	A	559	ILE	2.6
1	A	376	ALA	2.6
1	A	540	ALA	2.6
1	A	578	LEU	2.6
1	A	570	GLY	2.6
1	A	536	ARG	2.6
1	B	547	VAL	2.5
1	A	341	TYR	2.5
1	A	358	LEU	2.5
1	B	371	GLY	2.5
1	A	469	ASN	2.5
1	A	449	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	CYS	2.4
1	A	467	VAL	2.4
1	A	539	VAL	2.4
1	B	614	ARG	2.4
1	A	331	ALA	2.3
1	A	418	VAL	2.3
1	B	386	GLY	2.3
1	A	553	ARG	2.3
1	A	427	ALA	2.3
1	B	372	GLY	2.3
1	A	405	PRO	2.2
1	A	357	ASP	2.2
1	A	574	GLY	2.2
1	A	472	LEU	2.2
1	A	545	THR	2.2
1	A	489	CYS	2.2
1	B	613	SER	2.2
1	A	377	VAL	2.1
1	A	440	VAL	2.1
1	A	441	GLU	2.1
1	A	359	GLN	2.1
1	B	539	VAL	2.1
1	B	422	ASP	2.1
1	A	494	ARG	2.1
1	B	576	THR	2.0
1	A	473	TYR	2.0
1	A	532	ASN	2.0
1	A	557	LEU	2.0
1	A	529	ASP	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.