



# Full wwPDB X-ray Structure Validation Report i

Nov 5, 2023 – 08:54 PM EST

PDB ID : 7K2O  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

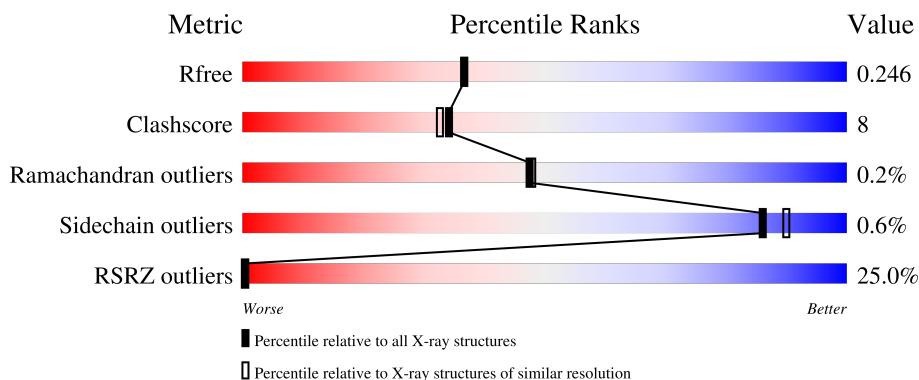
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

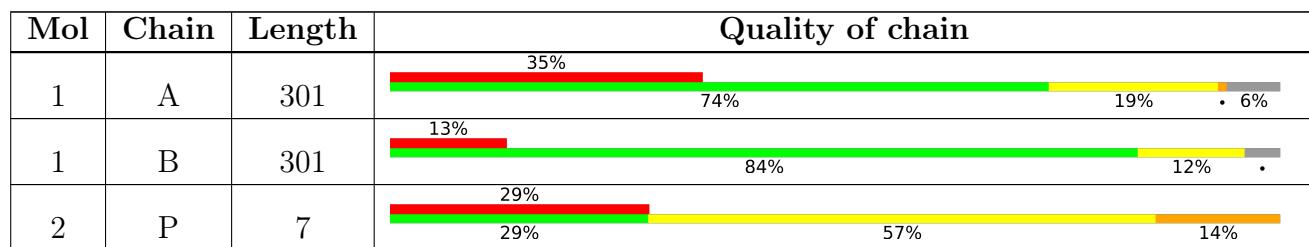
The reported resolution of this entry is 2.11 Å.

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))
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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  $\geq 3$ , 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.



## 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			

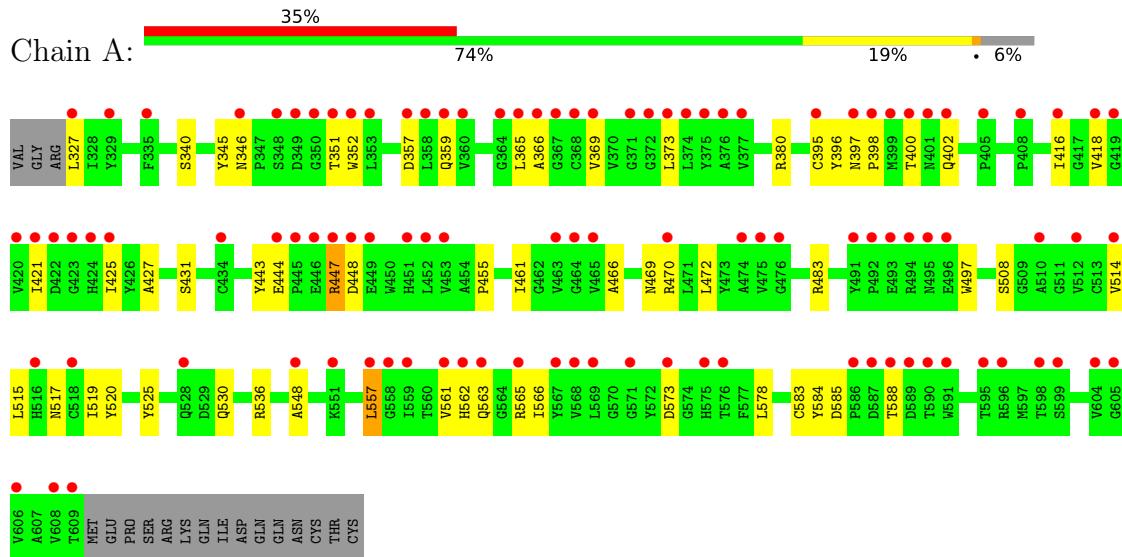
- Molecule 3 is water.

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		

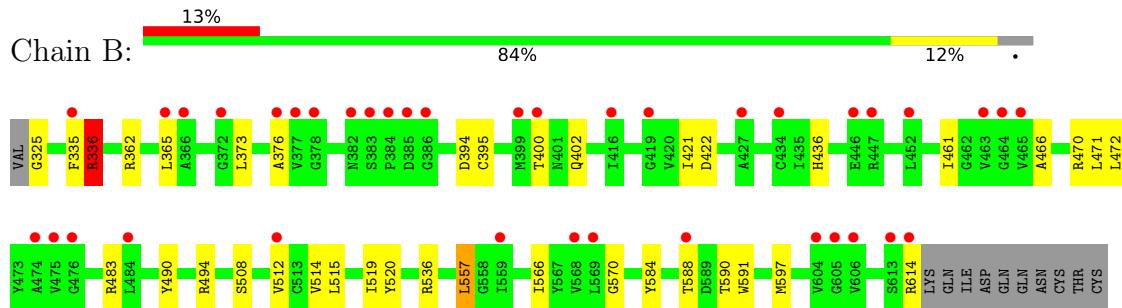
### 3 Residue-property plots [\(i\)](#)

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: (ABU)DPETGE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.3 (29.33-2.11)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.79 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R$ , $R_{free}$	0.208 , 0.246 0.208 , 0.246	Depositor DCC
$R_{free}$ test set	2004 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.5	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [\(i\)](#)

### 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	0.41	0/2223	0.63	0/3029
1	B	0.47	1/2286 (0.0%)	0.71	4/3112 (0.1%)
2	P	1.00	0/45	2.01	2/61 (3.3%)
All	All	0.45	1/4554 (0.0%)	0.70	6/6202 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	ARG	CB-CG	-6.19	1.35	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ARG	NE-CZ-NH2	-12.54	114.03	120.30
2	P	76	ABU	O-C-N	-11.15	104.85	122.70
2	P	76	ABU	C-N-CA	9.13	144.53	121.70
1	B	336	ARG	NH1-CZ-NH2	6.43	126.48	119.40
1	B	336	ARG	CB-CG-CD	-6.25	95.34	111.60
1	B	336	ARG	CG-CD-NE	-5.39	100.47	111.80

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	31	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	73	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 8.

All (73) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:471:LEU:HD12	1:B:471:LEU:N	2.30	0.47
1:A:517:ASN:CG	1:B:471:LEU:HD11	2.35	0.46
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: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:B:570:GLY:N	1:B:597:MET:HE1	2.33	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:470:ARG:C	1:B:471:LEU:HD12	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41 40
2	P	5/7 (71%)	5 (100%)	0	0	100 100
All	All	575/609 (94%)	551 (96%)	23 (4%)	1 (0%)	47 48

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%)	226 (99%)	2 (1%)	78	83
1	B	235/247 (95%)	234 (100%)	1 (0%)	91	94
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	468/499 (94%)	465 (99%)	3 (1%)	86	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	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	562	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 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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	283/301 (94%)	1.72	105 (37%) 0   0	30, 64, 117, 157	0
1	B	290/301 (96%)	0.82	38 (13%) 3   4	28, 39, 65, 103	0
2	P	6/7 (85%)	1.11	2 (33%) 0   0	40, 48, 52, 69	0
All	All	579/609 (95%)	1.26	145 (25%) 0   0	28, 47, 109, 157	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	GLN	8.2
1	A	353	LEU	7.7
1	A	400	THR	7.6
1	A	349	ASP	6.9
1	B	385	ASP	6.8
1	A	548	ALA	6.0
1	A	397	ASN	5.5
1	A	447	ARG	5.5
1	A	452	LEU	5.3
1	A	399	MET	5.3
1	A	588	THR	5.0
1	A	559	ILE	5.0
1	A	348	SER	5.0
1	A	516	HIS	5.0
1	A	371	GLY	5.0
1	A	351	THR	4.8
1	A	604	VAL	4.7
1	A	423	GLY	4.7
1	A	608	VAL	4.7
1	A	470	ARG	4.7
1	A	576	THR	4.6
1	A	329	TYR	4.5
1	A	563	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	346	ASN	4.3
1	A	557	LEU	4.3
1	A	365	LEU	4.3
1	A	352	TRP	4.2
1	A	408	PRO	4.2
1	B	365	LEU	4.2
1	A	421	ILE	4.1
1	A	451	HIS	4.1
1	A	359	GLN	4.0
1	A	416	ILE	4.0
1	A	561	VAL	4.0
1	A	350	GLY	4.0
1	B	366	ALA	4.0
1	A	401	ASN	3.9
1	A	575	HIS	3.9
1	B	416	ILE	3.9
1	B	613	SER	3.9
1	B	614	ARG	3.9
1	A	562	HIS	3.8
1	A	569	LEU	3.8
1	A	494	ARG	3.7
1	A	327	LEU	3.7
1	A	512	VAL	3.7
1	B	465	VAL	3.7
1	A	425	ILE	3.6
1	B	399	MET	3.6
1	A	373	LEU	3.6
1	B	512	VAL	3.6
1	A	567	TYR	3.6
1	A	446	GLU	3.6
1	B	447	ARG	3.6
1	A	598	THR	3.5
1	B	386	GLY	3.5
1	A	377	VAL	3.5
1	A	367	GLY	3.5
1	A	368	CYS	3.5
1	A	418	VAL	3.4
1	B	606	VAL	3.4
1	A	398	PRO	3.2
1	A	606	VAL	3.2
1	A	590	THR	3.2
1	A	463	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	377	VAL	3.2
1	A	374	LEU	3.2
1	A	605	GLY	3.1
1	B	434	CYS	3.0
1	A	589	ASP	3.0
1	B	604	VAL	3.0
1	A	491	TYR	3.0
1	B	605	GLY	3.0
1	B	384	PRO	3.0
1	B	383	SER	2.9
1	B	335	PHE	2.9
1	A	493	GLU	2.9
1	A	453	VAL	2.9
1	B	588	THR	2.9
1	A	492	PRO	2.9
1	A	420	VAL	2.9
1	A	495	ASN	2.9
1	B	463	VAL	2.8
1	B	464	GLY	2.8
1	A	518	CYS	2.8
1	A	558	GLY	2.8
1	A	551	LYS	2.7
1	A	395	CYS	2.7
1	A	358	LEU	2.7
1	A	422	ASP	2.7
1	A	419	GLY	2.7
1	A	366	ALA	2.7
1	A	335	PHE	2.6
1	A	514	VAL	2.5
1	A	510	ALA	2.5
1	A	599	SER	2.5
1	A	372	GLY	2.5
1	A	448	ASP	2.5
1	B	372	GLY	2.5
1	A	609	THR	2.5
1	A	465	VAL	2.5
1	A	595	THR	2.5
1	A	360	VAL	2.5
1	B	378	GLY	2.4
1	A	449	GLU	2.4
1	B	484	LEU	2.4
1	B	569	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	568	VAL	2.4
1	A	375	TYR	2.4
1	A	405	PRO	2.4
1	A	475	VAL	2.4
1	A	424	HIS	2.4
1	A	586	PRO	2.4
1	A	464	GLY	2.4
1	A	528	GLN	2.3
1	A	474	ALA	2.3
1	A	587	ASP	2.3
1	B	475	VAL	2.3
1	A	573	ASP	2.3
1	A	376	ALA	2.3
1	B	476	GLY	2.3
1	A	445	PRO	2.3
1	A	565	ARG	2.3
1	B	419	GLY	2.2
1	A	496	GLU	2.2
1	B	559	ILE	2.2
2	P	77	ASP	2.2
1	A	444	GLU	2.2
1	A	434	CYS	2.2
1	A	476	GLY	2.2
1	B	474	ALA	2.2
1	B	400	THR	2.2
2	P	78	PRO	2.2
1	B	446	GLU	2.1
1	A	364	GLY	2.1
1	B	427	ALA	2.1
1	B	382	ASN	2.1
1	A	568	VAL	2.0
1	B	452	LEU	2.0
1	B	376	ALA	2.0
1	A	369	VAL	2.0
1	A	357	ASP	2.0
1	A	591	TRP	2.0
1	A	596	ARG	2.0
1	A	571	GLY	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 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.