Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:57 am BST

PDB ID	:	2GOP
Title	:	The beta-propeller domain of the Trilobed protease from Pyrococcus furiosus reveals an open velcro topology
Authors	:	Bosch, J.; Tamura, T.; Tamura, N.; Baumeister, W.; Essen, L.-O.
Deposited on	:	2006-04-13
Resolution	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

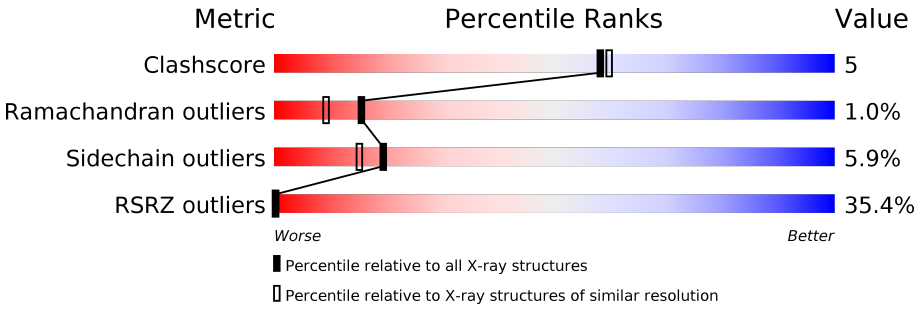
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	347	30% 81% 9% • 8%
1	B	347	34% 73% 13% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5479 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 Trilobed Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	6	0
			2708	1757	444	500	7			
1	B	304	Total	C	N	O	S	8	1	0
			2529	1635	414	474	6			

- Molecule 2 is water.

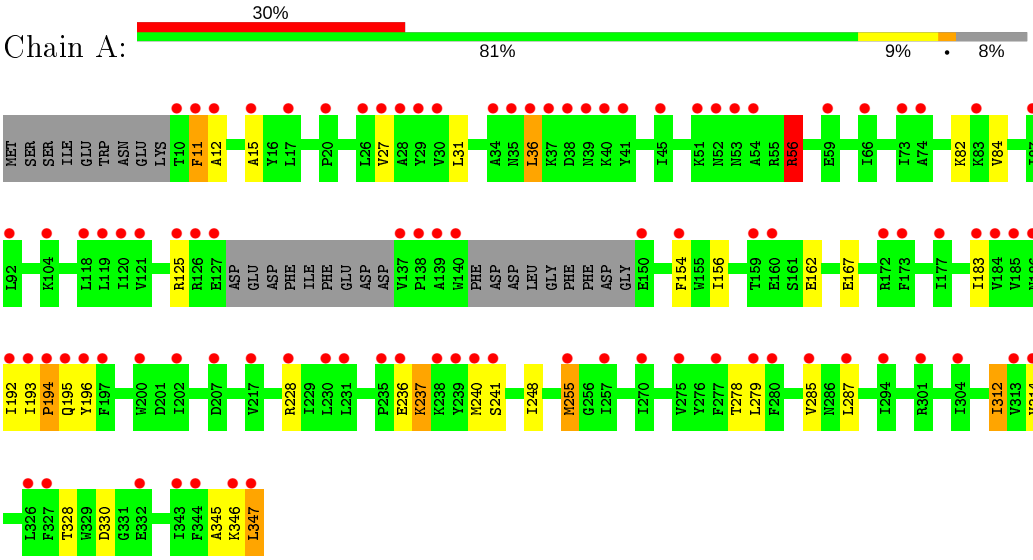
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	156	Total	O	0	0
			156	156		
2	B	86	Total	O	0	0
			86	86		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

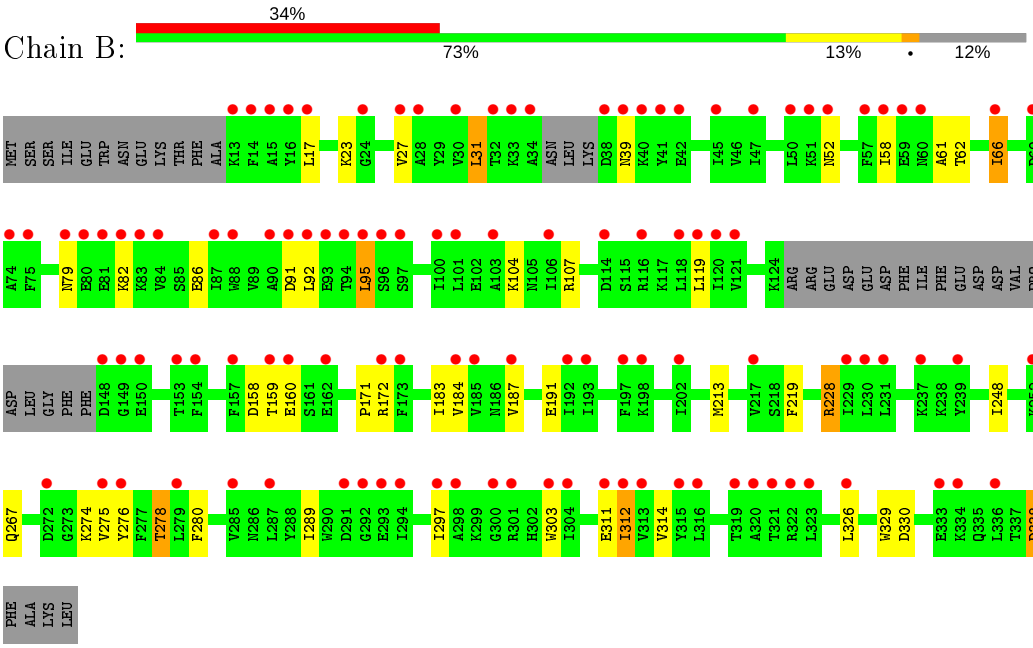
- Molecule 1: Trilobed Protease

Chain A:



- Molecule 1: Trilobed Protease

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.75Å 88.50Å 153.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.72 – 2.00 18.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (18.72-2.00) 80.2 (18.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.258 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5479	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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	0.44	0/2789	0.65	2/3755 (0.1%)
1	B	0.57	4/2589 (0.2%)	0.58	3/3484 (0.1%)
All	All	0.51	4/5378 (0.1%)	0.61	5/7239 (0.1%)

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	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	PRO	C-N	-14.56	1.00	1.34
1	B	326	LEU	CA-CB	-11.76	1.26	1.53
1	B	338	ASP	CA-CB	-11.71	1.28	1.53
1	B	172	ARG	C-N	7.27	1.50	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	338	ASP	N-CA-CB	7.14	123.45	110.60
1	B	342	PRO	N-CA-CB	6.28	110.84	103.30
1	B	338	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	56	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TYR	Peptide
1	A	240	MET	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	2708	0	2704	28	0
1	B	2529	0	2489	24	0
2	A	156	0	0	1	0
2	B	86	0	0	0	0
All	All	5479	0	5193	50	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 5.

All (50) 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:156:ILE:HD11	1:A:183:ILE:HD11	1.53	0.89
1:A:314[B]:VAL:HG22	1:A:328:THR:HG22	1.57	0.87
1:B:267:GLN:H	1:B:278:THR:HG22	1.51	0.76
1:A:193:ILE:HG22	1:A:193:ILE:O	1.85	0.75
1:A:15:ALA:HB1	1:A:31:LEU:HD11	1.74	0.69
1:B:276:TYR:CE2	1:B:289:ILE:HD13	2.30	0.67
1:A:156:ILE:HD11	1:A:183:ILE:CD1	2.24	0.65
1:B:23:LYS:HB2	1:B:66:ILE:HD11	1.81	0.64
1:A:56:ARG:HH11	1:A:56:ARG:HG3	1.62	0.63
1:A:312:ILE:HD11	1:A:330:ASP:HB3	1.81	0.61
1:B:17:LEU:HD21	1:B:31:LEU:HD22	1.84	0.60
1:B:27:VAL:HG21	1:B:314:VAL:HG21	1.85	0.58
1:B:274:LYS:HB3	1:B:289:ILE:HD11	1.85	0.57
1:A:236:GLU:O	1:A:237:LYS:HG2	2.05	0.56
1:B:184:VAL:HG13	1:B:213:MET:HE3	1.87	0.56
1:B:119:LEU:HD22	1:B:183:ILE:HD12	1.88	0.55
1:A:241:SER:HB3	1:B:280:PHE:CE1	2.40	0.55
1:A:15:ALA:HB1	1:A:31:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278[B]:THR:HG23	1:A:285:VAL:HG13	1.91	0.53
1:B:17:LEU:CD2	1:B:31:LEU:HD22	2.39	0.53
1:B:70:GLY:O	1:B:92:LEU:HD12	2.10	0.52
1:A:36:LEU:H	1:A:36:LEU:HD23	1.76	0.51
1:A:278[B]:THR:CG2	1:A:285:VAL:CG1	2.89	0.51
1:A:278[B]:THR:HG23	1:A:285:VAL:CG1	2.40	0.51
1:A:345:ALA:O	1:A:347:LEU:HD22	2.11	0.50
1:A:278[B]:THR:CG2	1:A:285:VAL:HG13	2.43	0.48
1:B:91:ASP:O	1:B:95:LEU:HA	2.13	0.48
1:A:193:ILE:O	1:A:194:PRO:O	2.32	0.48
1:A:241:SER:HB3	1:B:280:PHE:CD1	2.48	0.48
1:B:27:VAL:CG2	1:B:314:VAL:HG21	2.45	0.47
1:A:156:ILE:CD1	1:A:183:ILE:HD11	2.36	0.46
1:B:276:TYR:CD2	1:B:289:ILE:HD13	2.50	0.46
1:B:158:ASP:OD1	1:B:160:GLU:N	2.48	0.45
1:A:193:ILE:O	1:A:193:ILE:CG2	2.57	0.45
1:A:255[B]:MET:HE3	2:A:459:HOH:O	2.16	0.45
1:B:23:LYS:HB2	1:B:66:ILE:CD1	2.47	0.44
1:B:79:ASN:HD22	1:B:86:GLU:CD	2.20	0.44
1:B:184:VAL:HG13	1:B:213:MET:CE	2.48	0.44
1:A:190:ARG:O	1:A:191:GLU:O	2.35	0.44
1:A:56:ARG:CG	1:A:56:ARG:HH11	2.28	0.43
1:B:267:GLN:N	1:B:278:THR:HG22	2.28	0.43
1:B:58:ILE:HG22	1:B:61:ALA:HB2	2.01	0.43
1:B:297:ILE:HG23	1:B:329:TRP:CD2	2.54	0.43
1:B:228:ARG:HB3	1:B:248:ILE:HG23	2.00	0.43
1:A:27:VAL:HG12	1:A:314[B]:VAL:HG21	2.01	0.42
1:A:154:PHE:O	1:A:167:GLU:HA	2.18	0.42
1:B:312:ILE:HD11	1:B:330:ASP:HB3	2.03	0.41
1:A:82:LYS:HB3	1:A:84:VAL:HG22	2.03	0.40
1:A:192:ILE:HG22	1:A:192:ILE:O	2.22	0.40
1:A:228[A]:ARG:HD3	1:A:248:ILE:HG21	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	320/347 (92%)	298 (93%)	18 (6%)	4 (1%)	12 6
1	B	299/347 (86%)	281 (94%)	16 (5%)	2 (1%)	22 16
All	All	619/694 (89%)	579 (94%)	34 (6%)	6 (1%)	15 9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLU
1	A	194	PRO
1	A	12	ALA
1	B	52	ASN
1	A	11	PHE
1	B	39	ASN

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	293/312 (94%)	279 (95%)	14 (5%)	25 22
1	B	270/312 (86%)	249 (92%)	21 (8%)	12 8
All	All	563/624 (90%)	528 (94%)	35 (6%)	19 13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	36	LEU
1	A	56	ARG
1	A	125	ARG
1	A	162	GLU
1	A	195	GLN

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Mol	Chain	Res	Type
1	A	237	LYS
1	A	255[A]	MET
1	A	255[B]	MET
1	A	279	LEU
1	A	287	LEU
1	A	312	ILE
1	A	346	LYS
1	A	347	LEU
1	B	31	LEU
1	B	62	THR
1	B	66	ILE
1	B	82	LYS
1	B	95	LEU
1	B	104	LYS
1	B	107	ARG
1	B	159	THR
1	B	187	VAL
1	B	191	GLU
1	B	219	PHE
1	B	228	ARG
1	B	253	GLU
1	B	255	MET
1	B	275	VAL
1	B	278	THR
1	B	303	TRP
1	B	311[A]	GLU
1	B	311[B]	GLU
1	B	312	ILE
1	B	338	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	171:PRO	C	172:ARG	N	1.00

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	320/347 (92%)	1.70	103 (32%)	0	0	32, 44, 71, 101	0
1	B	304/347 (87%)	1.97	118 (38%)	0	0	20, 62, 86, 97	2 (0%)
All	All	624/694 (89%)	1.83	221 (35%)	0	0	20, 50, 83, 101	2 (0%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	PHE	12.7
1	A	192	ILE	11.6
1	A	10	THR	10.1
1	A	196	TYR	10.1
1	B	149	GLY	9.6
1	A	197	PHE	8.3
1	B	173	PHE	7.7
1	B	39	ASN	7.4
1	A	193	ILE	7.3
1	B	192	ILE	7.0
1	A	137	VAL	7.0
1	B	320	ALA	6.6
1	B	92	LEU	6.6
1	A	126	ARG	6.5
1	A	235	PRO	6.3
1	B	15	ALA	6.3
1	A	150	GLU	6.3
1	B	321	THR	6.1
1	A	191	GLU	5.9
1	A	347	LEU	5.9
1	B	254	VAL	5.8
1	B	97	SER	5.6
1	B	34	ALA	5.5
1	B	93	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	41	TYR	5.4
1	B	303	TRP	5.3
1	A	51	LYS	5.2
1	A	190	ARG	5.1
1	A	37	LYS	5.1
1	B	59	GLU	5.1
1	B	14	PHE	4.8
1	A	195	GLN	4.7
1	B	322	ARG	4.6
1	A	194	PRO	4.6
1	B	52	ASN	4.6
1	B	339	TYR	4.5
1	B	287	LEU	4.5
1	B	275	VAL	4.5
1	A	127	GLU	4.5
1	A	236	GLU	4.5
1	B	81	GLU	4.4
1	B	311[A]	GLU	4.4
1	A	240	MET	4.3
1	B	185	VAL	4.3
1	B	312	ILE	4.3
1	B	57	PHE	4.2
1	A	39	ASN	4.2
1	B	47	ILE	4.2
1	A	239	TYR	4.2
1	B	66	ILE	4.1
1	B	150	GLU	4.1
1	B	148	ASP	4.1
1	A	316	LEU	4.1
1	B	83	LYS	4.1
1	B	88	TRP	4.1
1	A	202	ILE	4.0
1	A	343	ILE	4.0
1	B	160	GLU	4.0
1	B	69	ASP	4.0
1	A	314[A]	VAL	4.0
1	A	304	ILE	4.0
1	B	73	ILE	4.0
1	B	202	ILE	3.9
1	B	17	LEU	3.9
1	B	231	LEU	3.9
1	A	125	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	3.8
1	A	346	LYS	3.8
1	A	187	VAL	3.8
1	A	17	LEU	3.7
1	A	139	ALA	3.7
1	B	298	ALA	3.7
1	A	185	VAL	3.7
1	B	87	ILE	3.7
1	A	118	LEU	3.6
1	B	184	VAL	3.6
1	B	16	TYR	3.6
1	B	38	ASP	3.6
1	B	72	LYS	3.6
1	A	38	ASP	3.6
1	A	173	PHE	3.5
1	B	96	SER	3.5
1	B	95	LEU	3.4
1	B	51	LYS	3.4
1	A	54	ALA	3.4
1	B	13	LYS	3.4
1	B	293	GLU	3.4
1	B	80	GLU	3.3
1	B	239	TYR	3.3
1	A	74	ALA	3.3
1	A	36	LEU	3.3
1	B	255	MET	3.3
1	B	323	LEU	3.3
1	A	140	TRP	3.3
1	B	300	GLY	3.3
1	A	28	ALA	3.3
1	B	172	ARG	3.2
1	B	50	LEU	3.2
1	B	193	ILE	3.2
1	A	238	LYS	3.2
1	A	270	ILE	3.2
1	B	279	LEU	3.2
1	B	276	TYR	3.2
1	B	316	LEU	3.2
1	B	315	TYR	3.2
1	B	24	GLY	3.1
1	A	200	TRP	3.1
1	B	198	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	3.1
1	B	40	LYS	3.1
1	A	119	LEU	3.1
1	B	304	ILE	3.0
1	B	272	ASP	3.0
1	A	332	GLU	3.0
1	A	52	ASN	3.0
1	A	66	ILE	2.9
1	B	187	VAL	2.9
1	B	103	ALA	2.9
1	B	297	ILE	2.9
1	B	162	GLU	2.9
1	A	30	VAL	2.9
1	B	101	LEU	2.9
1	B	230	LEU	2.9
1	A	277	PHE	2.8
1	B	60	ASN	2.8
1	B	94	THR	2.8
1	B	229	ILE	2.8
1	A	326	LEU	2.8
1	B	336	LEU	2.8
1	A	73	ILE	2.8
1	A	183	ILE	2.8
1	A	217	VAL	2.8
1	B	74	ALA	2.8
1	A	26	LEU	2.8
1	A	285	VAL	2.8
1	B	106	ILE	2.8
1	A	172	ARG	2.8
1	A	255[A]	MET	2.7
1	A	83	LYS	2.7
1	A	160	GLU	2.7
1	B	319	THR	2.7
1	A	184	VAL	2.7
1	A	15	ALA	2.7
1	B	79	ASN	2.7
1	B	121	VAL	2.6
1	B	237	LYS	2.6
1	A	344	PHE	2.6
1	A	287	LEU	2.6
1	B	90	ALA	2.6
1	A	53	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	27	VAL	2.6
1	A	275	VAL	2.6
1	B	32	THR	2.5
1	A	88	TRP	2.5
1	A	313	VAL	2.5
1	A	29	TYR	2.5
1	B	84	VAL	2.4
1	B	42	GLU	2.4
1	A	87	ILE	2.4
1	B	153	THR	2.4
1	A	186	ASN	2.4
1	B	120	ILE	2.4
1	A	207	ASP	2.4
1	B	253	GLU	2.4
1	B	116	ARG	2.4
1	A	230	LEU	2.4
1	B	301	ARG	2.3
1	A	120	ILE	2.3
1	A	294	ILE	2.3
1	B	294	ILE	2.3
1	A	228[A]	ARG	2.3
1	B	45	ILE	2.3
1	A	41	TYR	2.3
1	B	75	PHE	2.3
1	B	119	LEU	2.3
1	B	82	LYS	2.3
1	B	114	ASP	2.3
1	A	321	THR	2.3
1	B	91	ASP	2.3
1	A	138	PRO	2.3
1	B	100	ILE	2.3
1	A	279	LEU	2.3
1	A	154	PHE	2.3
1	A	327	PHE	2.3
1	A	301	ARG	2.3
1	A	257	ILE	2.3
1	A	34	ALA	2.2
1	B	157	PHE	2.2
1	B	30	VAL	2.2
1	B	285	VAL	2.2
1	A	59	GLU	2.2
1	A	40	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	2.2
1	A	35	ASN	2.2
1	A	241	SER	2.2
1	B	33	LYS	2.2
1	B	252	LYS	2.2
1	A	45	ILE	2.2
1	B	118	LEU	2.2
1	B	334	LYS	2.2
1	B	197	PHE	2.2
1	A	159	THR	2.2
1	A	20	PRO	2.2
1	B	326	LEU	2.1
1	B	313	VAL	2.1
1	A	92	LEU	2.1
1	A	121	VAL	2.1
1	B	292	GLY	2.1
1	B	333	GLU	2.1
1	A	177	ILE	2.1
1	B	159	THR	2.1
1	B	58	ILE	2.1
1	A	27	VAL	2.1
1	B	217	VAL	2.1
1	A	90	ALA	2.1
1	B	28	ALA	2.1
1	B	154	PHE	2.1
1	A	315	TYR	2.1
1	B	291	ASP	2.0
1	A	280	PHE	2.0
1	A	104	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 carbohydrates 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.