



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 4JEP / pdb_00004jep
Title : Crystal structure of Toxoplasma gondii nucleoside triphosphate diphosphohydrolase 1 (NTPDase1)
Authors : Krug, U.; Totzauer, R.; Strater, N.
Deposited on : 2013-02-27
Resolution : 3.10 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

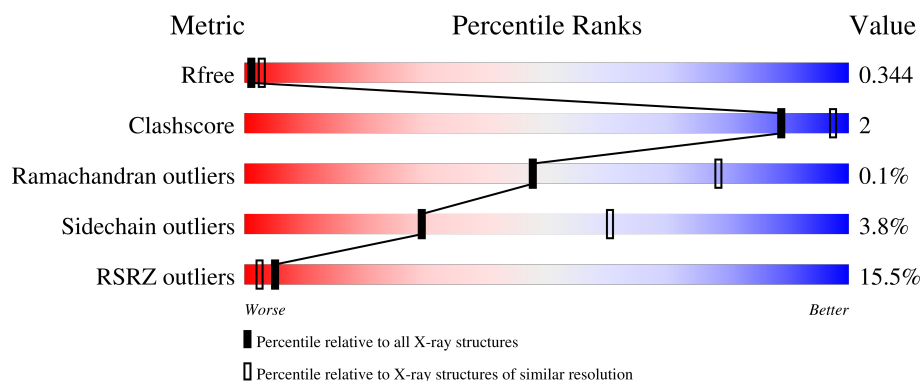
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	611	13% 85% 8% 6%
1	B	611	16% 82% 8% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8772 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 Nucleoside-triphosphatase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4471	2805	789	853	24			
1	B	552	Total	C	N	O	S	0	0	0
			4301	2703	756	816	26			

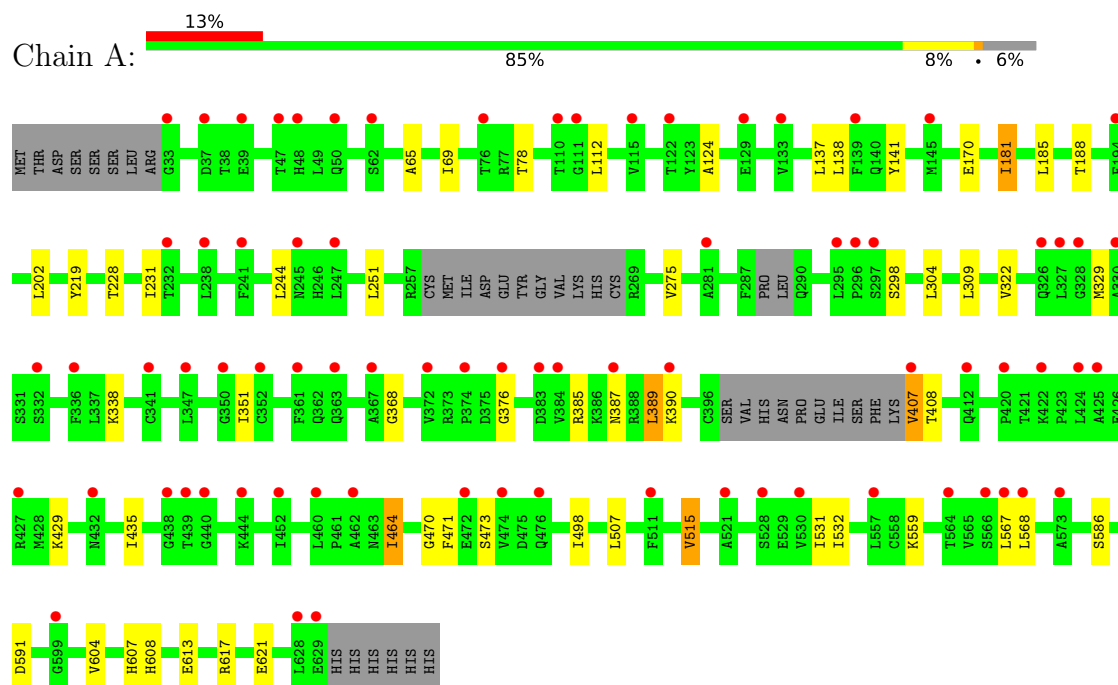
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP Q27895
A	629	GLU	-	expression tag	UNP Q27895
A	630	HIS	-	expression tag	UNP Q27895
A	631	HIS	-	expression tag	UNP Q27895
A	632	HIS	-	expression tag	UNP Q27895
A	633	HIS	-	expression tag	UNP Q27895
A	634	HIS	-	expression tag	UNP Q27895
A	635	HIS	-	expression tag	UNP Q27895
B	25	MET	-	expression tag	UNP Q27895
B	629	GLU	-	expression tag	UNP Q27895
B	630	HIS	-	expression tag	UNP Q27895
B	631	HIS	-	expression tag	UNP Q27895
B	632	HIS	-	expression tag	UNP Q27895
B	633	HIS	-	expression tag	UNP Q27895
B	634	HIS	-	expression tag	UNP Q27895
B	635	HIS	-	expression tag	UNP Q27895

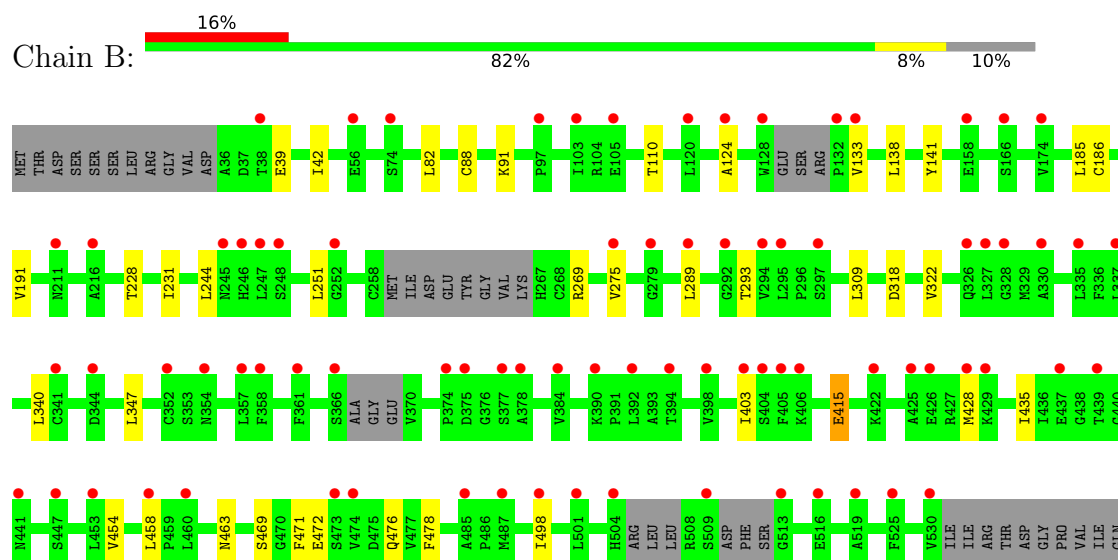
3 Residue-property plots

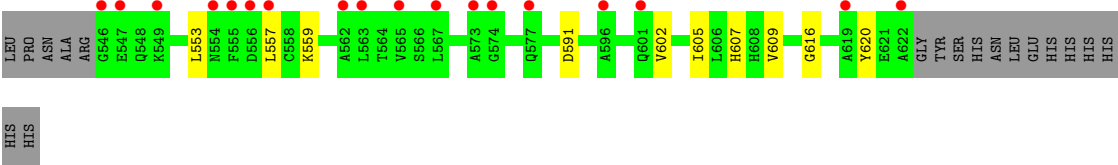
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoside-triphosphatase 2



• Molecule 1: Nucleoside-triphosphatase 2





HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 161.52Å 236.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.31 – 3.10 36.31 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.31-3.10) 99.6 (36.31-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.270 , 0.305 0.303 , 0.344	Depositor DCC
R_{free} test set	1306 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	8772	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 ⓘ

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	0.70	0/4554	1.28	8/6161 (0.1%)
1	B	0.71	0/4381	1.29	6/5922 (0.1%)
All	All	0.71	0/8935	1.29	14/12083 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ILE	N-CA-C	6.66	114.14	107.55
1	B	454	VAL	N-CA-C	5.81	115.94	110.30
1	A	608	HIS	CA-C-N	5.49	127.47	120.56
1	A	608	HIS	C-N-CA	5.49	127.47	120.56
1	B	478	PHE	N-CA-C	5.24	117.89	111.82
1	A	141	TYR	CA-C-N	5.22	124.50	120.33
1	A	141	TYR	C-N-CA	5.22	124.50	120.33
1	A	170	GLU	N-CA-C	5.18	116.92	111.28
1	B	141	TYR	CA-C-N	5.16	124.45	120.33
1	B	141	TYR	C-N-CA	5.16	124.45	120.33
1	A	473	SER	CA-C-N	5.15	127.78	120.53
1	A	473	SER	C-N-CA	5.15	127.78	120.53
1	B	191	VAL	CA-C-N	5.11	128.10	120.90
1	B	191	VAL	C-N-CA	5.11	128.10	120.90

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	4471	0	4420	19	0
1	B	4301	0	4249	16	0
All	All	8772	0	8669	33	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 2.

All (33) 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:338:LYS:HB2	1:A:389:LEU:HD11	1.86	0.56
1:B:616:GLY:HA2	1:B:620:TYR:HD1	1.73	0.54
1:B:185:LEU:HB3	1:B:228:THR:HG23	1.89	0.54
1:A:69:ILE:HG12	1:A:78:THR:HG22	1.89	0.53
1:B:289:LEU:HD11	1:B:293:THR:HG21	1.90	0.53
1:A:185:LEU:HB3	1:A:228:THR:HG23	1.91	0.52
1:A:368:GLY:HA2	1:A:387:ASN:HA	1.92	0.52
1:B:322:VAL:HG11	1:B:471:PHE:HB2	1.91	0.51
1:A:124:ALA:HB2	1:A:138:LEU:HD21	1.93	0.50
1:A:407:VAL:HG22	1:B:476:GLN:HE21	1.76	0.49
1:B:244:LEU:HD22	1:B:275:VAL:HB	1.96	0.47
1:B:415:GLU:HG2	1:B:458:LEU:HD13	1.96	0.47
1:A:188:THR:HG22	1:A:231:ILE:HD11	1.95	0.46
1:B:124:ALA:HB2	1:B:138:LEU:HD21	1.97	0.46
1:B:269:ARG:HH21	1:B:318:ASP:HB2	1.81	0.46
1:B:309:LEU:HA	1:B:607:HIS:HD2	1.81	0.45
1:B:39:GLU:HA	1:B:42:ILE:HD12	1.98	0.45
1:A:244:LEU:HD22	1:A:275:VAL:HB	1.98	0.44
1:A:112:LEU:HD22	1:A:202:LEU:HD21	1.98	0.44
1:A:464:ILE:HG12	1:A:470:GLY:HA2	2.00	0.44
1:A:376:GLY:HA3	1:A:532:ILE:HG12	2.00	0.43
1:B:602:VAL:HA	1:B:605:ILE:HD12	1.99	0.43
1:A:181:ILE:HD12	1:A:219:TYR:HB3	2.01	0.43
1:B:322:VAL:HG13	1:B:469:SER:HB2	2.00	0.43
1:A:322:VAL:HG11	1:A:471:PHE:HB2	2.00	0.43
1:A:385:ARG:HA	1:A:390:LYS:HD2	2.00	0.43
1:B:88:CYS:HB2	1:B:91:LYS:HB2	2.00	0.43
1:A:617:ARG:HA	1:A:621:GLU:HB2	2.00	0.42
1:A:298:SER:HB3	1:B:463:ASN:HD22	1.85	0.41
1:A:304:LEU:HD23	1:A:309:LEU:HD13	2.02	0.41
1:A:515:VAL:HG22	1:A:568:LEU:HB3	2.03	0.41
1:B:186:CYS:HB3	1:B:231:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HB3	1:A:181:ILE:HG12	2.04	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	566/611 (93%)	545 (96%)	20 (4%)	1 (0%)	43	73
1	B	538/611 (88%)	516 (96%)	22 (4%)	0	100	100
All	All	1104/1222 (90%)	1061 (96%)	42 (4%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	MET

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	491/527 (93%)	471 (96%)	20 (4%)	27	59
1	B	475/527 (90%)	458 (96%)	17 (4%)	31	62
All	All	966/1054 (92%)	929 (96%)	37 (4%)	29	60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	251	LEU
1	A	351	ILE
1	A	389	LEU
1	A	407	VAL
1	A	408	THR
1	A	429	LYS
1	A	435	ILE
1	A	464	ILE
1	A	498	ILE
1	A	507	LEU
1	A	515	VAL
1	A	531	ILE
1	A	559	LYS
1	A	567	LEU
1	A	586	SER
1	A	591	ASP
1	A	604	VAL
1	A	607	HIS
1	A	613	GLU
1	B	82	LEU
1	B	110	THR
1	B	133	VAL
1	B	251	LEU
1	B	340	LEU
1	B	347	LEU
1	B	403	ILE
1	B	415	GLU
1	B	428	MET
1	B	435	ILE
1	B	472	GLU
1	B	498	ILE
1	B	553	LEU
1	B	557	LEU
1	B	559	LYS
1	B	591	ASP
1	B	609	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	409	ASN
1	A	448	GLN
1	A	576	ASN
1	A	627	ASN
1	B	167	GLN
1	B	211	ASN
1	B	284	GLN
1	B	290	GLN
1	B	441	ASN
1	B	448	GLN
1	B	463	ASN
1	B	576	ASN
1	B	607	HIS
1	B	608	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 [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, 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	574/611 (93%)	1.10	77 (13%) 7 4	32, 61, 99, 128	0
1	B	552/611 (90%)	1.26	98 (17%) 4 2	38, 78, 112, 173	0
All	All	1126/1222 (92%)	1.18	175 (15%) 5 2	32, 69, 107, 173	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	CYS	6.2
1	B	567	LEU	4.8
1	A	39	GLU	4.7
1	A	566	SER	4.7
1	A	372	VAL	4.2
1	A	111	GLY	4.1
1	B	366	SER	4.1
1	A	472	GLU	4.0
1	B	97	PRO	3.9
1	A	48	HIS	3.8
1	A	110	THR	3.8
1	B	357	LEU	3.7
1	B	132	PRO	3.7
1	B	252	GLY	3.6
1	A	247	LEU	3.6
1	B	297	SER	3.6
1	B	337	LEU	3.6
1	B	390	LYS	3.5
1	B	384	VAL	3.5
1	B	405	PHE	3.5
1	B	557	LEU	3.5
1	B	394	THR	3.3
1	B	361	PHE	3.2
1	B	375	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	439	THR	3.2
1	B	120	LEU	3.2
1	A	139	PHE	3.1
1	B	103	ILE	3.1
1	A	528	SER	3.1
1	B	378	ALA	3.1
1	B	428	MET	3.1
1	A	564	THR	3.1
1	A	568	LEU	3.0
1	B	525	PHE	3.0
1	B	453	LEU	3.0
1	A	37	ASP	3.0
1	B	335	LEU	2.9
1	B	549	LYS	2.9
1	B	530	VAL	2.9
1	B	158	GLU	2.9
1	A	573	ALA	2.9
1	B	248	SER	2.9
1	A	438	GLY	2.9
1	B	403	ILE	2.9
1	B	289	LEU	2.9
1	B	406	LYS	2.9
1	B	509	SER	2.8
1	A	557	LEU	2.8
1	B	562	ALA	2.8
1	B	374	PRO	2.8
1	B	563	LEU	2.8
1	B	513	GLY	2.7
1	A	295	LEU	2.7
1	B	554	ASN	2.7
1	A	33	GLY	2.7
1	B	377	SER	2.7
1	B	327	LEU	2.7
1	B	504	HIS	2.7
1	B	547	GLU	2.7
1	B	622	ALA	2.7
1	B	565	VAL	2.7
1	A	245	ASN	2.7
1	A	326	GLN	2.6
1	A	444	LYS	2.6
1	A	530	VAL	2.6
1	B	439	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	628	LEU	2.6
1	A	384	VAL	2.6
1	A	361	PHE	2.6
1	B	392	LEU	2.6
1	A	412	GLN	2.6
1	A	452	ILE	2.5
1	A	567	LEU	2.5
1	B	425	ALA	2.5
1	B	546	GLY	2.5
1	B	577	GLN	2.5
1	A	129	GLU	2.5
1	A	241	PHE	2.5
1	A	352	CYS	2.5
1	B	473	SER	2.5
1	B	601	GLN	2.5
1	B	573	ALA	2.5
1	B	344	ASP	2.5
1	B	38	THR	2.5
1	A	347	LEU	2.5
1	B	352	CYS	2.5
1	A	629	GLU	2.5
1	B	498	ILE	2.5
1	B	245	ASN	2.5
1	A	407	VAL	2.5
1	B	474	VAL	2.5
1	A	387	ASN	2.4
1	A	47	THR	2.4
1	A	327	LEU	2.4
1	B	501	LEU	2.4
1	A	474	VAL	2.4
1	A	460	LEU	2.4
1	B	447	SER	2.4
1	B	292	GLY	2.4
1	B	487	MET	2.4
1	A	115	VAL	2.4
1	A	599	GLY	2.3
1	A	281	ALA	2.3
1	A	50	GLN	2.3
1	A	76	THR	2.3
1	B	211	ASN	2.3
1	B	437	GLU	2.3
1	A	376	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	247	LEU	2.3
1	B	128	TRP	2.3
1	B	279	GLY	2.3
1	A	194	PHE	2.3
1	B	105	GLU	2.3
1	B	133	VAL	2.3
1	B	294	VAL	2.3
1	A	328	GLY	2.3
1	B	460	LEU	2.3
1	A	133	VAL	2.3
1	A	420	PRO	2.2
1	B	574	GLY	2.2
1	A	238	LEU	2.2
1	A	62	SER	2.2
1	B	74	SER	2.2
1	B	166	SER	2.2
1	A	296	PRO	2.2
1	B	485	ALA	2.2
1	A	332	SER	2.2
1	B	330	ALA	2.2
1	A	297	SER	2.2
1	B	441	ASN	2.2
1	A	350	GLY	2.2
1	A	367	ALA	2.2
1	B	619	ALA	2.2
1	B	422	LYS	2.2
1	A	427	ARG	2.2
1	A	232	THR	2.2
1	B	295	LEU	2.2
1	B	596	ALA	2.2
1	A	341	CYS	2.2
1	A	476	GLN	2.1
1	B	429	LYS	2.1
1	A	145	MET	2.1
1	A	521	ALA	2.1
1	A	440	GLY	2.1
1	B	404	SER	2.1
1	A	383	ASP	2.1
1	B	246	HIS	2.1
1	A	122	THR	2.1
1	A	422	LYS	2.1
1	A	363	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	426	GLU	2.1
1	B	326	GLN	2.1
1	A	336	PHE	2.1
1	B	516	GLU	2.1
1	B	174	VAL	2.1
1	B	398	VAL	2.1
1	A	432	ASN	2.1
1	A	330	ALA	2.1
1	A	462	ALA	2.1
1	B	124	ALA	2.1
1	B	56	GLU	2.1
1	B	275	VAL	2.0
1	B	354	ASN	2.0
1	B	458	LEU	2.0
1	A	425	ALA	2.0
1	B	216	ALA	2.0
1	B	556	ASP	2.0
1	A	424	LEU	2.0
1	B	519	ALA	2.0
1	A	511	PHE	2.0
1	B	328	GLY	2.0
1	B	358	PHE	2.0
1	B	555	PHE	2.0
1	A	374	PRO	2.0
1	A	390	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.