



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:50 AM UTC

PDB ID : 5RDH / pdb_00005rdh
Title : PanDDA analysis group deposition – Endothiapepsin ground state model 39
Authors : Weiss, M.S.; Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.;
Mueller, U.; Klebe, G.
Deposited on : 2020-03-24
Resolution : 0.85 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

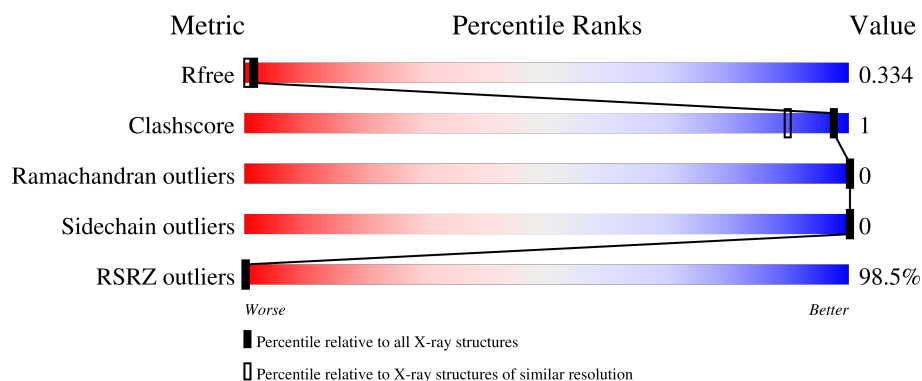
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.85 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	1405 (1.00-0.72)
Clashscore	190562	1457 (1.00-0.72)
Ramachandran outliers	187476	1376 (1.00-0.72)
Sidechain outliers	187428	1377 (1.00-0.72)
RSRZ outliers	180081	1400 (1.00-0.72)

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	419	78% 77% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2462 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.

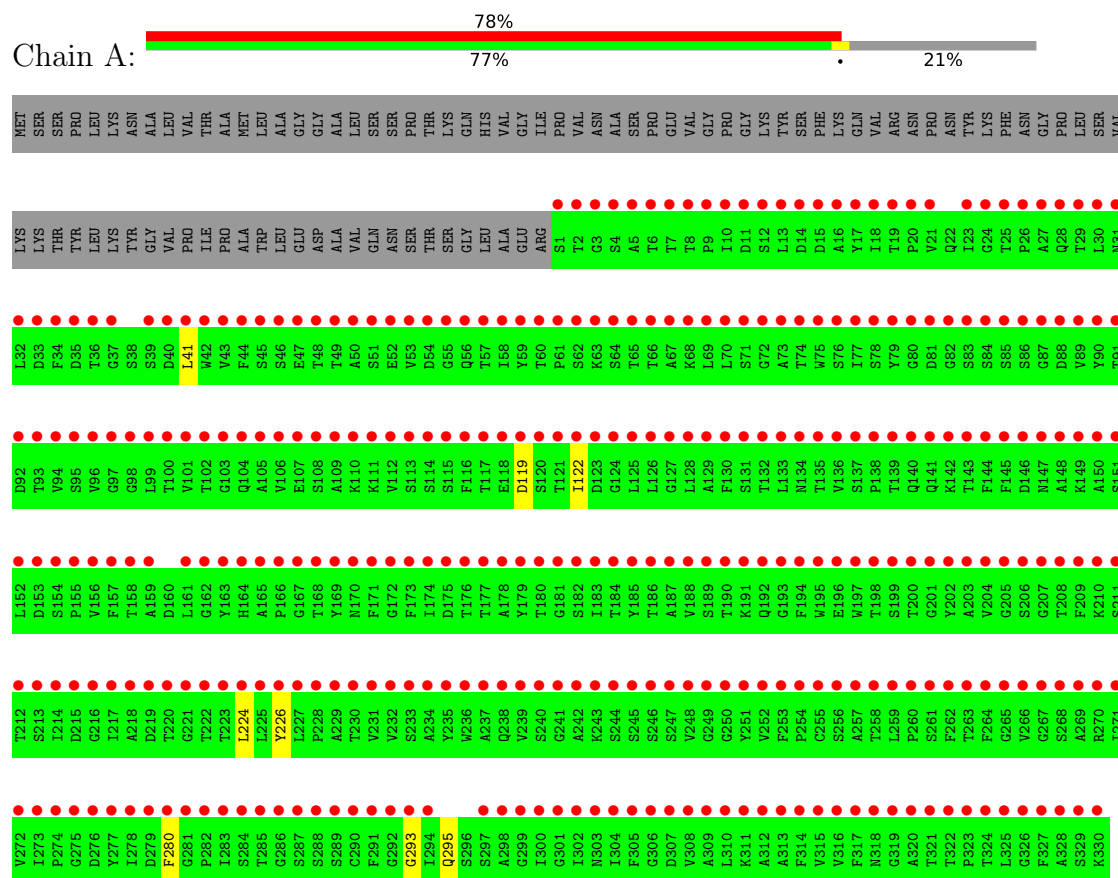
- Molecule 1 is a protein called Endothiapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	19	0
			2462	1566	367	527	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: Endothiapepsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.27Å 72.92Å 52.51Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	42.75 – 0.85 42.75 – 0.85	Depositor EDS
% Data completeness (in resolution range)	69.3 (42.75-0.85) 69.3 (42.75-0.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 0.85Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.334 , 0.334 0.338 , 0.334	Depositor DCC
R_{free} test set	9534 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	9.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 15.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	2462	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% 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](#)

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	1.01	0/2552	1.02	1/3496 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PHE	CA-CB-CG	-6.02	107.78	113.80

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	2462	0	2329	4	0
All	All	2462	0	2329	4	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 1.

All (4) 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:119:ASP:OD2	1:A:122:ILE:HD12	2.14	0.46
1:A:41:LEU:C	1:A:41:LEU:HD23	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:HA	1:A:295:GLN:O	2.21	0.41
1:A:224:LEU:HD22	1:A:293:GLY:HA2	2.02	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	347/419 (83%)	342 (99%)	5 (1%)	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	270/336 (80%)	270 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN

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	330/419 (78%)	5.36	325 (98%) 0 0	4, 10, 16, 21	19 (5%)

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	SER	13.8
1	A	300[A]	ILE	12.4
1	A	82	GLY	12.2
1	A	50	ALA	11.8
1	A	109	ALA	11.5
1	A	298[A]	ALA	11.0
1	A	53	VAL	10.8
1	A	117	THR	10.7
1	A	320	ALA	10.7
1	A	116	PHE	10.5
1	A	299[A]	GLY	10.5
1	A	138	PRO	10.2
1	A	194	PHE	10.1
1	A	145	PHE	10.0
1	A	321	THR	10.0
1	A	209	PHE	10.0
1	A	302	ILE	9.9
1	A	90	TYR	9.7
1	A	119	ASP	9.7
1	A	150	ALA	9.4
1	A	211	SER	9.4
1	A	58	ILE	9.1
1	A	179	TYR	9.1
1	A	149[A]	LYS	9.1
1	A	75	TRP	9.1
1	A	94	VAL	8.9
1	A	221	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	322	THR	8.8
1	A	17	TYR	8.6
1	A	133	LEU	8.6
1	A	112	VAL	8.2
1	A	248	VAL	8.2
1	A	152	LEU	8.1
1	A	80	GLY	8.0
1	A	156	VAL	8.0
1	A	136	VAL	7.9
1	A	130	PHE	7.9
1	A	272	VAL	7.8
1	A	77	ILE	7.8
1	A	174[A]	ILE	7.8
1	A	78	SER	7.7
1	A	13	LEU	7.7
1	A	106	VAL	7.6
1	A	41	LEU	7.6
1	A	49	THR	7.6
1	A	208	THR	7.6
1	A	65	THR	7.5
1	A	204	VAL	7.5
1	A	66	THR	7.5
1	A	121	THR	7.5
1	A	304	ILE	7.4
1	A	34	PHE	7.4
1	A	135	THR	7.4
1	A	308	VAL	7.4
1	A	51	SER	7.4
1	A	36	THR	7.4
1	A	132	THR	7.3
1	A	257	ALA	7.3
1	A	217	ILE	7.2
1	A	283	ILE	7.2
1	A	258	THR	7.2
1	A	323	PRO	7.1
1	A	10	ILE	7.1
1	A	187	ALA	7.1
1	A	69	LEU	7.0
1	A	268[A]	SER	7.0
1	A	9[A]	PRO	7.0
1	A	197	TRP	6.9
1	A	81	ASP	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	88	ASP	6.9
1	A	280	PHE	6.9
1	A	314	PHE	6.9
1	A	79	TYR	6.9
1	A	59	TYR	6.9
1	A	188	VAL	6.8
1	A	151	SER	6.8
1	A	305	PHE	6.8
1	A	44	PHE	6.7
1	A	190	THR	6.7
1	A	325[A]	LEU	6.7
1	A	245	SER	6.7
1	A	46	SER	6.6
1	A	202	TYR	6.6
1	A	176	THR	6.6
1	A	327	PHE	6.6
1	A	246[A]	SER	6.6
1	A	144	PHE	6.6
1	A	206[A]	SER	6.5
1	A	171	PHE	6.5
1	A	195	TRP	6.5
1	A	214	ILE	6.5
1	A	242	ALA	6.4
1	A	181	GLY	6.3
1	A	285	THR	6.3
1	A	301	GLY	6.3
1	A	42	TRP	6.2
1	A	244	SER	6.2
1	A	212	THR	6.2
1	A	266	VAL	6.2
1	A	164	HIS	6.2
1	A	277	TYR	6.1
1	A	101	VAL	6.1
1	A	249	GLY	6.1
1	A	163	TYR	6.1
1	A	27	ALA	6.1
1	A	247	SER	6.1
1	A	259	LEU	6.1
1	A	154[A]	SER	6.0
1	A	312	ALA	6.0
1	A	118	GLU	6.0
1	A	25	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	SER	5.9
1	A	191	LYS	5.9
1	A	232	VAL	5.8
1	A	74	THR	5.8
1	A	177	THR	5.8
1	A	30	LEU	5.8
1	A	70	LEU	5.8
1	A	180	THR	5.8
1	A	201	GLY	5.8
1	A	67	ALA	5.7
1	A	96	VAL	5.7
1	A	55	GLY	5.7
1	A	165	ALA	5.7
1	A	45	SER	5.6
1	A	71[A]	SER	5.6
1	A	48	THR	5.6
1	A	61	PRO	5.6
1	A	125	LEU	5.5
1	A	178	ALA	5.5
1	A	262	PHE	5.5
1	A	14	ASP	5.5
1	A	162	GLY	5.5
1	A	219	ASP	5.5
1	A	216	GLY	5.5
1	A	72	GLY	5.5
1	A	226	TYR	5.4
1	A	120	SER	5.4
1	A	271	ILE	5.4
1	A	126	LEU	5.4
1	A	269	ALA	5.4
1	A	264	PHE	5.4
1	A	99	LEU	5.3
1	A	286	GLY	5.3
1	A	158	THR	5.3
1	A	282	PRO	5.3
1	A	235	TYR	5.3
1	A	21	VAL	5.3
1	A	43	VAL	5.3
1	A	16	ALA	5.3
1	A	294	ILE	5.3
1	A	227	LEU	5.2
1	A	236	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	60	THR	5.2
1	A	324	THR	5.2
1	A	54	ASP	5.2
1	A	254	PRO	5.2
1	A	218	ALA	5.2
1	A	192	GLN	5.2
1	A	175	ASP	5.2
1	A	185	TYR	5.1
1	A	203	ALA	5.1
1	A	225	LEU	5.1
1	A	89	VAL	5.1
1	A	128	LEU	5.0
1	A	317	PHE	5.0
1	A	98	GLY	5.0
1	A	239	VAL	5.0
1	A	315	VAL	5.0
1	A	240[A]	SER	4.9
1	A	256	SER	4.9
1	A	313	ALA	4.9
1	A	330	LYS	4.9
1	A	251	TYR	4.9
1	A	291	PHE	4.9
1	A	32	LEU	4.8
1	A	124	GLY	4.8
1	A	237	ALA	4.8
1	A	284	SER	4.8
1	A	73	ALA	4.7
1	A	316	VAL	4.7
1	A	86	SER	4.7
1	A	173	PHE	4.7
1	A	84	SER	4.6
1	A	122	ILE	4.6
1	A	207	GLY	4.6
1	A	253	PHE	4.6
1	A	100	THR	4.6
1	A	2	THR	4.5
1	A	319	GLY	4.5
1	A	8	THR	4.5
1	A	1	SER	4.5
1	A	260	PRO	4.4
1	A	52	GLU	4.4
1	A	270	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	148	ALA	4.4
1	A	18	ILE	4.4
1	A	134	ASN	4.4
1	A	153	ASP	4.4
1	A	255	CYS	4.4
1	A	5	ALA	4.4
1	A	157	PHE	4.4
1	A	12	SER	4.4
1	A	87	GLY	4.4
1	A	168	THR	4.4
1	A	275	GLY	4.3
1	A	184	THR	4.3
1	A	108	SER	4.3
1	A	131	SER	4.3
1	A	155	PRO	4.3
1	A	200	THR	4.3
1	A	83	SER	4.2
1	A	93	THR	4.2
1	A	161	LEU	4.2
1	A	250	GLY	4.2
1	A	293	GLY	4.2
1	A	234	ALA	4.2
1	A	7	THR	4.2
1	A	91	THR	4.2
1	A	139	THR	4.2
1	A	224	LEU	4.2
1	A	290	CYS	4.2
1	A	303	ASN	4.2
1	A	23	ILE	4.2
1	A	63	LYS	4.2
1	A	220	THR	4.2
1	A	142	LYS	4.2
1	A	169	TYR	4.1
1	A	103	GLY	4.1
1	A	205	GLY	4.1
1	A	4	SER	4.1
1	A	85	SER	4.1
1	A	105	ALA	4.1
1	A	273	ILE	4.0
1	A	76	SER	4.0
1	A	114	SER	4.0
1	A	318	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	26	PRO	4.0
1	A	143	THR	4.0
1	A	182[A]	SER	4.0
1	A	252	VAL	4.0
1	A	267	GLY	4.0
1	A	140	GLN	3.9
1	A	189	SER	3.9
1	A	3	GLY	3.9
1	A	213	SER	3.9
1	A	281	GLY	3.9
1	A	102	THR	3.9
1	A	186	THR	3.9
1	A	57	THR	3.8
1	A	39	SER	3.8
1	A	183	ILE	3.8
1	A	129	ALA	3.7
1	A	228	PRO	3.7
1	A	137	SER	3.6
1	A	233	SER	3.6
1	A	274	PRO	3.6
1	A	146	ASP	3.6
1	A	263	THR	3.5
1	A	279	ASP	3.5
1	A	223	THR	3.5
1	A	47	GLU	3.5
1	A	329	SER	3.5
1	A	6	THR	3.5
1	A	24	GLY	3.5
1	A	241	GLY	3.5
1	A	215[A]	ASP	3.5
1	A	288	SER	3.4
1	A	198	THR	3.4
1	A	166	PRO	3.4
1	A	28	GLN	3.4
1	A	238	GLN	3.4
1	A	231	VAL	3.4
1	A	56	GLN	3.4
1	A	310	LEU	3.4
1	A	107	GLU	3.3
1	A	172	GLY	3.3
1	A	110	LYS	3.3
1	A	35	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLN	3.3
1	A	229	ALA	3.3
1	A	196	GLU	3.2
1	A	31	ASN	3.2
1	A	111	LYS	3.2
1	A	147	ASN	3.2
1	A	222	THR	3.2
1	A	278	ILE	3.2
1	A	261	SER	3.1
1	A	276[A]	ASP	3.1
1	A	141	GLN	3.1
1	A	40	ASP	3.0
1	A	289[A]	SER	3.0
1	A	193	GLY	3.0
1	A	33	ASP	3.0
1	A	113	SER	3.0
1	A	92	ASP	2.9
1	A	64	SER	2.9
1	A	230	THR	2.9
1	A	328	ALA	2.9
1	A	29	THR	2.9
1	A	159	ALA	2.9
1	A	11	ASP	2.8
1	A	199	SER	2.8
1	A	37	GLY	2.8
1	A	19	THR	2.8
1	A	309	ALA	2.8
1	A	210	LYS	2.8
1	A	95	SER	2.7
1	A	170	ASN	2.7
1	A	167	GLY	2.7
1	A	292	GLY	2.7
1	A	15	ASP	2.6
1	A	287	SER	2.5
1	A	297	SER	2.5
1	A	68[A]	LYS	2.5
1	A	20	PRO	2.4
1	A	326	GLY	2.4
1	A	127	GLY	2.3
1	A	97	GLY	2.2
1	A	306	GLY	2.2
1	A	123	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	2.2
1	A	265	GLY	2.2
1	A	307	ASP	2.1
1	A	311[A]	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.