



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 2ZHV / pdb_00002zhv
Title : Crystal structure of BACE1 at pH 7.0
Authors : Shimizu, H.; Nukina, N.
Deposited on : 2008-02-08
Resolution : 1.85 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

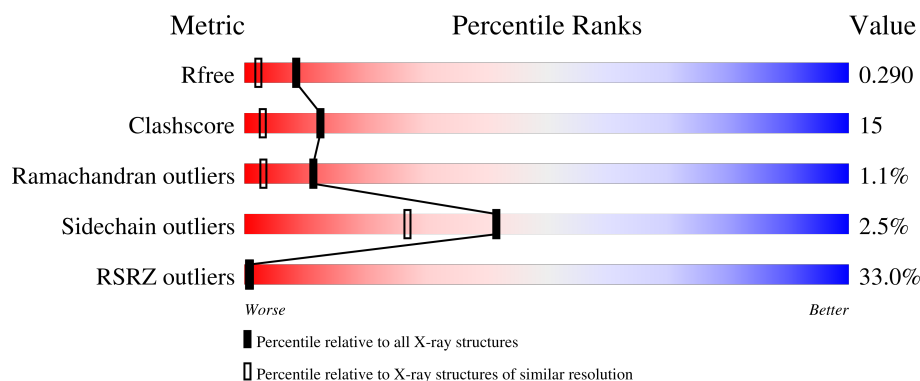
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	411	30% 63% 24% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3179 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2914	1869	485	546	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P56817

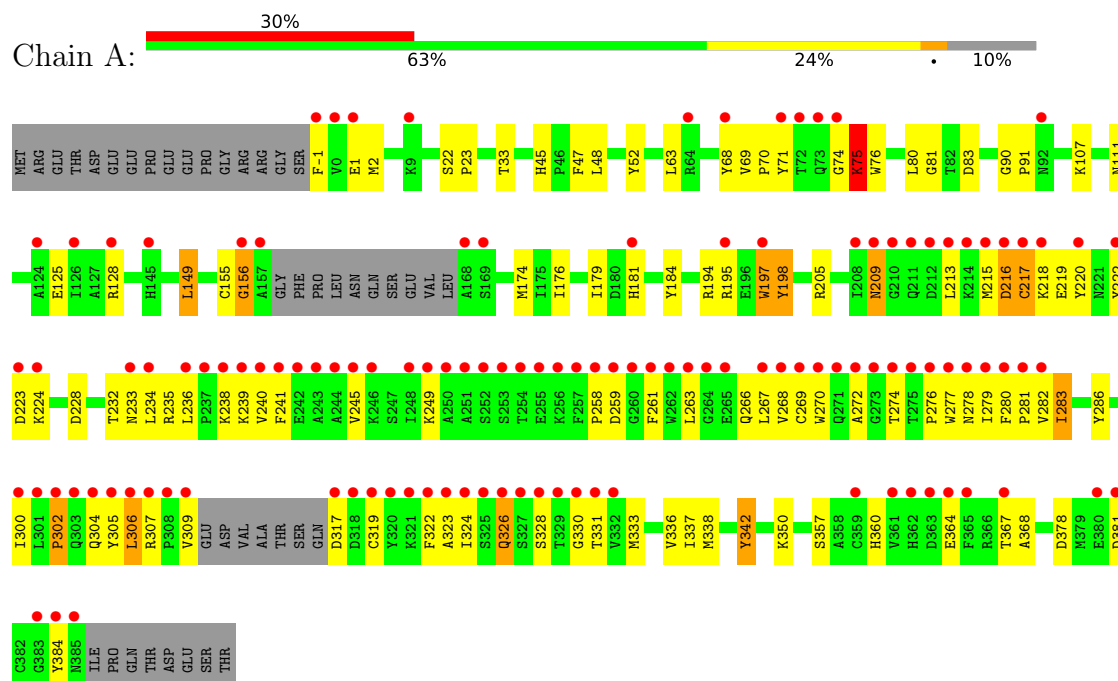
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	265	Total	O	0	0
			265	265		

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: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.33Å 102.33Å 170.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 1.85 49.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.01-1.85) 95.9 (49.01-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.290 0.246 , 0.290	Depositor DCC
R_{free} test set	2199 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3179	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.36	0/2988	0.90	9/4059 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	N-CA-C	-8.09	97.82	110.36
1	A	342	TYR	N-CA-C	-6.89	98.01	108.96
1	A	338	MET	N-CA-C	6.13	117.96	111.28
1	A	328	SER	N-CA-C	-5.60	106.34	114.12
1	A	45	HIS	N-CA-C	-5.34	103.05	109.83
1	A	307	ARG	CA-C-N	5.30	125.24	119.78
1	A	307	ARG	C-N-CA	5.30	125.24	119.78
1	A	302	PRO	N-CA-C	-5.26	107.29	113.86
1	A	48	LEU	N-CA-C	5.22	118.13	109.46

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	2914	0	2833	88	0
2	A	265	0	0	0	0
All	All	3179	0	2833	88	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 15.

All (88) 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:333:MET:HE2	1:A:337:ILE:HG21	1.65	0.78
1:A:71:TYR:HD1	1:A:75:LYS:HA	1.53	0.72
1:A:259:ASP:O	1:A:263:LEU:HD23	1.91	0.71
1:A:282:VAL:C	1:A:283:ILE:HD12	2.17	0.69
1:A:75:LYS:HD2	1:A:75:LYS:C	2.18	0.68
1:A:300:ILE:HD13	1:A:337:ILE:HD13	1.78	0.66
1:A:197:TRP:CH2	1:A:224:LYS:HD3	2.31	0.65
1:A:71:TYR:CD1	1:A:75:LYS:HA	2.33	0.64
1:A:233:ASN:HB3	1:A:323:ALA:O	1.98	0.62
1:A:74:GLY:HA3	1:A:107:LYS:HB2	1.85	0.58
1:A:283:ILE:HD12	1:A:283:ILE:N	2.19	0.57
1:A:235:ARG:O	1:A:331:THR:HA	2.06	0.56
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.88	0.56
1:A:278:ASN:HD22	1:A:278:ASN:N	2.02	0.56
1:A:-1:PHE:HB3	1:A:2:MET:HE3	1.88	0.56
1:A:91:PRO:HD3	1:A:176:ILE:HB	1.88	0.56
1:A:197:TRP:CG	1:A:198:TYR:H	2.22	0.56
1:A:68:TYR:HE1	1:A:70:PRO:HB3	1.70	0.55
1:A:245:VAL:O	1:A:249:LYS:HG3	2.07	0.55
1:A:74:GLY:O	1:A:75:LYS:HB3	2.07	0.54
1:A:268:VAL:O	1:A:319:CYS:HA	2.07	0.54
1:A:333:MET:CE	1:A:337:ILE:HG21	2.36	0.54
1:A:283:ILE:HD13	1:A:305:TYR:CE2	2.43	0.53
1:A:149:LEU:C	1:A:149:LEU:HD23	2.33	0.53
1:A:367:THR:HG22	1:A:368:ALA:O	2.10	0.51
1:A:241:PHE:CZ	1:A:245:VAL:HG21	2.45	0.51
1:A:276:PRO:HB2	1:A:279:ILE:CG1	2.41	0.51
1:A:232:THR:O	1:A:336:VAL:HG23	2.11	0.51
1:A:209:ASN:HD21	1:A:281:PRO:HA	1.76	0.51
1:A:258:PRO:HG3	1:A:266:GLN:NE2	2.26	0.51
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.75	0.50
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.93	0.50
1:A:233:ASN:HA	1:A:336:VAL:HG23	1.95	0.49
1:A:224:LYS:O	1:A:331:THR:N	2.42	0.49
1:A:209:ASN:ND2	1:A:281:PRO:HA	2.27	0.49
1:A:181:HIS:HA	1:A:184:TYR:CE2	2.47	0.49
1:A:305:TYR:HA	1:A:323:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:CE1	1:A:367:THR:HG23	2.49	0.48
1:A:283:ILE:N	1:A:283:ILE:CD1	2.77	0.48
1:A:219:GLU:CD	1:A:239:LYS:HD3	2.39	0.47
1:A:198:TYR:CE2	1:A:224:LYS:HE3	2.49	0.47
1:A:277:TRP:CE3	1:A:302:PRO:HB2	2.49	0.47
1:A:33:THR:OG1	1:A:228:ASP:HA	2.14	0.47
1:A:322:PHE:CE1	1:A:324:ILE:HB	2.49	0.47
1:A:378:ASP:HB3	1:A:381:ASP:OD2	2.15	0.47
1:A:245:VAL:HG12	1:A:249:LYS:HD2	1.97	0.47
1:A:267:LEU:HD11	1:A:309:VAL:HG11	1.96	0.46
1:A:277:TRP:HZ3	1:A:306:LEU:HB3	1.80	0.46
1:A:222:TYR:HA	1:A:223:ASP:HA	1.62	0.46
1:A:304:GLN:HB3	1:A:336:VAL:O	2.15	0.46
1:A:350:LYS:HE2	1:A:350:LYS:HB3	1.80	0.46
1:A:236:LEU:O	1:A:326:GLN:HA	2.15	0.45
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.98	0.45
1:A:52:TYR:OH	1:A:83:ASP:OD2	2.35	0.45
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.56	0.45
1:A:63:LEU:HG	1:A:81:GLY:HA2	1.98	0.44
1:A:128:ARG:HH21	1:A:128:ARG:HG2	1.81	0.44
1:A:215:MET:O	1:A:217:CYS:N	2.50	0.44
1:A:215:MET:HE1	1:A:240:VAL:HA	1.98	0.44
1:A:270:TRP:O	1:A:317:ASP:HB3	2.18	0.43
1:A:269:CYS:HA	1:A:319:CYS:HA	2.00	0.43
1:A:22:SER:HA	1:A:23:PRO:C	2.42	0.43
1:A:197:TRP:CD1	1:A:198:TYR:H	2.36	0.43
1:A:63:LEU:HD12	1:A:80:LEU:HB3	2.00	0.43
1:A:125:GLU:OE1	1:A:195:ARG:NH1	2.40	0.43
1:A:215:MET:O	1:A:216:ASP:C	2.61	0.43
1:A:222:TYR:O	1:A:330:GLY:HA2	2.19	0.42
1:A:197:TRP:CG	1:A:198:TYR:N	2.88	0.42
1:A:1:GLU:HG3	1:A:2:MET:HG3	2.01	0.42
1:A:70:PRO:HA	1:A:75:LYS:HB3	2.00	0.42
1:A:213:LEU:N	1:A:213:LEU:CD1	2.82	0.42
1:A:47:PHE:CZ	1:A:111:ASN:HB2	2.54	0.42
1:A:364:GLU:O	1:A:364:GLU:HG3	2.20	0.42
1:A:194:ARG:HH12	1:A:384:TYR:N	2.18	0.41
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.55	0.41
1:A:280:PHE:HB2	1:A:302:PRO:CG	2.50	0.41
1:A:47:PHE:CE2	1:A:111:ASN:HB2	2.55	0.41
1:A:68:TYR:HD1	1:A:70:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:O	1:A:156:GLY:C	2.63	0.41
1:A:216:ASP:O	1:A:218:LYS:N	2.54	0.41
1:A:258:PRO:O	1:A:261:PHE:HB3	2.21	0.41
1:A:302:PRO:O	1:A:306:LEU:HB2	2.21	0.41
1:A:69:VAL:HG21	1:A:76:TRP:CZ2	2.56	0.40
1:A:272:ALA:O	1:A:274:THR:HG23	2.21	0.40
1:A:205:ARG:HD3	1:A:286:TYR:CE1	2.56	0.40
1:A:357:SER:O	1:A:360:HIS:HD2	2.04	0.40
1:A:238:LYS:HE3	1:A:238:LYS:HB2	1.91	0.40
1:A:209:ASN:ND2	1:A:282:VAL:H	2.19	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	364/411 (89%)	347 (95%)	13 (4%)	4 (1%)	11 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	CYS
1	A	216	ASP
1	A	75	LYS
1	A	156	GLY

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	315/352 (90%)	307 (98%)	8 (2%)	42 27

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	149	LEU
1	A	197	TRP
1	A	209	ASN
1	A	234	LEU
1	A	283	ILE
1	A	306	LEU
1	A	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	73	GLN
1	A	89	HIS
1	A	114	ASN
1	A	209	ASN
1	A	271	GLN
1	A	278	ASN
1	A	326	GLN
1	A	360	HIS

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 [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	370/411 (90%)	1.39	122 (32%) 1 1	15, 30, 64, 93	3 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	8.3
1	A	276	PRO	7.2
1	A	279	ILE	7.0
1	A	272	ALA	6.0
1	A	168	ALA	5.5
1	A	254	THR	5.4
1	A	275	THR	5.3
1	A	72	THR	5.2
1	A	245	VAL	5.2
1	A	277	TRP	5.1
1	A	280	PHE	4.9
1	A	322	PHE	4.8
1	A	270	TRP	4.8
1	A	257	PHE	4.7
1	A	384	TYR	4.5
1	A	307	ARG	4.4
1	A	222	TYR	4.4
1	A	367	THR	4.4
1	A	323	ALA	4.4
1	A	269	CYS	4.3
1	A	242	GLU	4.3
1	A	256	LYS	4.3
1	A	263	LEU	4.2
1	A	328	SER	4.2
1	A	253	SER	4.1
1	A	319	CYS	4.1
1	A	237	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	4.0
1	A	241	PHE	4.0
1	A	213	LEU	3.9
1	A	365	PHE	3.9
1	A	362	HIS	3.9
1	A	274	THR	3.9
1	A	260	GLY	3.9
1	A	236	LEU	3.8
1	A	262	TRP	3.8
1	A	317	ASP	3.7
1	A	215	MET	3.7
1	A	306	LEU	3.7
1	A	74	GLY	3.7
1	A	305	TYR	3.7
1	A	243	ALA	3.7
1	A	250	ALA	3.7
1	A	73	GLN	3.7
1	A	281	PRO	3.7
1	A	302	PRO	3.7
1	A	301	LEU	3.6
1	A	329	THR	3.6
1	A	233	ASN	3.5
1	A	320	TYR	3.5
1	A	273	GLY	3.4
1	A	211	GLN	3.4
1	A	244	ALA	3.4
1	A	363	ASP	3.4
1	A	361	VAL	3.3
1	A	324	ILE	3.3
1	A	71	TYR	3.3
1	A	0	VAL	3.2
1	A	209	ASN	3.2
1	A	261	PHE	3.2
1	A	309	VAL	3.2
1	A	385	ASN	3.2
1	A	214	LYS	3.1
1	A	240	VAL	3.1
1	A	255	GLU	3.1
1	A	238	LYS	3.1
1	A	145	HIS	3.1
1	A	181	HIS	3.1
1	A	381	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	212	ASP	3.0
1	A	239	LYS	3.0
1	A	332	VAL	3.0
1	A	259	ASP	3.0
1	A	217	CYS	3.0
1	A	265	GLU	3.0
1	A	197	TRP	3.0
1	A	308	PRO	3.0
1	A	258	PRO	2.9
1	A	92	ASN	2.9
1	A	318	ASP	2.9
1	A	210	GLY	2.9
1	A	216	ASP	2.9
1	A	208	ILE	2.9
1	A	330	GLY	2.9
1	A	383	GLY	2.9
1	A	278	ASN	2.8
1	A	169	SER	2.8
1	A	327	SER	2.8
1	A	64	ARG	2.8
1	A	224	LYS	2.8
1	A	156	GLY	2.7
1	A	249	LYS	2.7
1	A	331	THR	2.7
1	A	271	GLN	2.6
1	A	68	TYR	2.6
1	A	246	LYS	2.6
1	A	195	ARG	2.6
1	A	251	ALA	2.6
1	A	304	GLN	2.5
1	A	364	GLU	2.5
1	A	303	GLN	2.5
1	A	264	GLY	2.5
1	A	282	VAL	2.5
1	A	128	ARG	2.4
1	A	220	TYR	2.4
1	A	234	LEU	2.4
1	A	300	ILE	2.4
1	A	359	CYS	2.4
1	A	267	LEU	2.3
1	A	-1	PHE	2.3
1	A	9	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLU	2.3
1	A	218	LYS	2.3
1	A	124	ALA	2.2
1	A	325	SER	2.2
1	A	248	ILE	2.2
1	A	126	ILE	2.1
1	A	321	LYS	2.1
1	A	223	ASP	2.1
1	A	1	GLU	2.0
1	A	252	SER	2.0
1	A	326	GLN	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.