



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 AM UTC

PDB ID : 3OG5 / pdb_00003og5
Title : Crystal Structure of BamA POTRA45 tandem
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Deposited on : 2010-08-16
Resolution : 2.69 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

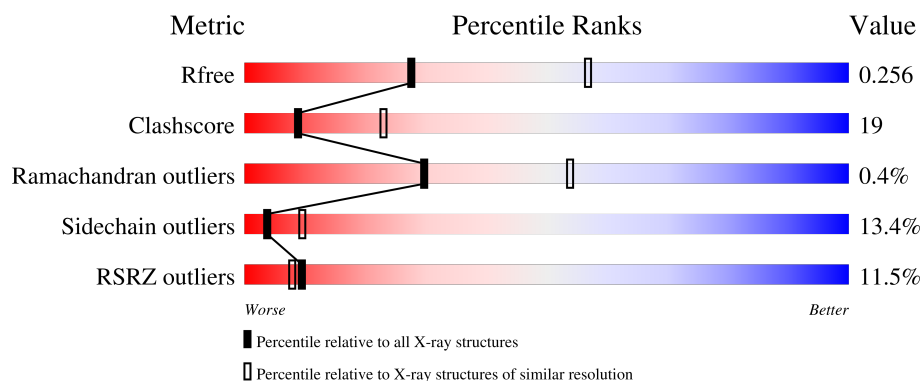
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	166	66% 24% 6% .
1	B	166	19% 50% 25% 7% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2351 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 Outer membrane protein assembly complex, YaeT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	Se	0	0	0
			1261	782	226	248	5			
1	B	136	Total	C	N	O	Se	0	0	0
			1040	653	183	200	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLY	-	expression tag	UNP D5CVA9
A	262	ALA	-	expression tag	UNP D5CVA9
A	263	MSE	-	expression tag	UNP D5CVA9
A	425	PRO	-	expression tag	UNP D5CVA9
A	426	GLY	-	expression tag	UNP D5CVA9
B	261	GLY	-	expression tag	UNP D5CVA9
B	262	ALA	-	expression tag	UNP D5CVA9
B	263	MSE	-	expression tag	UNP D5CVA9
B	425	PRO	-	expression tag	UNP D5CVA9
B	426	GLY	-	expression tag	UNP D5CVA9

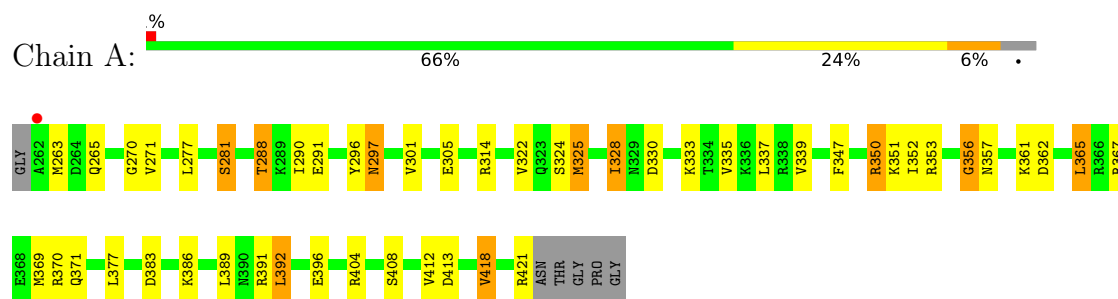
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		
2	B	11	Total	O	0	0
			11	11		

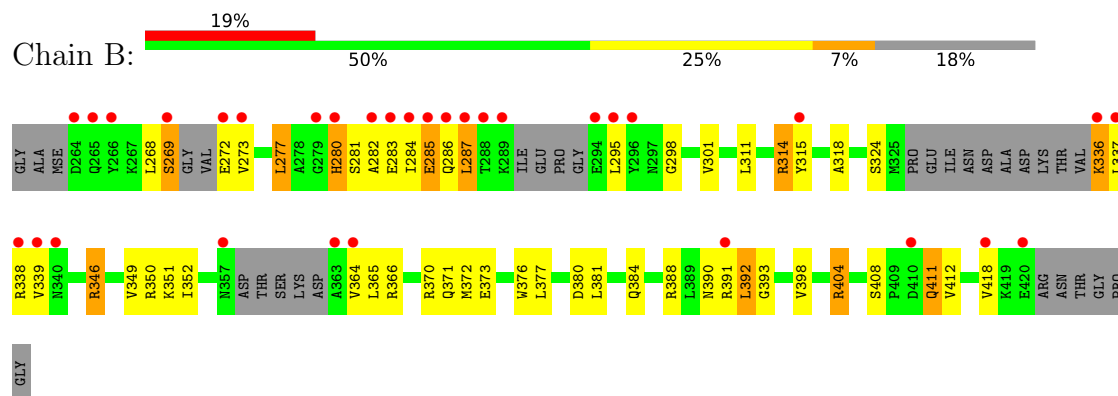
3 Residue-property plots [i](#)

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: Outer membrane protein assembly complex, YaeT protein



- Molecule 1: Outer membrane protein assembly complex, YaeT protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.49Å 118.49Å 69.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.79 – 2.69 38.79 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.5 (38.79-2.69) 93.9 (38.79-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.260 0.213 , 0.256	Depositor DCC
R_{free} test set	1529 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2351	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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	0.60	0/1274	0.96	6/1708 (0.4%)
1	B	0.49	0/1048	0.95	2/1404 (0.1%)
All	All	0.55	0/2322	0.96	8/3112 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	SER	CA-C-N	10.12	129.89	119.56
1	B	408	SER	C-N-CA	10.12	129.89	119.56
1	A	356	GLY	N-CA-C	-6.88	106.27	115.21
1	A	325	MSE	CA-C-N	6.16	126.37	119.90
1	A	325	MSE	C-N-CA	6.16	126.37	119.90
1	A	408	SER	CA-C-N	5.55	125.25	119.64
1	A	408	SER	C-N-CA	5.55	125.25	119.64
1	A	370	ARG	N-CA-C	-5.26	107.52	114.31

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	1261	0	1232	37	0
1	B	1040	0	986	49	0
2	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	11	0	0	1	0
All	All	2351	0	2218	84	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 19.

All (84) 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:271:VAL:HB	1:A:288:THR:HG23	1.62	0.80
1:B:277:LEU:HD23	1:B:284:ILE:HD13	1.63	0.80
1:B:350:ARG:HB2	1:B:411:GLN:HG2	1.62	0.80
1:A:263:MSE:HG2	1:A:328:ILE:HD11	1.64	0.77
1:B:277:LEU:O	1:B:280:HIS:HB2	1.86	0.75
1:A:389:LEU:O	1:A:392:LEU:HD22	1.86	0.75
1:B:384:GLN:O	1:B:388:ARG:HG3	1.89	0.72
1:B:349:VAL:O	1:B:373:GLU:O	2.11	0.68
1:B:272:GLU:O	1:B:339:VAL:HB	1.95	0.66
1:B:324:SER:HA	1:B:338:ARG:O	1.94	0.66
1:A:377:LEU:HD22	1:A:412:VAL:HG21	1.78	0.66
1:A:296:TYR:CD1	1:A:335:VAL:HG11	2.32	0.63
1:A:396:GLU:HG3	1:A:421:ARG:HA	1.80	0.63
1:B:273:VAL:HG23	1:B:273:VAL:O	1.98	0.62
1:B:315:TYR:O	1:B:346:ARG:HD2	2.01	0.60
1:B:269:SER:HB2	1:B:336:LYS:HD3	1.84	0.60
1:A:389:LEU:O	1:A:392:LEU:CD2	2.51	0.58
1:A:404:ARG:HH22	1:B:380:ASP:CG	2.11	0.58
1:B:392:LEU:C	1:B:392:LEU:HD12	2.29	0.57
1:B:280:HIS:C	1:B:282:ALA:H	2.12	0.56
1:B:370:ARG:HH21	1:B:388:ARG:NH1	2.03	0.56
1:B:404:ARG:HH11	1:B:404:ARG:CG	2.18	0.56
1:B:311:LEU:O	1:B:314:ARG:HG3	2.05	0.56
1:B:398:VAL:O	1:B:398:VAL:HG13	2.05	0.56
1:B:280:HIS:C	1:B:282:ALA:N	2.60	0.56
1:B:350:ARG:HH21	1:B:351:LYS:HD2	1.71	0.55
1:A:296:TYR:HD1	1:A:335:VAL:HG11	1.73	0.54
1:A:357:ASN:ND2	1:A:362:ASP:OD1	2.40	0.54
1:B:269:SER:HB2	1:B:336:LYS:CD	2.38	0.54
1:B:404:ARG:NH1	1:B:404:ARG:HG2	2.22	0.53
1:B:298:GLY:O	1:B:301:VAL:HG12	2.08	0.53
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD22	1:B:281:SER:HA	1.91	0.52
1:B:277:LEU:CD2	1:B:284:ILE:HD13	2.35	0.52
1:A:356:GLY:HA3	1:A:418:VAL:O	2.10	0.52
1:B:390:ASN:ND2	1:B:398:VAL:HG12	2.25	0.51
1:B:339:VAL:HG12	1:B:339:VAL:O	2.10	0.51
1:A:263:MSE:CG	1:A:328:ILE:HD11	2.38	0.51
1:A:367:ARG:HG3	1:A:367:ARG:HH11	1.76	0.51
1:B:318:ALA:HB2	1:B:377:LEU:CD2	2.40	0.50
1:A:301:VAL:HG22	1:A:337:LEU:HD11	1.95	0.49
1:B:370:ARG:HE	1:B:388:ARG:HH11	1.61	0.49
1:B:284:ILE:O	1:B:287:LEU:N	2.39	0.48
1:B:346:ARG:HG2	1:B:376:TRP:CZ3	2.48	0.48
1:B:352:ILE:O	1:B:366:ARG:NH2	2.47	0.48
1:A:352:ILE:HD11	1:A:371:GLN:O	2.14	0.47
1:A:367:ARG:HG3	1:A:367:ARG:NH1	2.29	0.47
1:B:404:ARG:CG	1:B:404:ARG:NH1	2.78	0.47
1:B:392:LEU:C	1:B:392:LEU:CD1	2.89	0.46
1:B:281:SER:O	1:B:285:GLU:CD	2.59	0.46
1:B:380:ASP:OD1	1:B:380:ASP:N	2.48	0.45
1:A:290:ILE:HG22	1:A:291:GLU:O	2.16	0.45
1:A:365:LEU:HD23	1:A:365:LEU:N	2.31	0.45
1:B:318:ALA:HB2	1:B:377:LEU:HD23	1.99	0.45
1:A:305:GLU:HG2	1:A:322:VAL:HG12	1.97	0.45
1:A:330:ASP:OD2	1:A:333:LYS:HE2	2.17	0.45
1:B:277:LEU:HD22	1:B:281:SER:CA	2.47	0.45
1:B:314:ARG:HB3	1:B:380:ASP:CG	2.41	0.45
1:B:390:ASN:C	1:B:392:LEU:H	2.25	0.45
1:A:369:MSE:HE2	1:A:369:MSE:HA	1.98	0.44
1:B:273:VAL:O	1:B:273:VAL:CG2	2.63	0.44
1:A:296:TYR:CD2	1:A:296:TYR:C	2.95	0.44
1:B:398:VAL:HG23	1:B:418:VAL:HG12	1.98	0.44
1:A:350:ARG:HD2	1:A:413:ASP:OD1	2.18	0.44
1:A:290:ILE:HG22	1:A:291:GLU:N	2.32	0.43
1:B:346:ARG:HG2	1:B:376:TRP:CE3	2.53	0.43
1:B:404:ARG:HG3	2:B:1:HOH:O	2.17	0.43
1:A:277:LEU:HD23	1:A:281:SER:HA	2.00	0.43
1:A:270:GLY:HA2	1:A:290:ILE:HD11	2.01	0.42
1:B:371:GLN:HE21	1:B:372:MSE:H	1.67	0.42
1:A:324:SER:HB2	1:A:339:VAL:HG22	2.01	0.42
1:B:285:GLU:N	1:B:285:GLU:OE1	2.53	0.42
1:A:270:GLY:CA	1:A:290:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ARG:NH2	1:B:381:LEU:HG	2.35	0.42
1:A:270:GLY:N	1:A:290:ILE:HD11	2.35	0.41
1:A:351:LYS:HD3	1:A:353:ARG:NH1	2.35	0.41
1:A:383:ASP:O	1:A:386:LYS:HB3	2.20	0.41
1:A:290:ILE:CG2	1:A:291:GLU:N	2.82	0.41
1:A:297:ASN:OD1	1:A:297:ASN:C	2.63	0.41
1:B:280:HIS:NE2	1:B:315:TYR:CE1	2.86	0.41
1:A:324:SER:CB	1:A:339:VAL:HG22	2.51	0.41
1:A:296:TYR:HB2	1:A:335:VAL:HG11	2.02	0.40
1:B:392:LEU:HD12	1:B:393:GLY:N	2.36	0.40
1:A:347:PHE:CD1	1:A:412:VAL:HG13	2.56	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	158/166 (95%)	153 (97%)	5 (3%)	0	100	100
1	B	126/166 (76%)	115 (91%)	10 (8%)	1 (1%)	16	37
All	All	284/332 (86%)	268 (94%)	15 (5%)	1 (0%)	30	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	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	134/136 (98%)	121 (90%)	13 (10%)	8	20
1	B	105/136 (77%)	86 (82%)	19 (18%)	2	5
All	All	239/272 (88%)	207 (87%)	32 (13%)	4	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	281	SER
1	A	288	THR
1	A	297	ASN
1	A	314	ARG
1	A	325	MSE
1	A	328	ILE
1	A	350	ARG
1	A	361	LYS
1	A	365	LEU
1	A	391	ARG
1	A	392	LEU
1	A	418	VAL
1	B	268	LEU
1	B	269	SER
1	B	277	LEU
1	B	280	HIS
1	B	283	GLU
1	B	285	GLU
1	B	286	GLN
1	B	287	LEU
1	B	295	LEU
1	B	314	ARG
1	B	336	LYS
1	B	337	LEU
1	B	346	ARG
1	B	364	VAL
1	B	365	LEU
1	B	392	LEU
1	B	404	ARG
1	B	411	GLN
1	B	412	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	B	276	ASN
1	B	345	ASN
1	B	357	ASN

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	155/166 (93%)	-0.25	1 (0%) 85 85	11, 26, 50, 74	0
1	B	132/166 (79%)	1.07	32 (24%) 2 1	23, 57, 98, 146	0
All	All	287/332 (86%)	0.36	33 (11%) 9 8	11, 35, 90, 146	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ASP	5.9
1	B	363	ALA	5.9
1	B	294	GLU	4.7
1	B	282	ALA	4.5
1	B	279	GLY	4.5
1	A	262	ALA	4.2
1	B	285	GLU	4.2
1	B	272	GLU	4.1
1	B	420	GLU	3.7
1	B	286	GLN	3.7
1	B	364	VAL	3.5
1	B	289	LYS	3.5
1	B	269	SER	3.4
1	B	280	HIS	3.3
1	B	391	ARG	3.3
1	B	273	VAL	3.3
1	B	287	LEU	3.3
1	B	315	TYR	3.1
1	B	296	TYR	2.9
1	B	340	ASN	2.9
1	B	336	LYS	2.9
1	B	265	GLN	2.8
1	B	288	THR	2.8
1	B	266	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	337	LEU	2.8
1	B	339	VAL	2.8
1	B	284	ILE	2.6
1	B	338	ARG	2.5
1	B	410	ASP	2.3
1	B	283	GLU	2.2
1	B	357	ASN	2.2
1	B	295	LEU	2.2
1	B	418	VAL	2.2

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.