



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 PM UTC

PDB ID : 8GUM / pdb_00008gum
Title : Chitin-active AA10 LPMO (GbpA) from *Vibrio campbellii*
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Deposited on : 2022-09-12
Resolution : 2.35 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

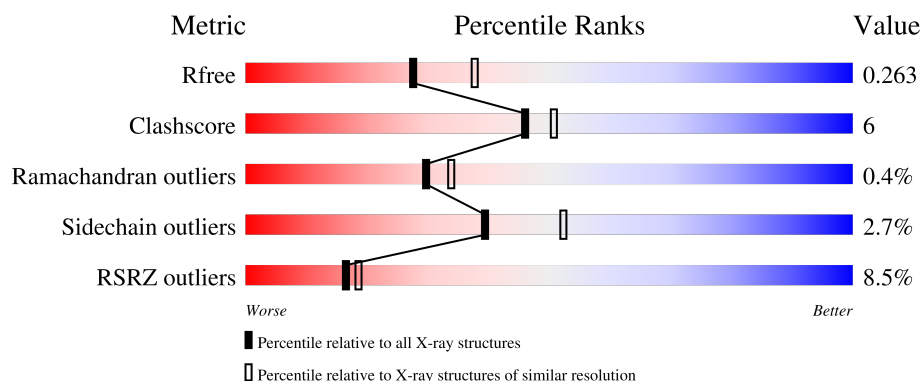
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	464	5% 85% 15%
1	B	464	10% 64% 12% • 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6514 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 GlcNAc-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3607	2260	601	734	12			
1	B	360	Total	C	N	O	S	0	0	0
			2795	1741	480	564	10			

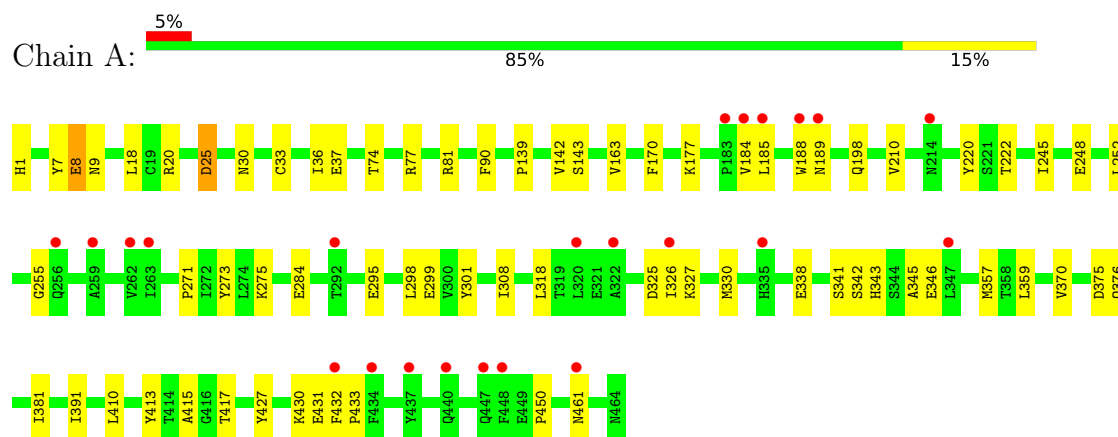
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total	O	0	0
			57	57		
2	B	55	Total	O	0	0
			55	55		

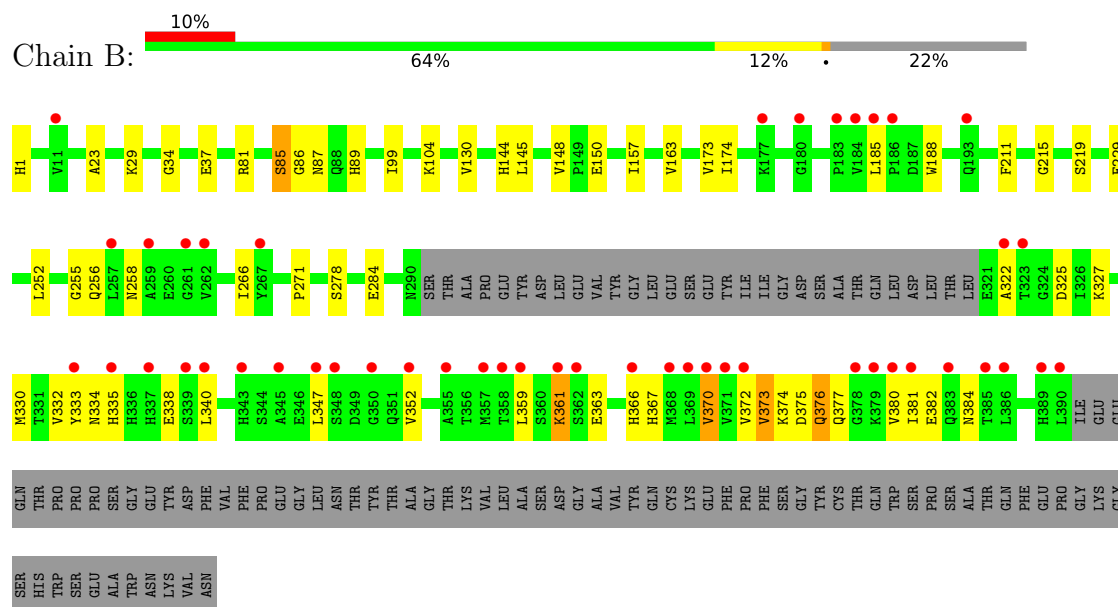
3 Residue-property plots [i](#)

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: GlcNAc-binding protein A



• Molecule 1: GlcNAc-binding protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.61Å 113.61Å 215.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.10 – 2.35 25.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.10-2.35) 99.6 (25.10-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.262 0.220 , 0.263	Depositor DCC
R_{free} test set	2926 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.43	0/3700	0.60	2/5048 (0.0%)
1	B	0.42	0/2860	0.61	0/3895
All	All	0.42	0/6560	0.60	2/8943 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	VAL	CA-C-N	6.47	127.12	119.94
1	A	163	VAL	C-N-CA	6.47	127.12	119.94

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	3607	0	3364	41	0
1	B	2795	0	2628	34	0
2	A	57	0	0	3	0
2	B	55	0	0	1	0
All	All	6514	0	5992	72	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 6.

All (72) 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:210:VAL:HG21	1:A:220:TYR:HB2	1.48	0.92
1:A:327:LYS:HG2	1:A:346:GLU:HG2	1.52	0.90
1:B:327:LYS:HG3	1:B:376:GLN:HA	1.65	0.78
1:A:222:THR:HG21	1:A:245:ILE:HA	1.74	0.69
1:A:248:GLU:OE1	2:A:501:HOH:O	2.09	0.69
1:B:322:ALA:HB2	1:B:347:LEU:HD23	1.76	0.68
1:B:325:ASP:HB3	1:B:376:GLN:HG3	1.79	0.64
1:A:25:ASP:OD1	1:A:25:ASP:N	2.26	0.64
1:A:430:LYS:HD3	1:A:461:ASN:OD1	1.99	0.61
2:A:503:HOH:O	1:B:29:LYS:NZ	2.35	0.60
1:A:284:GLU:HG3	1:B:1:HIS:CG	2.36	0.59
1:B:173:VAL:O	2:B:501:HOH:O	2.16	0.57
1:A:415:ALA:HB1	1:A:431:GLU:HG2	1.86	0.57
1:B:256:GLN:HG3	1:B:266:ILE:HD13	1.87	0.56
1:A:318:LEU:HD12	1:A:357:MET:HE3	1.87	0.56
1:B:334:ASN:HA	1:B:367:HIS:HA	1.86	0.56
1:A:375:ASP:HB3	1:A:381:ILE:HD11	1.89	0.55
1:B:332:VAL:HB	1:B:340:LEU:HB2	1.89	0.55
1:A:308:ILE:HG12	1:A:391:ILE:HD11	1.90	0.54
1:A:325:ASP:HB3	1:A:376:GLN:HG2	1.90	0.53
1:A:198:GLN:NE2	2:A:510:HOH:O	2.38	0.52
1:B:34:GLY:O	1:B:37:GLU:HG2	2.10	0.51
1:B:185:LEU:HB3	1:B:188:TRP:HD1	1.75	0.50
1:B:255:GLY:O	1:B:271:PRO:HG2	2.11	0.50
1:B:332:VAL:HG11	1:B:359:LEU:HD21	1.93	0.49
1:A:255:GLY:O	1:A:271:PRO:HG2	2.12	0.49
1:B:330:MET:HG2	1:B:370:VAL:O	2.12	0.49
1:A:330:MET:HA	1:A:370:VAL:O	2.12	0.48
1:A:341:SER:OG	1:A:357:MET:HB3	2.13	0.48
1:B:361:LYS:HD2	1:B:363:GLU:OE2	2.13	0.48
1:A:139:PRO:HD2	1:A:142:VAL:CG1	2.44	0.47
1:B:327:LYS:O	1:B:374:LYS:HB2	2.14	0.47
1:B:375:ASP:C	1:B:377:GLN:H	2.23	0.47
1:A:8:GLU:HB2	1:A:9:ASN:H	1.50	0.47
1:A:20:ARG:HB2	1:A:37:GLU:O	2.15	0.47
1:B:211:PHE:CE1	1:B:215:GLY:HA2	2.50	0.47
1:A:25:ASP:OD1	1:A:81:ARG:NH2	2.48	0.46
1:B:89:HIS:HA	1:B:144:HIS:O	2.16	0.46
1:A:1:HIS:HA	1:A:170:PHE:CZ	2.51	0.45
1:A:298:LEU:HD13	1:A:326:ILE:HD11	1.99	0.45
1:A:413:TYR:CD1	1:A:417:THR:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:C	1:A:8:GLU:HG2	2.42	0.45
1:A:427:TYR:CD1	1:A:450:PRO:HB3	2.52	0.45
1:B:325:ASP:HB3	1:B:376:GLN:CG	2.46	0.45
1:A:18:LEU:HB2	1:A:30:ASN:ND2	2.32	0.44
1:A:427:TYR:CG	1:A:450:PRO:HB3	2.52	0.44
1:A:330:MET:O	1:A:342:SER:HA	2.17	0.44
1:B:104:LYS:HG2	1:B:130:VAL:HG22	1.99	0.44
1:A:410:LEU:HA	1:A:413:TYR:CE2	2.53	0.44
1:A:1:HIS:CG	1:B:284:GLU:HG3	2.53	0.43
1:A:284:GLU:HG3	1:B:1:HIS:CD2	2.54	0.43
1:B:87:ASN:ND2	1:B:145:LEU:HD21	2.34	0.43
1:B:335:HIS:HB2	1:B:366:HIS:HB3	2.00	0.43
1:A:299:GLU:HG2	1:A:301:TYR:CZ	2.54	0.43
1:A:189:ASN:O	1:A:273:TYR:HA	2.18	0.42
1:B:85:SER:HB3	1:B:150:GLU:HA	2.02	0.42
1:B:157:ILE:O	1:B:174:ILE:N	2.51	0.42
1:B:372:VAL:HG11	1:B:374:LYS:HE3	2.01	0.42
1:A:188:TRP:CZ2	1:A:275:LYS:HD3	2.55	0.42
1:B:86:GLY:O	1:B:148:VAL:N	2.52	0.42
1:A:90:PHE:O	1:A:143:SER:HA	2.20	0.41
1:A:343:HIS:NE2	1:A:345:ALA:HB2	2.35	0.41
1:A:432:PHE:HA	1:A:433:PRO:HA	1.74	0.41
1:B:333:TYR:HA	1:B:338:GLU:O	2.19	0.41
1:B:373:VAL:O	1:B:381:ILE:HB	2.19	0.41
1:A:74:THR:OG1	1:A:77:ARG:HB2	2.21	0.41
1:A:33:CYS:O	1:A:36:ILE:HG22	2.20	0.41
1:A:430:LYS:HG3	1:A:431:GLU:N	2.36	0.41
1:B:23:ALA:HB1	1:B:81:ARG:NH1	2.36	0.41
1:B:382:GLU:HG2	1:B:384:ASN:HD21	1.84	0.41
1:A:185:LEU:HB3	1:A:188:TRP:HB2	2.02	0.41
1:B:335:HIS:N	1:B:366:HIS:O	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	462/464 (100%)	434 (94%)	28 (6%)	0	100	100
1	B	356/464 (77%)	319 (90%)	34 (10%)	3 (1%)	16	17
All	All	818/928 (88%)	753 (92%)	62 (8%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	LYS
1	B	258	ASN
1	B	376	GLN

5.3.2 Protein sidechains ⓘ

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	392/392 (100%)	384 (98%)	8 (2%)	48	63
1	B	304/392 (78%)	293 (96%)	11 (4%)	31	41
All	All	696/784 (89%)	677 (97%)	19 (3%)	39	52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	25	ASP
1	A	177	LYS
1	A	184	VAL
1	A	252	LEU
1	A	295	GLU
1	A	338	GLU
1	A	359	LEU
1	B	85	SER
1	B	99	ILE

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Mol	Chain	Res	Type
1	B	163	VAL
1	B	219	SER
1	B	229	GLU
1	B	252	LEU
1	B	278	SER
1	B	352	VAL
1	B	370	VAL
1	B	373	VAL
1	B	380	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	198	GLN
1	A	213	GLN
1	A	239	HIS
1	A	376	GLN
1	B	1	HIS
1	B	24	ASN
1	B	201	ASN
1	B	239	HIS
1	B	253	GLN
1	B	290	ASN
1	B	384	ASN

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 oligosaccharides 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

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	464/464 (100%)	0.56	23 (4%) 34 40	56, 84, 133, 175	0
1	B	360/464 (77%)	0.77	47 (13%) 7 8	48, 81, 164, 190	0
All	All	824/928 (88%)	0.65	70 (8%) 16 18	48, 83, 153, 190	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	VAL	5.0
1	B	259	ALA	4.7
1	B	352	VAL	4.4
1	B	337	HIS	4.1
1	B	386	LEU	4.0
1	B	257	LEU	3.8
1	B	390	LEU	3.7
1	A	183	PRO	3.6
1	B	347	LEU	3.6
1	B	359	LEU	3.5
1	A	437	TYR	3.4
1	B	184	VAL	3.4
1	B	183	PRO	3.3
1	B	361	LYS	3.3
1	B	261	GLY	3.2
1	B	333	TYR	3.2
1	B	185	LEU	3.1
1	A	259	ALA	3.1
1	B	323	THR	3.1
1	B	369	LEU	3.0
1	A	185	LEU	2.9
1	B	370	VAL	2.9
1	B	366	HIS	2.9
1	A	262	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLY	2.8
1	B	267	TYR	2.8
1	A	432	PHE	2.8
1	A	434	PHE	2.8
1	B	357	MET	2.7
1	A	322	ALA	2.7
1	B	389	HIS	2.7
1	A	448	PHE	2.6
1	B	335	HIS	2.6
1	B	345	ALA	2.6
1	B	355	ALA	2.6
1	A	189	ASN	2.6
1	B	371	VAL	2.6
1	A	440	GLN	2.5
1	B	381	ILE	2.5
1	A	214	ASN	2.5
1	B	322	ALA	2.5
1	B	343	HIS	2.5
1	B	348	SER	2.5
1	B	350	GLY	2.4
1	A	335	HIS	2.4
1	B	11	VAL	2.4
1	B	339	SER	2.4
1	A	347	LEU	2.4
1	B	379	LYS	2.3
1	B	193	GLN	2.3
1	B	362	SER	2.3
1	A	461	ASN	2.3
1	B	372	VAL	2.3
1	B	186	PRO	2.2
1	A	326	ILE	2.2
1	B	380	VAL	2.2
1	A	292	THR	2.2
1	B	358	THR	2.2
1	B	340	LEU	2.1
1	A	184	VAL	2.1
1	B	378	GLY	2.1
1	A	320	LEU	2.1
1	A	263	ILE	2.1
1	A	447	GLN	2.1
1	A	256	GLN	2.0
1	B	383	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	177	LYS	2.0
1	A	188	TRP	2.0
1	B	368	MET	2.0
1	B	385	THR	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.