



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:07 am BST

PDB ID : 3OF0
Title : crystal structure of the L317I mutant of the chicken c-Src tyrosine kinase domain
Authors : Boubeva, R.; Pernot, L.; Perozzo, R.; Scapozza, L.
Deposited on : 2010-08-13
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

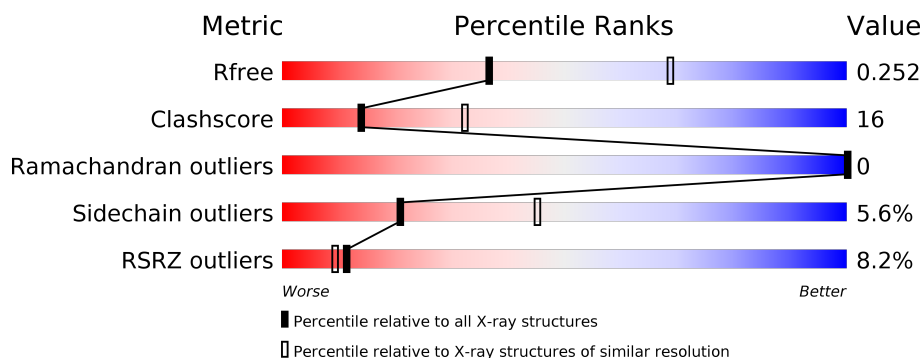
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	286	<div> <div>7%</div> <div>61%</div> <div>28%</div> <div>• 9%</div> </div>
1	B	286	<div> <div>7%</div> <div>57%</div> <div>29%</div> <div>• 12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4297 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 Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2066	1325	348	377	16			
1	B	251	Total	C	N	O	S	0	0	0
			1990	1277	332	365	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P00523
A	249	HIS	-	EXPRESSION TAG	UNP P00523
A	250	MET	-	EXPRESSION TAG	UNP P00523
A	317	ILE	LEU	ENGINEERED MUTATION	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523
B	317	ILE	LEU	ENGINEERED MUTATION	UNP P00523

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	133	Total	O	0	0
			133	133		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.07Å 63.50Å 74.13Å 78.66° 89.41° 90.00°	Depositor
Resolution (Å)	32.78 – 2.70 32.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (32.78-2.70) 97.4 (32.78-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.233 , 0.262 0.224 , 0.252	Depositor DCC
R_{free} test set	977 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.69% 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	0.26	0/2116	0.43	0/2866
1	B	0.23	0/2036	0.41	0/2755
All	All	0.25	0/4152	0.42	0/5621

There are no bond length outliers.

There are no bond angle outliers.

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	2066	0	2027	63	0
1	B	1990	0	1942	63	0
2	A	108	0	0	3	0
2	B	133	0	0	3	0
All	All	4297	0	3969	126	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 16.

All (126) 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:279:GLY:HA2	1:A:298:LYS:HD3	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ARG:HD3	1:B:505:GLU:HB3	1.53	0.89
1:A:280:GLU:HG3	1:A:298:LYS:HE2	1.54	0.88
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.53	0.87
1:A:260:TRP:HE1	1:A:315:LYS:HG2	1.44	0.82
1:A:257:LYS:CG	1:A:258:ASP:H	1.93	0.81
1:B:359:ARG:HD3	2:B:191:HOH:O	1.84	0.77
1:A:260:TRP:HB3	1:A:328:VAL:HG22	1.66	0.77
1:B:257:LYS:HG2	1:B:261:GLU:HG3	1.67	0.77
1:B:311:ALA:HB1	1:B:315:LYS:HE3	1.68	0.76
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.73	0.70
1:A:297:LEU:HD23	1:A:334:ILE:HG13	1.74	0.69
1:A:297:LEU:HD12	1:A:298:LYS:N	2.09	0.67
1:B:309:GLN:O	1:B:313:VAL:HG23	1.95	0.67
1:A:350:LEU:HD21	1:A:455:LEU:HA	1.74	0.67
1:A:359:ARG:HB3	1:A:361:PRO:HD2	1.76	0.67
1:B:257:LYS:CG	1:B:261:GLU:HG3	2.25	0.67
1:B:350:LEU:HD21	1:B:455:LEU:HA	1.76	0.67
1:A:279:GLY:HA3	1:A:296:THR:O	1.96	0.66
1:A:384:HIS:O	1:A:385:ARG:HB2	1.93	0.66
1:A:521:THR:O	1:A:525:PRO:HG3	1.96	0.66
1:B:384:HIS:O	1:B:385:ARG:HB2	1.97	0.63
1:A:257:LYS:HG2	1:A:258:ASP:H	1.62	0.63
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.81	0.62
1:B:320:GLU:O	1:B:401:LYS:HE2	1.98	0.62
1:B:382:TYR:HB3	1:B:405:PHE:HZ	1.63	0.62
1:A:309:GLN:O	1:A:313:VAL:HG23	1.99	0.61
1:A:257:LYS:CG	1:A:258:ASP:N	2.64	0.60
1:B:351:LYS:HB3	2:B:160:HOH:O	2.01	0.60
1:A:260:TRP:HE1	1:A:315:LYS:CG	2.15	0.59
1:B:267:LEU:HD21	1:B:337:VAL:HG21	1.84	0.58
1:A:380:MET:HB2	1:A:382:TYR:HD2	1.69	0.58
1:A:467:VAL:HG22	1:A:470:GLU:HG3	1.85	0.58
1:A:343:LYS:HB2	1:A:394:VAL:HB	1.86	0.57
1:A:319:HIS:HB3	1:A:322:LEU:HD12	1.85	0.57
1:B:359:ARG:HA	2:B:191:HOH:O	2.04	0.57
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.87	0.57
1:B:319:HIS:HB3	1:B:322:LEU:HD12	1.86	0.56
1:A:383:VAL:O	1:A:405:PHE:HE1	1.88	0.56
1:A:279:GLY:HA2	1:A:298:LYS:CD	2.28	0.56
1:A:275:GLN:OE1	1:A:280:GLU:HG2	2.07	0.54
1:A:269:LEU:HB3	1:A:282:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLU:HG3	1:B:284:GLY:HA2	1.91	0.52
1:B:275:GLN:NE2	1:B:280:GLU:HG2	2.24	0.52
1:B:346:LEU:O	1:B:350:LEU:HB2	2.10	0.52
1:A:278:PHE:O	1:A:297:LEU:HA	2.12	0.50
1:A:493:ASP:O	1:A:497:GLN:HG3	2.11	0.50
1:B:383:VAL:HG12	1:B:385:ARG:HG3	1.93	0.50
1:A:511:TYR:C	1:A:511:TYR:CD2	2.85	0.50
1:B:267:LEU:HD13	1:B:335:TYR:HD2	1.77	0.50
1:A:365:ASP:O	1:A:369:GLN:HG3	2.11	0.49
1:B:365:ASP:O	1:B:369:GLN:HG3	2.11	0.49
1:B:446:TRP:CE3	1:B:499:TRP:HA	2.47	0.49
1:B:277:CYS:O	1:B:278:PHE:HD1	1.96	0.49
1:B:313:VAL:HG12	1:B:405:PHE:HE1	1.78	0.49
1:A:432:GLU:HG2	1:A:433:ALA:N	2.27	0.48
1:B:380:MET:CB	1:B:382:TYR:HD2	2.26	0.48
1:B:511:TYR:C	1:B:511:TYR:CD2	2.86	0.48
1:B:276:GLY:C	1:B:278:PHE:H	2.17	0.48
1:A:321:LYS:HE3	2:A:67:HOH:O	2.13	0.48
1:B:269:LEU:HD22	1:B:294:ILE:HD12	1.94	0.48
1:B:363:LEU:HD23	1:B:366:MET:CE	2.44	0.47
1:A:277:CYS:C	1:A:278:PHE:HD1	2.18	0.47
1:B:311:ALA:HB1	1:B:315:LYS:CE	2.43	0.47
1:B:467:VAL:O	1:B:471:VAL:HG23	2.14	0.47
1:B:347:LEU:O	1:B:351:LYS:HG2	2.14	0.47
1:A:257:LYS:HD3	1:A:261:GLU:HG3	1.97	0.47
1:B:308:LEU:O	1:B:312:GLN:HG2	2.15	0.47
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.51	0.46
1:A:363:LEU:HD23	1:A:366:MET:CE	2.44	0.46
1:A:527:TYR:OH	1:A:533:LEU:OXT	2.33	0.46
1:A:257:LYS:HG3	1:A:258:ASP:H	1.75	0.46
1:B:277:CYS:C	1:B:278:PHE:HD1	2.19	0.46
1:A:273:LEU:HB2	1:A:281:VAL:HG12	1.97	0.46
1:A:511:TYR:HE2	1:A:515:PHE:HB2	1.81	0.46
1:A:511:TYR:CE2	1:A:515:PHE:HB2	2.51	0.45
1:B:424:PHE:HA	1:B:425:PRO:HD3	1.79	0.45
1:B:532:ASN:O	1:B:533:LEU:HD23	2.16	0.45
1:B:263:PRO:HD2	1:B:266:SER:OG	2.17	0.45
1:B:380:MET:HB3	1:B:382:TYR:CD2	2.51	0.45
1:B:438:ARG:HD3	1:B:438:ARG:HA	1.68	0.45
1:A:346:LEU:O	1:A:350:LEU:HB2	2.16	0.45
1:A:384:HIS:HA	1:A:405:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.51	0.44
1:A:511:TYR:C	1:A:511:TYR:HD2	2.21	0.44
1:A:297:LEU:HD12	1:A:298:LYS:H	1.83	0.44
1:B:325:LEU:HD12	1:B:337:VAL:O	2.18	0.44
1:B:493:ASP:O	1:B:497:GLN:HG3	2.18	0.44
1:A:360:LEU:N	1:A:361:PRO:CD	2.81	0.44
1:A:502:ASP:O	1:A:505:GLU:HB2	2.18	0.44
1:A:380:MET:HB2	1:A:382:TYR:CD2	2.52	0.44
1:B:511:TYR:CE2	1:B:515:PHE:HB2	2.53	0.44
1:B:500:ARG:O	1:B:506:ARG:NH1	2.42	0.43
1:A:491:LEU:O	1:A:495:MET:HG3	2.18	0.43
1:B:502:ASP:O	1:B:505:GLU:HB2	2.18	0.43
1:B:314:MET:O	1:B:317:ILE:HB	2.18	0.43
1:A:494:LEU:HD22	1:A:515:PHE:CE2	2.54	0.43
1:A:424:PHE:HA	1:A:425:PRO:HD3	1.84	0.43
1:B:340:TYR:CE2	1:B:342:SER:HA	2.54	0.43
1:B:446:TRP:HA	1:B:498:CYS:O	2.18	0.43
1:B:485:PRO:O	1:B:486:GLU:HB2	2.19	0.43
1:B:276:GLY:C	1:B:278:PHE:N	2.72	0.43
1:A:258:ASP:OD1	1:A:259:ALA:N	2.52	0.43
1:A:501:LYS:HE3	1:A:501:LYS:HB2	1.60	0.42
1:B:360:LEU:N	1:B:361:PRO:CD	2.82	0.42
1:B:380:MET:HB3	1:B:382:TYR:HD2	1.84	0.42
1:B:506:ARG:HA	1:B:507:PRO:HD3	1.87	0.42
1:A:467:VAL:O	1:A:471:VAL:HG23	2.19	0.42
1:B:432:GLU:HG2	1:B:433:ALA:N	2.35	0.42
1:A:277:CYS:HA	2:A:163:HOH:O	2.18	0.42
1:A:356:LYS:HB3	1:A:356:LYS:NZ	2.34	0.42
1:A:485:PRO:O	1:A:486:GLU:HB2	2.19	0.42
1:B:309:GLN:C	1:B:311:ALA:N	2.71	0.42
1:A:317:ILE:HG23	1:A:376:TYR:HE2	1.85	0.41
1:A:323:VAL:HG21	1:A:403:ALA:HB2	2.02	0.41
1:B:349:PHE:CE2	1:B:358:LEU:HD11	2.55	0.41
1:A:432:GLU:OE2	1:A:506:ARG:NH2	2.53	0.41
1:B:511:TYR:HE2	1:B:515:PHE:HB2	1.85	0.41
1:A:504:GLU:HB2	2:A:38:HOH:O	2.21	0.41
1:B:382:TYR:HB3	1:B:405:PHE:CZ	2.49	0.41
1:A:283:MET:HG2	1:A:291:ARG:HH11	1.85	0.41
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.56	0.41
1:A:461:VAL:HA	1:A:462:PRO:HD3	1.92	0.41
1:B:258:ASP:OD1	1:B:260:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:TYR:HD2	1:B:511:TYR:C	2.25	0.40
1:B:497:GLN:O	1:B:506:ARG:HG3	2.22	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	256/286 (90%)	242 (94%)	14 (6%)	0	100	100
1	B	243/286 (85%)	228 (94%)	15 (6%)	0	100	100
All	All	499/572 (87%)	470 (94%)	29 (6%)	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	217/245 (89%)	207 (95%)	10 (5%)	27	54
1	B	209/245 (85%)	195 (93%)	14 (7%)	16	37
All	All	426/490 (87%)	402 (94%)	24 (6%)	21	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	CYS
1	A	290	THR
1	A	315	LYS
1	A	356	LYS
1	A	360	LEU
1	A	397	ASN
1	A	474	GLN
1	A	477	ARG
1	A	493	ASP
1	A	511	TYR
1	B	258	ASP
1	B	269	LEU
1	B	275	GLN
1	B	289	THR
1	B	290	THR
1	B	291	ARG
1	B	318	ARG
1	B	336	ILE
1	B	351	LYS
1	B	360	LEU
1	B	397	ASN
1	B	438	ARG
1	B	501	LYS
1	B	511	TYR

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

Mol	Chain	Res	Type
1	A	312	GLN
1	A	397	ASN
1	B	312	GLN
1	B	397	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 [i](#)

There are no carbohydrates 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	260/286 (90%)	0.32	21 (8%) 12 10	11, 32, 104, 124	0
1	B	251/286 (87%)	0.48	21 (8%) 11 9	11, 30, 96, 128	0
All	All	511/572 (89%)	0.39	42 (8%) 11 9	11, 31, 101, 128	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	GLU	10.3
1	B	306	ALA	9.9
1	B	303	SER	7.6
1	B	311	ALA	7.2
1	B	278	PHE	7.1
1	B	276	GLY	6.5
1	B	307	PHE	6.4
1	B	277	CYS	5.3
1	B	289	THR	4.8
1	A	306	ALA	4.6
1	B	313	VAL	4.6
1	B	288	GLY	4.3
1	A	300	GLY	4.2
1	A	297	LEU	4.0
1	A	301	THR	4.0
1	A	271	VAL	4.0
1	A	477	ARG	3.9
1	A	473	ASP	3.7
1	B	309	GLN	3.6
1	A	278	PHE	3.4
1	A	311	ALA	3.3
1	A	299	PRO	3.2
1	B	477	ARG	3.2
1	A	309	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	308	LEU	3.0
1	B	274	GLY	3.0
1	B	269	LEU	2.9
1	B	424	PHE	2.9
1	A	277	CYS	2.9
1	B	275	GLN	2.8
1	A	316	LYS	2.8
1	B	271	VAL	2.8
1	A	313	VAL	2.8
1	B	473	ASP	2.8
1	B	304	PRO	2.7
1	A	305	GLU	2.7
1	A	275	GLN	2.4
1	A	307	PHE	2.3
1	A	405	PHE	2.2
1	A	288	GLY	2.1
1	A	289	THR	2.0
1	A	315	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 carbohydrates 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.