



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:17 PM EST

PDB ID : 5TUB
Title : Crystal Structure of the Shark TBC1D15 GAP Domain
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Deposited on : 2016-11-05
Resolution : 2.85 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

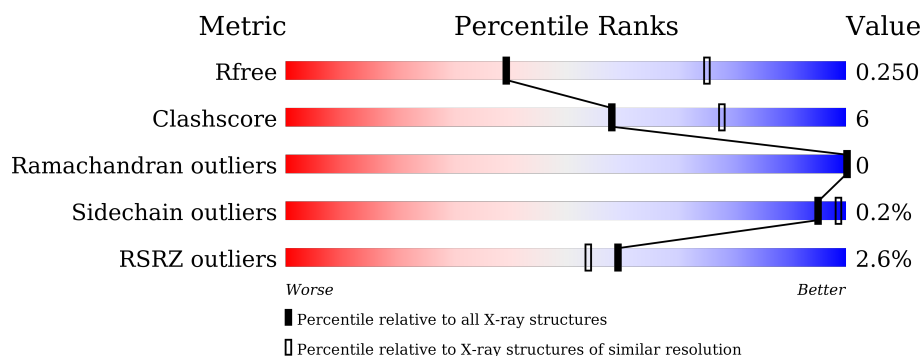
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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. 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	348	<div> <div>0%</div> <div>78% 19% .</div> </div>
1	B	348	<div> <div>2%</div> <div>84% 12% .</div> </div>
1	C	348	<div> <div>0%</div> <div>78% 17% 5%</div> </div>
1	D	348	<div> <div>6%</div> <div>82% 14% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11231 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 Shark TBC1D15 GTPase-activating Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2807	1811	466	505	25			
1	B	334	Total	C	N	O	S	0	0	0
			2798	1805	464	504	25			
1	C	330	Total	C	N	O	S	0	0	0
			2759	1779	458	497	25			
1	D	333	Total	C	N	O	S	0	0	0
			2784	1793	463	503	25			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	21	Total	O	0	0
			21	21		
2	C	26	Total	O	0	0
			26	26		
2	D	16	Total	O	0	0
			16	16		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.79 Å 149.74 Å 95.03 Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	47.26 – 2.85 48.59 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.26-2.85) 100.0 (48.59-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.86 Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.215 , 0.248 0.218 , 0.250	Depositor DCC
R_{free} test set	4813 reflections (6.94%)	DCC
Wilson B-factor (Å ²)	69.8	Xtrriage
Anisotropy	0.492	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11231	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.35	0/2872	0.51	0/3867
1	B	0.33	0/2863	0.49	0/3856
1	C	0.33	0/2823	0.49	0/3801
1	D	0.30	0/2848	0.50	1/3836 (0.0%)
All	All	0.33	0/11406	0.50	1/15360 (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	D	334	GLY	N-CA-C	7.51	131.87	113.10

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	2807	0	2789	44	0
1	B	2798	0	2776	25	0
1	C	2759	0	2736	40	0
1	D	2784	0	2758	28	0
2	A	20	0	0	0	0
2	B	21	0	0	0	0
2	C	26	0	0	1	0
2	D	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11231	0	11059	132	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 (132) 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:D:384:PRO:HG2	1:D:387:SER:HB3	1.64	0.79
1:B:384:PRO:HG2	1:B:387:SER:HB3	1.64	0.77
1:C:384:PRO:HG2	1:C:387:SER:HB3	1.68	0.75
1:C:433:LYS:HE2	1:C:437:ARG:HH22	1.58	0.68
1:A:384:PRO:HG2	1:A:387:SER:HB3	1.76	0.67
1:D:335:GLU:O	1:D:365:GLY:HA3	1.95	0.67
1:C:438:THR:HG22	1:C:439:ASP:H	1.60	0.67
1:A:595:GLN:NE2	1:C:602:TYR:O	2.28	0.66
1:C:350:GLY:O	1:C:392:ARG:NH2	2.28	0.65
1:C:376:TRP:HE1	1:C:570:GLU:HG2	1.61	0.65
1:D:402:GLU:HG3	1:D:405:ARG:HH21	1.63	0.64
1:D:362:ILE:HG12	1:D:367:LEU:HD21	1.80	0.64
1:A:436:ASN:O	1:A:440:ARG:NH2	2.32	0.62
1:A:514:GLY:HA2	1:A:517:THR:HB	1.80	0.62
1:B:402:GLU:HG3	1:B:405:ARG:HH21	1.65	0.61
1:B:427:TYR:CZ	1:B:471:GLY:HA3	2.36	0.61
1:C:514:GLY:HA2	1:C:517:THR:HB	1.83	0.61
1:B:366:GLY:HA3	1:B:567:ARG:HH21	1.68	0.59
1:C:372:ARG:NE	1:C:570:GLU:OE2	2.28	0.59
1:B:350:GLY:O	1:B:392:ARG:NH2	2.36	0.59
1:C:362:ILE:HG12	1:C:367:LEU:HD21	1.84	0.59
1:C:523:SER:HB2	1:C:534:TRP:HE1	1.68	0.59
1:A:402:GLU:HG3	1:A:405:ARG:HH21	1.68	0.59
1:A:322:ARG:HA	1:C:550:ARG:HD3	1.85	0.59
1:A:433:LYS:HE2	1:A:437:ARG:HH22	1.67	0.58
1:D:547:PHE:HB2	1:D:611:ILE:HD12	1.86	0.58
1:A:372:ARG:NE	1:A:570:GLU:OE2	2.28	0.57
1:B:438:THR:HG22	1:B:439:ASP:H	1.69	0.57
1:D:416:GLU:HG2	1:D:420:ARG:HH22	1.69	0.57
1:A:568:LEU:HD11	1:A:585:ILE:HD13	1.85	0.57
1:C:368:CYS:SG	1:C:371:VAL:HG23	2.45	0.57
1:A:416:GLU:HB3	1:A:420:ARG:HH22	1.70	0.55
1:C:402:GLU:HG3	1:C:405:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLU:HG3	1:A:614:LEU:HD11	1.88	0.55
1:C:433:LYS:HE2	1:C:437:ARG:NH2	2.21	0.54
1:A:383:PHE:CD2	1:A:392:ARG:HD3	2.43	0.54
1:D:400:THR:HG23	1:D:491:VAL:HG21	1.90	0.54
1:B:514:GLY:HA2	1:B:517:THR:HB	1.88	0.54
1:B:554:ILE:HG22	1:B:557:LYS:HB3	1.89	0.54
1:C:588:ALA:HB1	1:C:626:LYS:HB3	1.90	0.53
1:C:427:TYR:CZ	1:C:471:GLY:HA3	2.44	0.52
1:C:366:GLY:HA3	1:C:567:ARG:HH21	1.74	0.52
1:A:376:TRP:HE1	1:A:570:GLU:HG2	1.74	0.52
1:A:550:ARG:HD3	1:B:322:ARG:HA	1.92	0.52
1:C:354:ASP:OD2	1:C:357:ASN:ND2	2.43	0.52
1:A:514:GLY:H	1:A:517:THR:H	1.57	0.51
1:C:514:GLY:H	1:C:517:THR:H	1.57	0.51
1:D:342:TRP:HE1	1:D:374:LEU:HD23	1.75	0.51
1:D:416:GLU:HG2	1:D:420:ARG:HH12	1.76	0.51
1:D:333:ARG:HB2	1:D:364:ARG:O	2.11	0.51
1:A:536:TYR:CD1	1:C:541:GLU:HG2	2.46	0.50
1:A:554:ILE:HG22	1:A:557:LYS:HB3	1.94	0.50
1:B:528:LEU:HD22	1:B:644:VAL:HG21	1.93	0.50
1:B:377:LYS:HG2	1:B:382:TYR:HD2	1.75	0.50
1:C:528:LEU:HD22	1:C:644:VAL:HG21	1.94	0.50
1:B:362:ILE:HG12	1:B:367:LEU:HD21	1.94	0.50
1:D:547:PHE:HB2	1:D:611:ILE:CD1	2.42	0.49
1:A:434:ASP:O	1:A:438:THR:OG1	2.29	0.49
1:D:371:VAL:HG12	1:D:375:THR:HG23	1.94	0.49
1:C:620:VAL:HG23	2:C:704:HOH:O	2.13	0.49
1:D:472:TYR:CE1	1:D:476:MET:HB2	2.48	0.49
1:A:380:LEU:HD13	1:A:496:CYS:HB3	1.94	0.49
1:C:578:CYS:HB3	1:C:631:TYR:CE1	2.48	0.49
1:D:366:GLY:HA3	1:D:567:ARG:HH21	1.78	0.49
1:B:366:GLY:HA3	1:B:567:ARG:NH2	2.27	0.48
1:A:368:CYS:SG	1:A:371:VAL:HG23	2.54	0.48
1:C:413:VAL:HG13	1:C:417:GLN:HB3	1.94	0.48
1:A:320:ILE:O	1:A:323:ILE:HG22	2.14	0.48
1:A:366:GLY:HA3	1:A:567:ARG:NH2	2.29	0.48
1:B:320:ILE:HD11	1:B:531:LEU:HD13	1.96	0.48
1:B:369:HIS:HA	1:B:372:ARG:HD2	1.94	0.48
1:C:402:GLU:HG3	1:C:405:ARG:HH21	1.78	0.47
1:A:350:GLY:O	1:A:392:ARG:NH2	2.38	0.47
1:A:386:ASP:OD1	1:A:386:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ASP:OD2	1:D:357:ASN:ND2	2.47	0.47
1:C:371:VAL:HG12	1:C:375:THR:HG23	1.96	0.47
1:B:342:TRP:HE1	1:B:374:LEU:HD23	1.79	0.47
1:C:376:TRP:NE1	1:C:570:GLU:HG2	2.30	0.47
1:D:448:HIS:CD2	1:D:449:GLU:HG3	2.50	0.47
1:D:386:ASP:OD1	1:D:386:ASP:N	2.44	0.47
1:A:377:LYS:HG2	1:A:382:TYR:HD2	1.80	0.46
1:C:568:LEU:HD11	1:C:585:ILE:HD13	1.98	0.46
1:C:325:LEU:HB3	1:C:633:GLN:HG2	1.98	0.46
1:A:440:ARG:O	1:A:446:GLU:HB3	2.16	0.46
1:C:377:LYS:HG2	1:C:382:TYR:HD2	1.80	0.46
1:C:366:GLY:HA3	1:C:567:ARG:NH2	2.30	0.46
1:D:536:TYR:CZ	1:D:598:MET:HA	2.51	0.46
1:B:317:PHE:HB2	1:B:527:LYS:NZ	2.31	0.46
1:A:377:LYS:HE3	1:A:487:MET:SD	2.57	0.45
1:A:362:ILE:HG12	1:A:367:LEU:HD21	1.99	0.45
1:C:489:ASN:HD22	1:C:492:ASP:CG	2.20	0.45
1:C:333:ARG:HG2	1:C:625:CYS:SG	2.57	0.45
1:A:366:GLY:HA3	1:A:567:ARG:HH21	1.82	0.44
1:A:450:ASN:HA	1:A:451:PRO:HD3	1.89	0.44
1:C:481:SER:HB3	1:C:482:PRO:HD3	1.99	0.44
1:D:358:VAL:O	1:D:362:ILE:HG13	2.18	0.44
1:C:337:VAL:HB	1:C:367:LEU:HD23	1.99	0.44
1:A:414:SER:OG	1:A:417:GLN:HB2	2.18	0.44
1:A:376:TRP:HE1	1:A:570:GLU:CG	2.30	0.44
1:C:376:TRP:HE1	1:C:570:GLU:CG	2.30	0.44
1:B:414:SER:OG	1:B:417:GLN:HB2	2.17	0.44
1:B:372:ARG:NE	1:B:570:GLU:OE2	2.34	0.44
1:B:386:ASP:N	1:B:386:ASP:OD1	2.47	0.44
1:C:586:CYS:O	1:C:590:LEU:HB2	2.17	0.44
1:D:514:GLY:HA2	1:D:517:THR:HB	2.00	0.44
1:A:367:LEU:HB2	1:A:570:GLU:OE2	2.18	0.43
1:B:578:CYS:HB3	1:B:631:TYR:CE1	2.53	0.43
1:D:562:PHE:O	1:D:566:LEU:HG	2.17	0.43
1:A:442:ASN:HA	1:A:443:PRO:HD3	1.89	0.43
1:A:626:LYS:O	1:A:630:ILE:HG13	2.19	0.42
1:A:481:SER:HB3	1:A:482:PRO:HD3	2.00	0.42
1:D:597:ILE:HA	1:D:602:TYR:CD2	2.54	0.42
1:A:371:VAL:HG12	1:A:375:THR:HG23	2.01	0.42
1:D:427:TYR:CZ	1:D:471:GLY:HA3	2.53	0.42
1:C:536:TYR:OH	1:C:540:GLN:NE2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:N	1:C:567:ARG:HH22	2.17	0.42
1:B:527:LYS:HG3	1:B:534:TRP:CD2	2.55	0.42
1:B:602:TYR:HB3	1:B:606:GLU:HB2	2.02	0.42
1:A:323:ILE:HD13	1:A:528:LEU:HD11	2.01	0.41
1:A:402:GLU:HG3	1:A:405:ARG:NH2	2.34	0.41
1:D:377:LYS:HE3	1:D:487:MET:SD	2.60	0.41
1:D:546:TYR:O	1:D:549:PHE:HB2	2.20	0.41
1:C:478:ASP:OD2	1:C:558:ARG:NH2	2.53	0.41
1:A:427:TYR:CZ	1:A:471:GLY:HA3	2.56	0.41
1:D:560:PHE:CD1	1:D:620:VAL:HG22	2.56	0.41
1:A:503:GLN:HG3	1:A:504:MET:HG3	2.03	0.41
1:D:402:GLU:HG3	1:D:405:ARG:NH2	2.32	0.41
1:A:413:VAL:HG13	1:A:417:GLN:HB3	2.04	0.40
1:A:333:ARG:HH21	1:A:624:LEU:HD13	1.87	0.40
1:B:376:TRP:HE1	1:B:570:GLU:HG2	1.85	0.40
1:A:541:GLU:HG2	1:B:536:TYR:CD1	2.57	0.40
1:D:594:LYS:O	1:D:598:MET:HG3	2.21	0.40

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	333/348 (96%)	326 (98%)	7 (2%)	0	100	100
1	B	332/348 (95%)	325 (98%)	7 (2%)	0	100	100
1	C	328/348 (94%)	323 (98%)	5 (2%)	0	100	100
1	D	331/348 (95%)	327 (99%)	4 (1%)	0	100	100
All	All	1324/1392 (95%)	1301 (98%)	23 (2%)	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	311/323 (96%)	311 (100%)	0	100	100
1	B	310/323 (96%)	309 (100%)	1 (0%)	94	98
1	C	305/323 (94%)	304 (100%)	1 (0%)	94	98
1	D	308/323 (95%)	308 (100%)	0	100	100
All	All	1234/1292 (96%)	1232 (100%)	2 (0%)	95	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	547	PHE
1	C	590	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	600	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 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	335/348 (96%)	0.06	4 (1%) 81 78	48, 69, 103, 135	0
1	B	334/348 (95%)	0.11	7 (2%) 67 62	49, 73, 108, 139	0
1	C	330/348 (94%)	0.16	4 (1%) 81 78	46, 71, 112, 141	0
1	D	333/348 (95%)	0.44	20 (6%) 25 18	53, 98, 136, 152	0
All	All	1332/1392 (95%)	0.19	35 (2%) 59 54	46, 77, 121, 152	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	610	HIS	5.1
1	B	546	TYR	4.0
1	D	319	VAL	3.6
1	D	321	THR	3.3
1	D	320	ILE	3.3
1	C	325	LEU	3.3
1	D	332	GLN	3.1
1	D	323	ILE	3.0
1	D	549	PHE	3.0
1	D	335	GLU	3.0
1	D	342	TRP	2.9
1	B	448	HIS	2.8
1	D	325	LEU	2.7
1	A	424	LEU	2.6
1	A	448	HIS	2.6
1	D	616	LEU	2.5
1	D	357	ASN	2.5
1	B	322	ARG	2.4
1	C	322	ARG	2.4
1	D	554	ILE	2.3
1	D	631	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	2.2
1	D	510	GLU	2.2
1	C	529	LEU	2.2
1	A	651	LYS	2.2
1	D	588	ALA	2.2
1	C	324	ASP	2.1
1	B	326	GLY	2.1
1	D	385	TRP	2.1
1	D	349	GLU	2.1
1	B	511	GLN	2.1
1	D	636	LYS	2.1
1	D	556	PHE	2.1
1	B	513	GLN	2.0
1	B	325	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.