



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 09:52 AM EDT

PDB ID : 3DPU
Title : RocCOR domain tandem of Rab family protein (Roco)
Authors : Gotthardt, K.; Weyand, M.; Kortholt, A.; Van Haastert, P.J.M.; Wittinghofer, A.
Deposited on : unknown
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

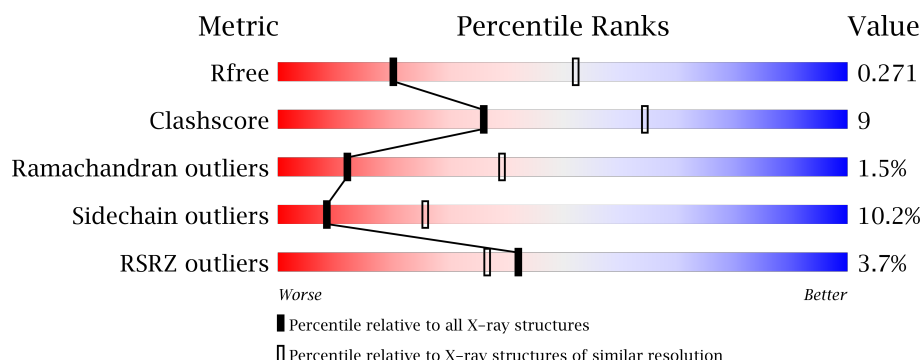
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	535	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	535	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>12%</div> <div>•</div> <div>39%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6235 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 Rab family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3695	2379	603	696	17			
1	B	328	Total	C	N	O	S	0	0	0
			2540	1640	414	475	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	917	ARG	GLU	ENGINEERED	UNP Q8KC98
B	917	ARG	GLU	ENGINEERED	UNP Q8KC98



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.20Å 106.10Å 139.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.90 47.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.90) 98.5 (47.66-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.270 0.230 , 0.271	Depositor DCC
R_{free} test set	1374 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.1	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	0.90	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	0.45	0/3772	0.62	2/5135 (0.0%)
1	B	0.48	0/2592	0.63	0/3527
All	All	0.46	0/6364	0.63	2/8662 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	506	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	518	GLY	N-CA-C	-5.29	99.87	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	517	GLY	Peptide

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	3695	0	3490	78	0
1	B	2540	0	2456	36	0
All	All	6235	0	5946	111	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 9.

All (111) 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:B:729:ASN:HD21	1:B:748:TYR:H	1.11	0.94
1:A:631:SER:HB3	1:A:663:ILE:HD11	1.55	0.88
1:A:421:GLU:HG3	1:A:422:ILE:N	1.95	0.79
1:A:578:ASN:HD22	1:A:579:ILE:H	1.31	0.76
1:A:487:LEU:HD13	1:A:706:TYR:CE1	2.22	0.75
1:A:549:HIS:O	1:A:553:ARG:HG2	1.94	0.68
1:A:812:ARG:HH12	1:A:882:ASN:ND2	1.93	0.66
1:A:453:ILE:CD1	1:A:535:VAL:HG23	2.26	0.66
1:A:553:ARG:NH1	1:B:850:LYS:HD2	2.13	0.64
1:A:487:LEU:HG	1:A:488:ASN:N	2.13	0.62
1:B:417:SER:N	1:B:418:PRO:HD2	2.15	0.61
1:B:875:GLU:O	1:B:879:ILE:HG12	2.00	0.61
1:A:577:TYR:O	1:A:597:ARG:NH1	2.34	0.60
1:A:469:LEU:HD21	1:A:490:VAL:HG21	1.82	0.60
1:A:553:ARG:O	1:A:557:LYS:HG2	2.02	0.59
1:A:453:ILE:HD11	1:A:535:VAL:HG23	1.86	0.58
1:B:429:ALA:HA	1:B:671:THR:HG21	1.84	0.58
1:A:421:GLU:HG2	1:A:675:TYR:HE1	1.69	0.58
1:B:701:VAL:O	1:B:705:VAL:HG12	2.02	0.58
1:A:729:ASN:HD21	1:A:748:TYR:H	1.50	0.58
1:B:917:ARG:HG3	1:B:917:ARG:HH11	1.69	0.58
1:A:578:ASN:HD21	1:A:581:GLN:HE21	1.51	0.57
1:B:729:ASN:HD21	1:B:748:TYR:N	1.94	0.56
1:A:596:HIS:HE1	1:A:612:SER:OG	1.89	0.56
1:B:939:LYS:O	1:B:940:GLU:CB	2.54	0.56
1:A:804:TYR:O	1:A:806:PRO:HD3	2.07	0.54
1:A:921:GLY:O	1:B:909:GLY:HA3	2.08	0.54
1:A:453:ILE:HD12	1:A:535:VAL:HG23	1.89	0.54
1:A:642:ALA:HB1	1:A:649:LEU:HD11	1.88	0.54
1:A:763:PHE:HB3	1:A:765:LEU:HD23	1.90	0.54
1:A:937:ILE:O	1:A:938:SER:CB	2.56	0.53
1:B:682:VAL:HG13	1:B:695:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:TYR:CE1	1:A:559:GLY:HA3	2.45	0.52
1:A:893:PRO:HA	1:A:901:LEU:HD23	1.91	0.52
1:B:795:PRO:HA	1:B:865:LYS:HE2	1.92	0.52
1:A:462:MET:CE	1:A:462:MET:HA	2.39	0.52
1:B:769:GLU:HB2	1:B:775:ILE:HD12	1.92	0.52
1:A:462:MET:HE2	1:A:462:MET:HA	1.92	0.52
1:A:796:LEU:HB2	1:A:865:LYS:HD2	1.92	0.52
1:A:937:ILE:O	1:A:938:SER:HB3	2.11	0.51
1:A:682:VAL:HG13	1:A:695:VAL:HG13	1.93	0.51
1:A:425:GLN:N	1:A:425:GLN:HE21	2.09	0.50
1:A:873:TRP:HZ3	1:A:937:ILE:HD11	1.75	0.50
1:B:417:SER:N	1:B:418:PRO:CD	2.74	0.50
1:A:460:ASP:O	1:A:461:GLY:C	2.50	0.50
1:A:635:VAL:CG2	1:A:672:LEU:HD21	2.42	0.49
1:A:667:GLY:O	1:A:671:THR:HG23	2.11	0.49
1:A:423:VAL:C	1:A:425:GLN:H	2.16	0.49
1:A:904:TYR:CE2	1:A:908:LEU:HD11	2.47	0.49
1:A:578:ASN:HD21	1:A:581:GLN:NE2	2.10	0.49
1:A:424:LYS:C	1:A:425:GLN:HE21	2.16	0.49
1:B:769:GLU:HB2	1:B:775:ILE:CD1	2.43	0.49
1:A:801:LYS:O	1:A:888:VAL:HA	2.13	0.49
1:A:928:SER:HB3	1:A:931:LYS:HB2	1.94	0.49
1:A:432:GLN:OE1	1:A:668:GLU:HB3	2.12	0.48
1:B:659:ASN:OD1	1:B:669:ARG:NH2	2.46	0.48
1:B:863:ARG:O	1:B:867:GLU:HB2	2.12	0.48
1:B:917:ARG:HG3	1:B:917:ARG:NH1	2.28	0.48
1:A:902:VAL:HG11	1:A:932:MET:HE1	1.96	0.47
1:A:564:VAL:HG22	1:A:591:ILE:HG12	1.96	0.47
1:A:421:GLU:CG	1:A:422:ILE:N	2.72	0.47
1:B:677:ASN:HA	1:B:682:VAL:O	2.15	0.47
1:A:646:GLN:O	1:A:648:TYR:N	2.47	0.47
1:A:805:LEU:HD11	1:A:854:ILE:HD11	1.96	0.47
1:B:647:ARG:HG2	1:B:700:TRP:CD1	2.50	0.47
1:B:666:PRO:HA	1:B:669:ARG:HD2	1.96	0.46
1:A:635:VAL:HG22	1:A:672:LEU:HD21	1.97	0.46
1:A:796:LEU:HD12	1:A:865:LYS:HB3	1.98	0.45
1:A:894:LEU:HD12	1:A:932:MET:HE1	1.99	0.45
1:B:835:SER:HB2	1:B:868:TYR:CZ	2.52	0.45
1:A:579:ILE:O	1:A:581:GLN:N	2.50	0.45
1:A:703:ILE:O	1:A:707:ARG:HG3	2.16	0.45
1:B:916:ASP:HA	1:B:929:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ILE:HD13	1:A:454:LYS:N	2.32	0.45
1:B:796:LEU:O	1:B:857:ALA:HA	2.17	0.45
1:B:419:PRO:HB3	1:B:626:THR:HG21	1.98	0.44
1:B:923:LEU:O	1:B:925:LYS:N	2.50	0.44
1:A:429:ALA:HA	1:A:671:THR:HG21	1.99	0.44
1:A:596:HIS:HB3	1:A:598:ILE:HD13	2.00	0.44
1:A:535:VAL:HG22	1:A:616:ALA:HB1	1.99	0.44
1:B:704:GLY:HA3	1:B:756:LEU:HD21	2.00	0.44
1:A:606:VAL:HA	1:A:609:ILE:HD12	2.00	0.44
1:A:553:ARG:CZ	1:B:850:LYS:HD2	2.48	0.44
1:A:498:LYS:O	1:A:501:GLU:CD	2.56	0.43
1:A:460:ASP:OD2	1:A:547:ASN:ND2	2.51	0.43
1:B:780:LEU:O	1:B:828:ARG:NH1	2.51	0.43
1:A:920:SER:OG	1:A:923:LEU:HB2	2.18	0.43
1:A:553:ARG:HG2	1:A:553:ARG:H	1.70	0.43
1:B:915:ARG:HG2	1:B:916:ASP:H	1.83	0.43
1:A:791:THR:HA	1:A:795:PRO:HG2	2.00	0.43
1:A:613:LEU:O	1:A:617:VAL:HG23	2.19	0.42
1:A:806:PRO:HB2	1:A:809:ILE:HG12	2.01	0.42
1:A:529:PHE:HD2	1:A:680:GLY:HA3	1.84	0.42
1:A:749:THR:N	1:A:752:GLU:OE2	2.35	0.42
1:A:529:PHE:CD2	1:A:680:GLY:HA3	2.55	0.42
1:A:527:GLN:H	1:A:527:GLN:HG3	1.39	0.42
1:A:868:TYR:O	1:A:871:ILE:HG13	2.20	0.42
1:A:516:PHE:O	1:A:517:GLY:O	2.38	0.42
1:A:791:THR:HA	1:A:795:PRO:CG	2.51	0.41
1:A:548:LYS:HD2	1:A:584:ILE:HD11	2.02	0.41
1:A:866:ARG:HD3	1:A:934:ASP:O	2.20	0.41
1:B:433:TYR:O	1:B:436:SER:HB2	2.20	0.41
1:A:868:TYR:O	1:A:872:ILE:HG12	2.21	0.41
1:B:768:ASP:OD2	1:B:770:GLY:HA3	2.21	0.41
1:B:766:CYS:HB2	1:B:775:ILE:O	2.20	0.40
1:A:677:ASN:HB2	1:A:684:TYR:HB3	2.03	0.40
1:A:705:VAL:HB	1:A:760:MET:SD	2.61	0.40
1:B:650:ASN:OD1	1:B:653:GLU:HG3	2.21	0.40
1:B:917:ARG:HA	1:B:927:PHE:O	2.21	0.40
1:A:613:LEU:HD23	1:A:613:LEU:HA	1.81	0.40
1:B:750:LEU:O	1:B:753:GLN:HG2	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	475/535 (89%)	445 (94%)	19 (4%)	11 (2%)	7	27
1	B	320/535 (60%)	305 (95%)	14 (4%)	1 (0%)	44	77
All	All	795/1070 (74%)	750 (94%)	33 (4%)	12 (2%)	12	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	ARG
1	A	822	LEU
1	A	884	THR
1	A	424	LYS
1	A	461	GLY
1	A	517	GLY
1	A	839	GLU
1	A	580	GLU
1	A	937	ILE
1	B	924	GLU
1	A	421	GLU
1	A	422	ILE

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	375/482 (78%)	338 (90%)	37 (10%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	263/482 (55%)	235 (89%)	28 (11%)	8	24
All	All	638/964 (66%)	573 (90%)	65 (10%)	8	26

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	GLU
1	A	425	GLN
1	A	450	LEU
1	A	453	ILE
1	A	462	MET
1	A	466	THR
1	A	467	SER
1	A	487	LEU
1	A	488	ASN
1	A	489	VAL
1	A	500	LEU
1	A	506	LEU
1	A	527	GLN
1	A	533	SER
1	A	538	LEU
1	A	539	LEU
1	A	541	ASP
1	A	548	LYS
1	A	553	ARG
1	A	562	SER
1	A	564	VAL
1	A	578	ASN
1	A	615	SER
1	A	623	ILE
1	A	635	VAL
1	A	649	LEU
1	A	652	THR
1	A	654	VAL
1	A	661	SER
1	A	664	THR
1	A	705	VAL
1	A	751	LEU
1	A	791	THR
1	A	853	THR
1	A	894	LEU
1	A	899	ASP

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Mol	Chain	Res	Type
1	A	926	VAL
1	B	421	GLU
1	B	628	LEU
1	B	647	ARG
1	B	688	LEU
1	B	703	ILE
1	B	705	VAL
1	B	710	ASN
1	B	743	ASN
1	B	773	LEU
1	B	783	GLN
1	B	799	ILE
1	B	815	ILE
1	B	817	MET
1	B	828	ARG
1	B	846	VAL
1	B	848	GLU
1	B	850	LYS
1	B	851	ASP
1	B	852	SER
1	B	867	GLU
1	B	869	LEU
1	B	884	THR
1	B	894	LEU
1	B	910	LEU
1	B	915	ARG
1	B	916	ASP
1	B	923	LEU
1	B	929	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	451	GLN
1	A	547	ASN
1	A	549	HIS
1	A	574	ASN
1	A	578	ASN
1	A	596	HIS
1	A	659	ASN
1	A	729	ASN

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Mol	Chain	Res	Type
1	A	779	ASN
1	A	859	GLN
1	A	880	ASN
1	A	882	ASN
1	B	710	ASN
1	B	716	ASN
1	B	729	ASN
1	B	779	ASN
1	B	820	GLN
1	B	885	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	485/535 (90%)	0.18	18 (3%) 42 37	39, 49, 61, 70	0
1	B	328/535 (61%)	0.12	12 (3%) 42 37	38, 52, 60, 66	0
All	All	813/1070 (75%)	0.16	30 (3%) 42 37	38, 50, 61, 70	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	664	THR	4.2
1	B	627	PRO	3.0
1	A	486	GLY	3.0
1	A	462	MET	3.0
1	A	663	ILE	2.9
1	A	838	HIS	2.8
1	B	681	ILE	2.8
1	A	706	TYR	2.8
1	B	680	GLY	2.8
1	B	436	SER	2.8
1	A	445	GLU	2.7
1	A	437	ILE	2.6
1	A	461	GLY	2.6
1	A	784	ILE	2.5
1	B	676	LEU	2.5
1	A	898	PRO	2.5
1	A	842	LEU	2.5
1	B	629	ALA	2.4
1	B	442	SER	2.4
1	A	843	ALA	2.3
1	B	630	PRO	2.3
1	A	474	GLY	2.3
1	B	743	ASN	2.2
1	A	659	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	660	ASP	2.2
1	B	916	ASP	2.2
1	A	772	GLY	2.1
1	B	661	SER	2.0
1	B	660	ASP	2.0
1	A	569	ASN	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.