



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 01:39 AM EDT

PDB ID : 6N8S
Title : Crystal structure of the human cell polarity protein Lethal Giant Larvae 2 (Lgl2). aPKC phosphorylated, crystal form 3.
Authors : Almagor, L.; Weis, W.I.
Deposited on : 2018-11-30
Resolution : 3.90 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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

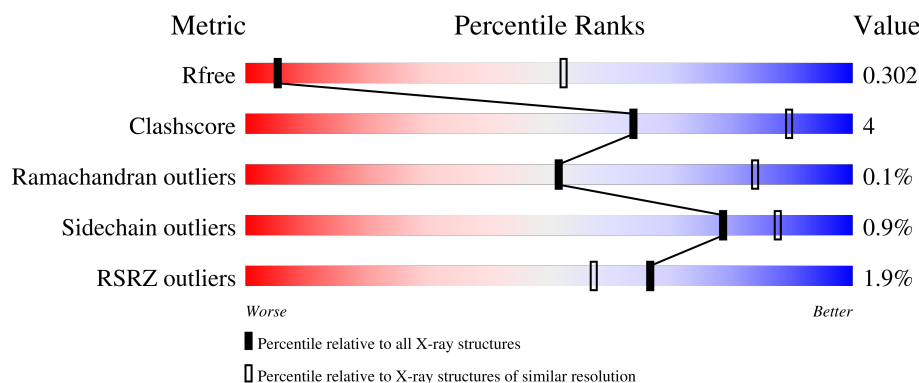
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	979	<div> <div> <div>0%</div> <div>74%</div> <div>11%</div> <div>15%</div> </div> </div>
1	D	979	<div> <div>2%</div> <div>75%</div> <div>9%</div> <div>15%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12829 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 Lethal(2) giant larvae protein homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6434	4116	1110	1185	23			
1	D	830	Total	C	N	O	S	0	0	0
			6395	4098	1101	1172	24			

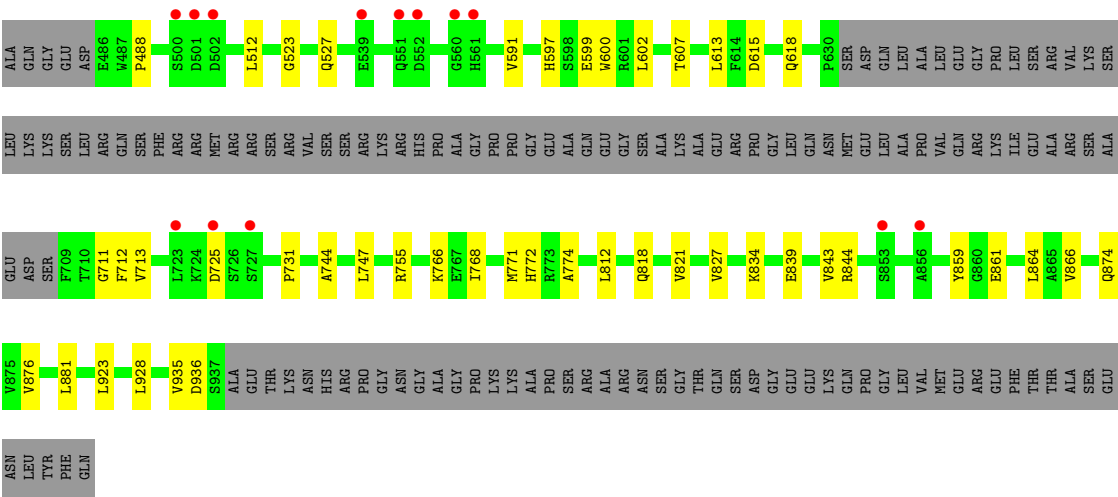
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP Q6P1M3
A	979	GLU	-	expression tag	UNP Q6P1M3
A	980	PHE	-	expression tag	UNP Q6P1M3
A	981	THR	-	expression tag	UNP Q6P1M3
A	982	THR	-	expression tag	UNP Q6P1M3
A	983	ALA	-	expression tag	UNP Q6P1M3
A	984	SER	-	expression tag	UNP Q6P1M3
A	985	GLU	-	expression tag	UNP Q6P1M3
A	986	ASN	-	expression tag	UNP Q6P1M3
A	987	LEU	-	expression tag	UNP Q6P1M3
A	988	TYR	-	expression tag	UNP Q6P1M3
A	989	PHE	-	expression tag	UNP Q6P1M3
A	990	GLN	-	expression tag	UNP Q6P1M3
D	12	MET	-	initiating methionine	UNP Q6P1M3
D	979	GLU	-	expression tag	UNP Q6P1M3
D	980	PHE	-	expression tag	UNP Q6P1M3
D	981	THR	-	expression tag	UNP Q6P1M3
D	982	THR	-	expression tag	UNP Q6P1M3
D	983	ALA	-	expression tag	UNP Q6P1M3
D	984	SER	-	expression tag	UNP Q6P1M3
D	985	GLU	-	expression tag	UNP Q6P1M3
D	986	ASN	-	expression tag	UNP Q6P1M3
D	987	LEU	-	expression tag	UNP Q6P1M3
D	988	TYR	-	expression tag	UNP Q6P1M3
D	989	PHE	-	expression tag	UNP Q6P1M3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	990	GLN	-	expression tag	UNP Q6P1M3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.87Å 130.87Å 277.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.66 – 3.90 39.66 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.66-3.90) 100.0 (39.66-3.90)	Depositor EDS
R_{merge}	1.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.87Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.252 , 0.298 0.259 , 0.302	Depositor DCC
R_{free} test set	1998 reflections (8.78%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtrriage
Anisotropy	0.220	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 22.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12829	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8136e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.25	0/6603	0.43	0/9008
1	D	0.25	0/6564	0.43	0/8957
All	All	0.25	0/13167	0.43	0/17965

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	6434	0	6262	61	0
1	D	6395	0	6240	48	0
All	All	12829	0	12502	106	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 4.

All (106) 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:64:VAL:HG11	1:D:425:GLY:HA3	1.74	0.68
1:D:744:ALA:HB3	1:D:766:LYS:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLN:NE2	1:D:236:ILE:O	2.27	0.67
1:A:410:ARG:HD3	1:A:575:PRO:HG2	1.76	0.66
1:A:195:GLN:NE2	1:A:236:ILE:O	2.28	0.66
1:A:618:GLN:NE2	1:A:755:ARG:O	2.31	0.64
1:A:602:LEU:HB3	1:A:613:LEU:HD11	1.81	0.63
1:A:240:ARG:NH2	1:A:342:ASP:O	2.31	0.63
1:D:768:ILE:HG12	1:D:827:VAL:HG11	1.80	0.63
1:D:199:ARG:NH2	1:D:345:ALA:O	2.33	0.60
1:D:253:SER:HB3	1:D:273:VAL:HG22	1.84	0.60
1:A:248:CYS:HB2	1:A:283:ILE:HB	1.85	0.59
1:A:744:ALA:HB3	1:A:766:LYS:HB2	1.85	0.58
1:D:342:ASP:HB2	1:D:343:PRO:HD2	1.85	0.58
1:A:57:LYS:HG2	1:A:67:MET:HG3	1.85	0.58
1:A:64:VAL:HG11	1:A:425:GLY:HA3	1.85	0.58
1:A:253:SER:HB3	1:A:273:VAL:HG22	1.86	0.58
1:A:239:GLN:NE2	1:A:241:ASP:OD1	2.37	0.57
1:D:239:GLN:NE2	1:D:241:ASP:OD1	2.36	0.57
1:A:18:ARG:HG2	1:D:24:ASN:ND2	2.19	0.57
1:A:41:SER:HB2	1:A:81:LEU:HD22	1.86	0.57
1:A:171:SER:OG	1:A:185:ARG:NH1	2.37	0.57
1:A:199:ARG:NH2	1:A:345:ALA:O	2.36	0.57
1:A:315:ILE:HD11	1:A:332:VAL:HG11	1.87	0.56
1:D:361:LEU:HD22	1:D:379:LEU:HD23	1.87	0.56
1:A:768:ILE:HG12	1:A:827:VAL:HG11	1.86	0.55
1:A:592:THR:OG1	1:A:713:VAL:O	2.22	0.55
1:D:821:VAL:HG23	1:D:881:LEU:HD11	1.87	0.55
1:D:57:LYS:HG2	1:D:67:MET:HG3	1.88	0.54
1:A:26:THR:OG1	1:A:27:VAL:N	2.41	0.54
1:A:240:ARG:NH1	1:A:348:ASP:OD1	2.40	0.54
1:A:504:ARG:HB3	1:A:525:ALA:HB2	1.90	0.54
1:D:731:PRO:HB2	1:D:747:LEU:HB2	1.89	0.54
1:D:818:GLN:HG2	1:D:834:LYS:HA	1.88	0.54
1:D:248:CYS:HB2	1:D:283:ILE:HB	1.91	0.52
1:D:600:TRP:O	1:D:755:ARG:NH2	2.42	0.52
1:A:256:GLN:HB2	1:A:269:LEU:HB2	1.90	0.52
1:D:602:LEU:HD13	1:D:613:LEU:HD21	1.92	0.52
1:D:602:LEU:HB3	1:D:613:LEU:HD11	1.92	0.52
1:A:240:ARG:HD3	1:A:346:THR:O	2.10	0.52
1:A:843:VAL:HG13	1:A:866:VAL:HG13	1.93	0.51
1:A:731:PRO:HB2	1:A:747:LEU:HB2	1.93	0.51
1:D:618:GLN:NE2	1:D:755:ARG:O	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LEU:HB2	1:A:876:VAL:HB	1.93	0.51
1:D:315:ILE:HD11	1:D:332:VAL:HG11	1.92	0.50
1:D:859:TYR:OH	1:D:861:GLU:OE2	2.26	0.50
1:A:359:GLU:OE1	1:A:383:HIS:NE2	2.32	0.50
1:A:821:VAL:HG23	1:A:881:LEU:HD11	1.94	0.50
1:D:597:HIS:CE1	1:D:599:GLU:HB3	2.47	0.49
1:A:710:THR:HG22	1:A:711:GLY:H	1.77	0.49
1:A:298:THR:HB	1:A:318:ILE:HB	1.94	0.49
1:D:591:VAL:HA	1:D:607:THR:HG22	1.93	0.49
1:A:936:ASP:OD1	1:A:936:ASP:N	2.45	0.49
1:A:603:VAL:HG13	1:A:614:PHE:HB3	1.95	0.49
1:A:353:LEU:HB3	1:A:364:ILE:HB	1.94	0.48
1:D:839:GLU:OE1	1:D:874:GLN:NE2	2.43	0.48
1:D:304:MET:HB3	1:D:309:TYR:HB2	1.96	0.48
1:D:372:PRO:HG2	1:D:416:SER:HB2	1.96	0.48
1:A:812:LEU:HD21	1:A:864:LEU:HD11	1.96	0.47
1:A:597:HIS:CE1	1:A:599:GLU:HB3	2.50	0.47
1:A:602:LEU:HD13	1:A:613:LEU:HD21	1.96	0.47
1:D:843:VAL:HG13	1:D:866:VAL:HG13	1.97	0.47
1:A:38:LEU:HD11	1:A:47:LEU:HD11	1.96	0.47
1:A:177:ARG:HG2	1:A:222:ARG:HA	1.96	0.47
1:D:151:GLY:HA3	1:D:189:GLU:HB2	1.96	0.47
1:D:711:GLY:O	1:D:713:VAL:N	2.48	0.46
1:A:59:TYR:CZ	1:A:379:LEU:HD21	2.49	0.46
1:A:914:SER:OG	1:A:917:GLU:HG2	2.15	0.46
1:A:197:HIS:HB3	1:A:200:ASP:O	2.17	0.45
1:A:383:HIS:HB3	1:A:915:PRO:O	2.17	0.45
1:A:821:VAL:HB	1:A:831:LEU:HB2	1.98	0.45
1:A:149:GLU:HA	1:A:190:MET:HA	1.99	0.45
1:A:372:PRO:HG2	1:A:416:SER:HB2	1.98	0.45
1:A:400:LEU:O	1:A:404:ILE:HG12	2.17	0.44
1:A:182:ALA:O	1:A:184:HIS:N	2.50	0.44
1:D:46:ILE:HD11	1:D:935:VAL:HG21	2.00	0.44
1:D:439:LEU:HD11	1:D:512:LEU:HD22	1.99	0.43
1:A:92:LEU:HB2	1:A:94:ASP:OD1	2.18	0.43
1:D:298:THR:HB	1:D:318:ILE:HB	2.00	0.43
1:A:46:ILE:HD11	1:A:935:VAL:HG21	2.01	0.43
1:A:144:LEU:HG	1:A:158:LEU:HD11	2.00	0.43
1:D:92:LEU:HB2	1:D:94:ASP:OD1	2.19	0.43
1:A:401:TRP:CG	1:A:435:ARG:HD2	2.53	0.43
1:A:721:THR:OG1	1:A:722:TYR:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ALA:HA	1:A:755:ARG:HB2	2.01	0.42
1:D:257:TRP:CH2	1:D:268:PRO:HG3	2.54	0.42
1:D:186:ARG:HG3	1:D:187:VAL:H	1.84	0.42
1:A:18:ARG:CZ	1:D:928:LEU:HD13	2.50	0.42
1:A:756:MET:SD	1:A:756:MET:N	2.93	0.42
1:D:812:LEU:HD21	1:D:864:LEU:HD11	1.99	0.42
1:D:615:ASP:OD1	1:D:755:ARG:NH2	2.53	0.42
1:A:504:ARG:HE	1:A:561:HIS:HB3	1.84	0.42
1:D:864:LEU:HB2	1:D:876:VAL:HB	2.02	0.41
1:A:14:GLU:HG2	1:D:26:THR:HA	2.02	0.41
1:D:523:GLY:HA3	1:D:527:GLN:NE2	2.35	0.41
1:A:267:GLU:H	1:A:267:GLU:CD	2.24	0.41
1:A:909:GLY:HA3	1:A:921:PHE:CZ	2.56	0.41
1:D:275:TYR:CE1	1:D:488:PRO:HB3	2.55	0.41
1:D:38:LEU:HD11	1:D:47:LEU:HD11	2.03	0.41
1:D:936:ASP:OD1	1:D:936:ASP:N	2.52	0.40
1:D:149:GLU:HA	1:D:190:MET:HA	2.03	0.40
1:D:772:HIS:HD2	1:D:774:ALA:HB3	1.87	0.40
1:A:388:THR:OG1	1:A:507:ILE:O	2.26	0.40
1:A:243:ARG:HA	1:A:259:VAL:HB	2.04	0.40
1:D:41:SER:HB2	1:D:81:LEU:HD22	2.03	0.40
1:D:339:THR:OG1	1:D:348:ASP:O	2.36	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	826/979 (84%)	760 (92%)	65 (8%)	1 (0%)	51	84
1	D	822/979 (84%)	764 (93%)	57 (7%)	1 (0%)	51	84
All	All	1648/1958 (84%)	1524 (92%)	122 (7%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	712	PHE
1	A	179	PRO

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	689/837 (82%)	682 (99%)	7 (1%)	76	86
1	D	686/837 (82%)	681 (99%)	5 (1%)	84	90
All	All	1375/1674 (82%)	1363 (99%)	12 (1%)	78	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	383	HIS
1	A	410	ARG
1	A	712	PHE
1	A	754	ARG
1	A	771	MET
1	A	923	LEU
1	D	120	ARG
1	D	725	ASP
1	D	771	MET
1	D	844	ARG
1	D	923	LEU

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

Mol	Chain	Res	Type
1	A	884	GLN

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 monosaccharides 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	834/979 (85%)	-0.03	12 (1%) 75 66	48, 95, 153, 223	0
1	D	830/979 (84%)	0.01	20 (2%) 59 48	52, 102, 161, 248	0
All	All	1664/1958 (84%)	-0.01	32 (1%) 66 57	48, 99, 158, 248	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	501	ASP	4.9
1	D	502	ASP	3.7
1	A	127	PRO	3.1
1	D	561	HIS	3.0
1	D	725	ASP	3.0
1	A	856	ALA	2.8
1	D	552	ASP	2.8
1	D	500	SER	2.7
1	D	560	GLY	2.6
1	A	104	VAL	2.6
1	A	840	GLY	2.5
1	D	856	ALA	2.5
1	D	551	GLN	2.5
1	A	855	ARG	2.5
1	D	727	SER	2.5
1	A	727	SER	2.5
1	D	310	GLY	2.4
1	A	758	GLU	2.4
1	D	178	LEU	2.3
1	A	107	GLY	2.3
1	D	71	GLN	2.3
1	D	123	PRO	2.3
1	D	723	LEU	2.3
1	A	264	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	188	PHE	2.2
1	A	936	ASP	2.2
1	A	490	LEU	2.2
1	A	836	THR	2.1
1	D	104	VAL	2.1
1	D	853	SER	2.1
1	D	539	GLU	2.1
1	D	177	ARG	2.1

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 monosaccharides 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.