WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 08:39 PM EDT

PDB ID	:	5V6R
Title	:	Structure of Plexin D1 intracellular domain
Authors	:	Shang, G.; Zhang, X.
Deposited on	:	2017-03-17
Resolution	:	2.70 Å(reported)

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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
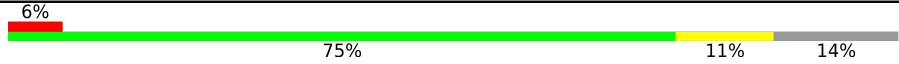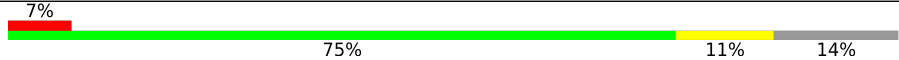*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.
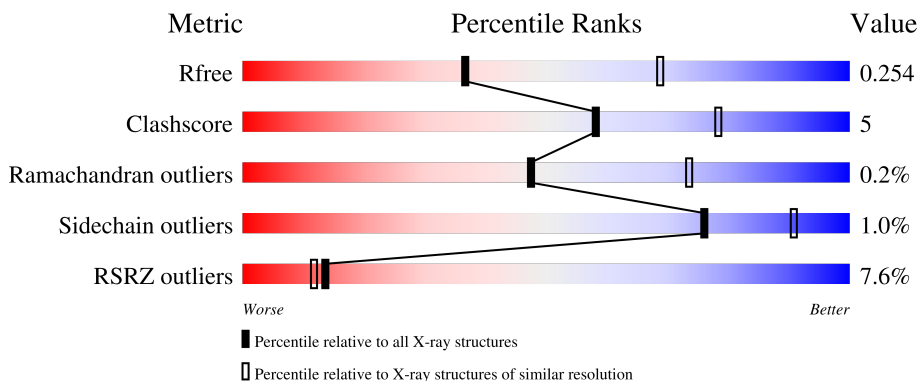
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	587	6% — 75% 11% 14%
1	B	587	7% — 75% 11% 14%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8190 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 Plexin-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			4068	2619	681	746	22			
1	B	503	Total	C	N	O	S	0	0	0
			4024	2590	677	735	22			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	45	Total	O	0	0
			45	45		

3 Residue-property plots ⓘ

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: Plexin-D1
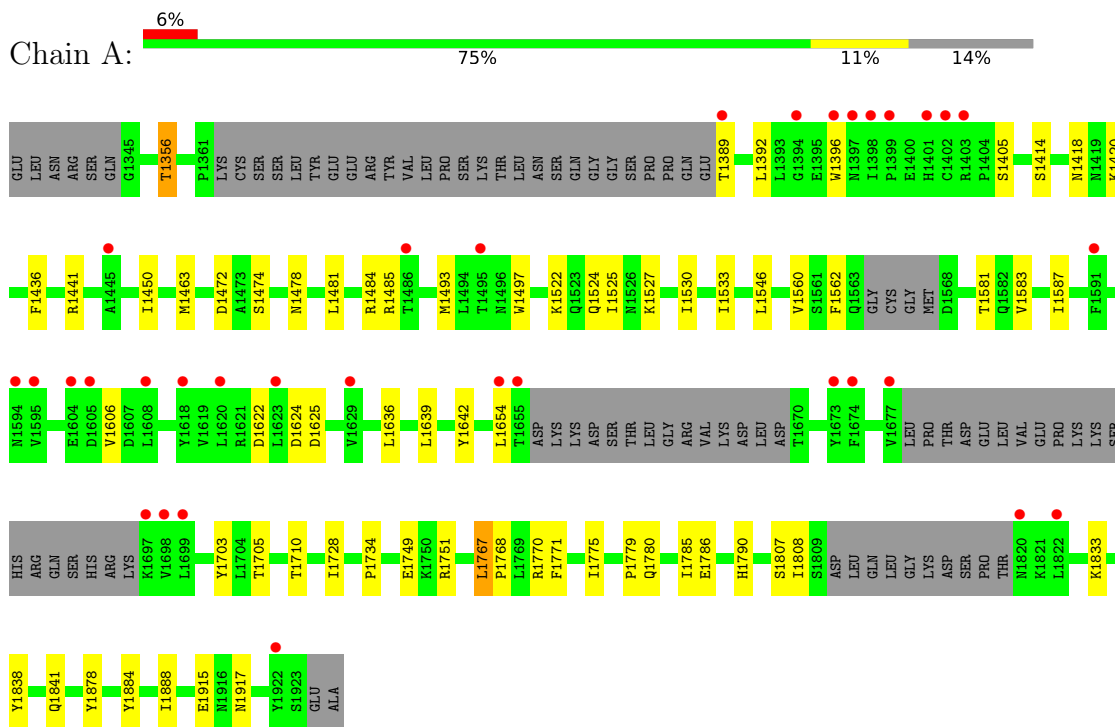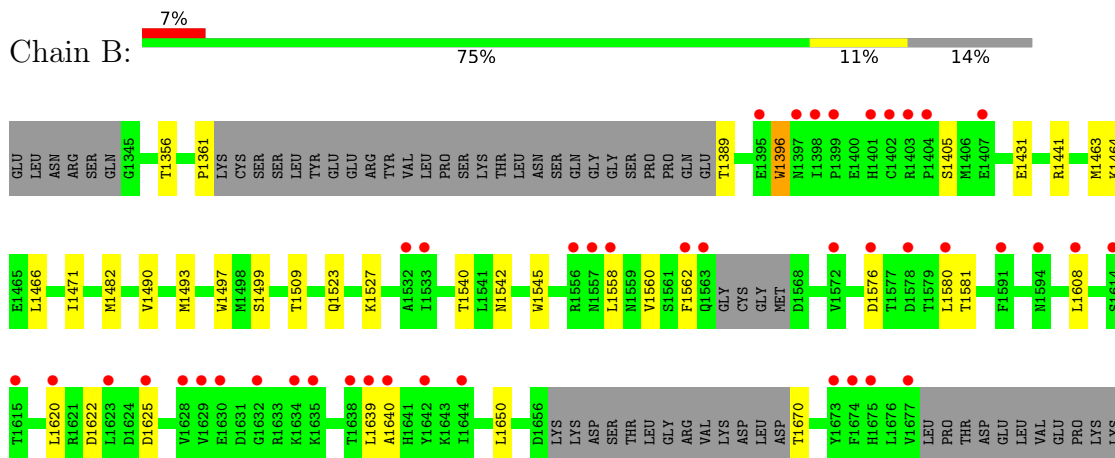
Chain A:

• Molecule 1: Plexin-D1

Chain B:

SER HIS ARG GLN SER HIS ARG LYS LYS V1698 L1699 P1700 L1704 K1711 I1725 I1728 R1729 P1734 Q1747 R1751 L1767 P1768 F1771 W1772 P1779 I1785 H1790 S1807 I1808 S1809 ASP LEU GLN LEU GLY LYS ASP SER PRO THR ASN K1821 L1822 L1823 Y1824 A1825 K1826

E1827 I1828 T1846 P1847 L1848 R1900 N1916 N1917 Y1922 SER GLU ALA

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.85Å 164.54Å 84.27Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	37.09 – 2.70 37.10 – 2.55	Depositor EDS
% Data completeness (in resolution range)	91.7 (37.09-2.70) 87.8 (37.10-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.256 0.218 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8190	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	0.23	0/4155	0.38	0/5625
1	B	0.23	0/4109	0.38	1/5566 (0.0%)
All	All	0.23	0/8264	0.38	1/11191 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1361	PRO	N-CA-CB	5.88	110.35	103.30

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	4068	0	4027	38	0
1	B	4024	0	3961	41	0
2	A	53	0	0	6	0
2	B	45	0	0	6	0
All	All	8190	0	7988	77	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 5.

All (77) 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:1846:THR:O	2:B:2001:HOH:O	1.92	0.88
1:A:1474:SER:O	2:A:2001:HOH:O	2.00	0.79
1:A:1779:PRO:HB2	1:A:1785:ILE:HD11	1.69	0.73
1:B:1540:THR:HG22	1:B:1542:ASN:H	1.56	0.71
1:A:1833:LYS:NZ	2:A:2007:HOH:O	2.25	0.70
1:B:1698:VAL:N	2:B:2006:HOH:O	2.31	0.64
1:B:1558:LEU:HD11	1:B:1639:LEU:HD21	1.82	0.61
1:B:1576:ASP:HB2	1:B:1640:ALA:HB2	1.83	0.59
1:A:1581:THR:OG1	1:A:1622:ASP:OD2	2.19	0.59
1:B:1431:GLU:OE1	2:B:2002:HOH:O	2.17	0.59
1:B:1670:THR:N	2:B:2009:HOH:O	2.34	0.59
1:A:1780:GLN:HB2	2:A:2010:HOH:O	2.04	0.57
1:A:1463:MET:HE1	1:A:1497:TRP:HB2	1.86	0.56
1:A:1420:LYS:HG2	2:A:2033:HOH:O	2.06	0.55
1:B:1540:THR:HG21	1:B:1545:TRP:HB2	1.89	0.55
1:A:1392:LEU:HD13	1:A:1450:ILE:HD12	1.89	0.54
1:A:1414:SER:O	1:A:1418:ASN:ND2	2.37	0.53
1:B:1356:THR:HG23	1:B:1389:THR:N	2.25	0.52
1:A:1606:VAL:HG12	1:A:1654:LEU:HD23	1.92	0.51
1:B:1826:LYS:NZ	2:B:2016:HOH:O	2.42	0.51
1:A:1546:LEU:HD13	1:A:1703:TYR:HB3	1.92	0.51
1:A:1485:ARG:O	1:A:1770:ARG:NH1	2.43	0.51
1:B:1608:LEU:HD21	1:B:1650:LEU:HD13	1.93	0.51
1:B:1767:LEU:HB3	1:B:1768:PRO:HD3	1.93	0.50
1:B:1540:THR:HG23	1:B:1790:HIS:NE2	2.27	0.50
1:B:1699:LEU:HD23	1:B:1704:LEU:HD12	1.94	0.50
1:A:1624:ASP:OD2	1:A:1642:TYR:OH	2.27	0.49
1:B:1728:ILE:HG23	1:B:1734:PRO:HD3	1.93	0.49
1:B:1779:PRO:HB2	1:B:1785:ILE:HD11	1.94	0.49
1:A:1405:SER:O	1:A:1917:ASN:ND2	2.46	0.48
1:A:1807:SER:OG	1:A:1808:ILE:N	2.44	0.48
1:B:1466:LEU:HD13	1:B:1490:VAL:HG22	1.95	0.48
1:A:1767:LEU:HB3	1:A:1768:PRO:HD3	1.95	0.48
1:B:1431:GLU:HG2	1:B:1441:ARG:HE	1.78	0.48
1:A:1522:LYS:NZ	1:A:1786:GLU:OE2	2.35	0.47
1:B:1464:LYS:NZ	2:B:2018:HOH:O	2.44	0.47
1:B:1463:MET:HE2	1:B:1493:MET:HB3	1.96	0.47
1:A:1525:ILE:HG22	1:A:1530:ILE:HD11	1.96	0.46
1:B:1699:LEU:HD12	1:B:1700:PRO:HD2	1.96	0.46
1:A:1472:ASP:OD1	1:A:1751:ARG:NH1	2.35	0.46
1:A:1728:ILE:HD12	1:A:1841:GLN:HB3	1.97	0.46
1:A:1356:THR:HG1	1:A:1389:THR:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1471:ILE:HG12	1:B:1482:MET:HE1	1.98	0.46
1:B:1581:THR:OG1	1:B:1622:ASP:OD2	2.19	0.45
1:A:1560:VAL:HG11	1:A:1587:ILE:HD13	1.99	0.45
1:A:1749:GLU:OE2	1:B:1900:ARG:HD3	2.16	0.45
1:B:1509:THR:HG22	1:B:1729:ARG:HH11	1.82	0.44
1:B:1807:SER:OG	1:B:1808:ILE:N	2.50	0.44
1:B:1560:VAL:HG22	1:B:1650:LEU:HB2	1.99	0.44
1:A:1484:ARG:HG3	1:A:1485:ARG:HG3	1.99	0.44
1:A:1583:VAL:HG21	1:A:1639:LEU:HD13	1.99	0.44
1:B:1725:ILE:HG23	1:B:1772:TRP:CE2	2.53	0.44
1:A:1878:TYR:OH	1:A:1915:GLU:OE2	2.27	0.44
1:B:1558:LEU:HD13	1:B:1650:LEU:HD11	1.99	0.44
1:B:1499:SER:HA	1:B:1771:PHE:CE1	2.52	0.43
1:B:1396:TRP:CD1	1:B:1396:TRP:N	2.86	0.43
1:A:1463:MET:HE2	1:A:1493:MET:HB3	2.01	0.43
1:A:1838:TYR:OH	2:A:2003:HOH:O	2.21	0.42
1:A:1884:TYR:O	1:A:1888:ILE:HG12	2.19	0.42
1:B:1405:SER:O	1:B:1917:ASN:ND2	2.53	0.42
1:B:1463:MET:HE1	1:B:1497:TRP:HB2	2.01	0.42
1:B:1747:GLN:OE1	1:B:1751:ARG:NH2	2.52	0.42
1:A:1749:GLU:OE2	1:B:1900:ARG:NH1	2.48	0.42
1:B:1580:LEU:HD13	1:B:1620:LEU:HB3	2.02	0.42
1:B:1482:MET:HE3	1:B:1482:MET:HB3	1.95	0.42
1:A:1436:PHE:CD2	1:A:1441:ARG:HG2	2.54	0.41
1:A:1728:ILE:HG23	1:A:1734:PRO:HD3	2.02	0.41
1:A:1524:GLN:O	1:A:1527:LYS:HB2	2.20	0.41
1:A:1771:PHE:O	1:A:1775:ILE:HG12	2.20	0.41
1:B:1463:MET:HE1	1:B:1493:MET:O	2.21	0.41
1:A:1478:ASN:HB3	1:A:1481:LEU:HG	2.02	0.41
1:B:1824:TYR:O	1:B:1828:ILE:HG12	2.21	0.41
1:A:1705:THR:OG1	2:A:2004:HOH:O	2.22	0.41
1:A:1524:GLN:HG2	1:A:1710:THR:HG23	2.03	0.41
1:A:1533:ILE:HD11	1:A:1636:LEU:HD11	2.04	0.40
1:B:1523:GLN:O	1:B:1527:LYS:HG3	2.22	0.40
1:B:1711:LYS:HD3	1:B:1823:LEU:HG	2.04	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	493/587 (84%)	474 (96%)	18 (4%)	1 (0%)	47	73
1	B	491/587 (84%)	473 (96%)	17 (4%)	1 (0%)	47	73
All	All	984/1174 (84%)	947 (96%)	35 (4%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1767	LEU
1	A	1767	LEU

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	440/532 (83%)	435 (99%)	5 (1%)	73	90
1	B	430/532 (81%)	426 (99%)	4 (1%)	78	92
All	All	870/1064 (82%)	861 (99%)	9 (1%)	76	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1356	THR
1	A	1396	TRP
1	A	1562	PHE
1	A	1625	ASP

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Mol	Chain	Res	Type
1	A	1790	HIS
1	B	1396	TRP
1	B	1562	PHE
1	B	1625	ASP
1	B	1916	ASN

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	1523	GLN

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 monosaccharides 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	505/587 (86%)	0.16	33 (6%)	18	17	42, 72, 114, 138	0
1	B	503/587 (85%)	0.29	44 (8%)	10	8	45, 80, 139, 160	0
All	All	1008/1174 (85%)	0.22	77 (7%)	13	12	42, 76, 128, 160	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1397	ASN	12.4
1	B	1674	PHE	8.9
1	B	1673	TYR	8.2
1	B	1562	PHE	6.8
1	A	1389	THR	5.7
1	A	1654	LEU	5.3
1	B	1591	PHE	5.2
1	A	1591	PHE	5.0
1	A	1397	ASN	4.5
1	B	1639	LEU	4.5
1	B	1635	LYS	4.4
1	B	1629	VAL	4.4
1	B	1628	VAL	4.3
1	B	1403	ARG	3.9
1	B	1632	GLY	3.9
1	A	1608	LEU	3.8
1	B	1558	LEU	3.8
1	A	1673	TYR	3.8
1	B	1677	VAL	3.7
1	B	1848	LEU	3.7
1	A	1595	VAL	3.6
1	A	1677	VAL	3.6
1	B	1398	ILE	3.6
1	B	1625	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1572	VAL	3.3
1	A	1618	TYR	3.2
1	A	1399	PRO	3.2
1	B	1563	GLN	3.2
1	B	1644	ILE	3.1
1	A	1698	VAL	3.1
1	B	1594	ASN	3.1
1	B	1404	PRO	3.0
1	A	1401	HIS	2.9
1	A	1699	LEU	2.8
1	B	1578	ASP	2.8
1	B	1614	SER	2.8
1	A	1620	LEU	2.8
1	B	1620	LEU	2.8
1	B	1402	CYS	2.8
1	A	1403	ARG	2.8
1	A	1402	CYS	2.7
1	B	1576	ASP	2.7
1	B	1638	THR	2.7
1	B	1608	LEU	2.7
1	A	1604	GLU	2.7
1	B	1642	TYR	2.6
1	B	1532	ALA	2.6
1	B	1533	ILE	2.6
1	B	1407	GLU	2.6
1	A	1922	TYR	2.6
1	B	1640	ALA	2.6
1	B	1401	HIS	2.5
1	A	1398	ILE	2.5
1	A	1445	ALA	2.5
1	A	1822	LEU	2.5
1	A	1594	ASN	2.5
1	A	1605	ASP	2.5
1	B	1675	HIS	2.5
1	B	1634	LYS	2.4
1	A	1495	THR	2.4
1	A	1396	TRP	2.4
1	A	1674	PHE	2.4
1	A	1697	LYS	2.3
1	B	1615	THR	2.3
1	B	1580	LEU	2.3
1	B	1556	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1655	THR	2.3
1	A	1820	ASN	2.2
1	B	1395	GLU	2.2
1	B	1399	PRO	2.2
1	B	1623	LEU	2.1
1	A	1486	THR	2.1
1	A	1623	LEU	2.0
1	B	1557	ASN	2.0
1	A	1394	GLY	2.0
1	A	1629	VAL	2.0
1	B	1630	GLU	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 monosaccharides 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.