



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 PM UTC

PDB ID : 5V6R / pdb_00005v6r
Title : Structure of Plexin D1 intracellular domain
Authors : Shang, G.; Zhang, X.
Deposited on : 2017-03-17
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

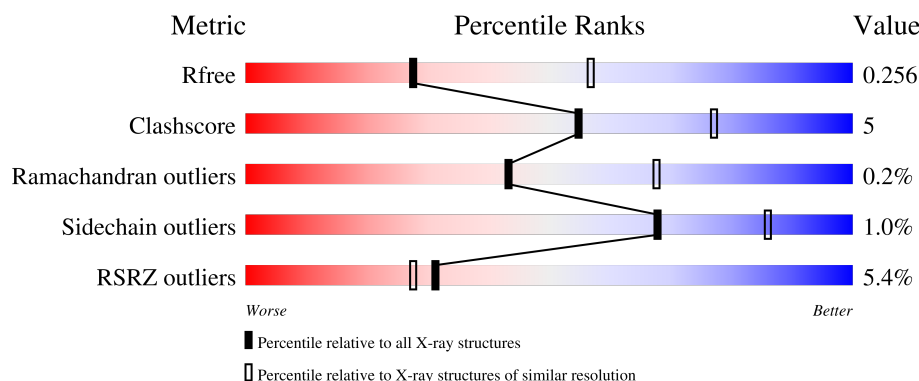
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	587	4% 74% 12% 14%
1	B	587	5% 75% 10% 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			

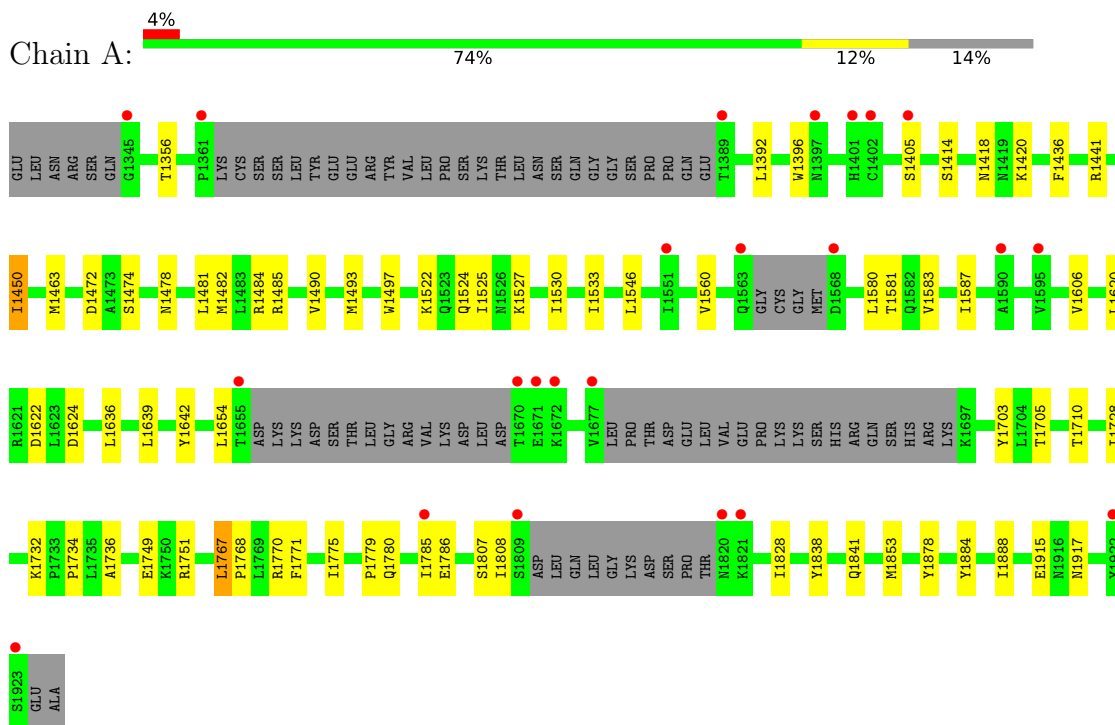
- Molecule 2 is water.

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

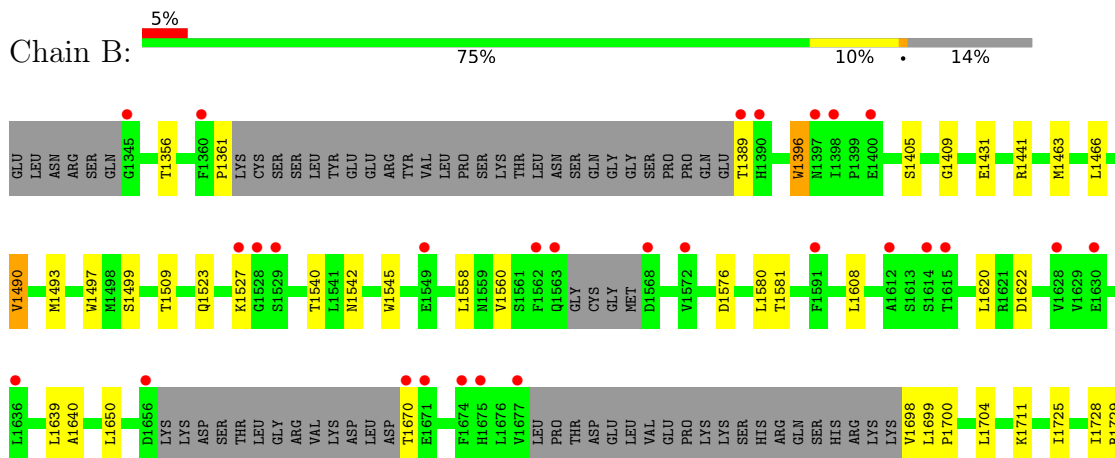
3 Residue-property plots

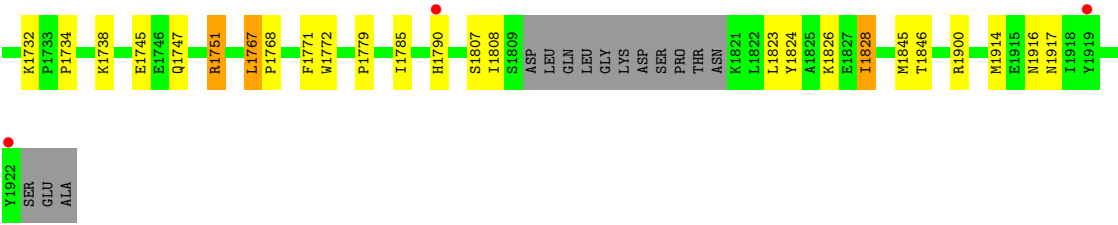
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Plexin-D1





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 37.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (37.09-2.70) 91.8 (37.09-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.256 0.221 , 0.256	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)	0.28 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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	0.30	0/4155	0.69	3/5625 (0.1%)
1	B	0.30	0/4109	0.71	4/5566 (0.1%)
All	All	0.30	0/8264	0.70	7/11191 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1361	PRO	N-CA-CB	6.68	110.35	103.00
1	B	1732	LYS	CA-C-N	6.27	124.23	119.66
1	B	1732	LYS	C-N-CA	6.27	124.23	119.66
1	B	1828	ILE	CB-CA-C	-5.79	108.21	114.35
1	A	1732	LYS	CA-C-N	5.66	123.79	119.66
1	A	1732	LYS	C-N-CA	5.66	123.79	119.66
1	A	1828	ILE	CB-CA-C	-5.52	108.50	114.35

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	39	0
1	B	4024	0	3961	40	0
2	A	53	0	0	5	0
2	B	45	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:1463:MET:HE1	1:A:1497:TRP:HB2	1.65	0.78
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:B:1463:MET:HE2	1:B:1493:MET:HB3	1.76	0.66
1:B:1463:MET:HE1	1:B:1497:TRP:HB2	1.75	0.66
1:B:1698:VAL:N	2:B:2006:HOH:O	2.31	0.64
1:B:1409:GLY:HA3	1:B:1914:MET:HE3	1.81	0.62
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: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:1522:LYS:NZ	1:A:1786:GLU:OE2	2.35	0.54
1:A:1414:SER:O	1:A:1418:ASN:ND2	2.37	0.53
1:A:1878:TYR:OH	1:A:1915:GLU:OE2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:SER:O	1:A:1917:ASN:ND2	2.46	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:1463:MET:HE2	1:A:1493:MET:HB3	1.95	0.47
1:A:1807:SER:OG	1:A:1808:ILE:N	2.44	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: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:1736:ALA:HA	1:A:1853:MET:HE1	1.99	0.44
1:B:1558:LEU:HD13	1:B:1650:LEU:HD11	1.99	0.44
1:B:1914:MET:HE2	1:B:1914:MET:HA	2.00	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: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: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: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:1738:LYS:HB2	1:B:1845:MET:HE3	2.03	0.41
1:A:1478:ASN:HB3	1:A:1481:LEU:HG	2.02	0.41
1:A:1482:MET:HE3	1:A:1482:MET:HB3	1.94	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:1580:LEU:HD13	1:A:1620:LEU:C	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	493/587 (84%)	474 (96%)	18 (4%)	1 (0%)	43	68
1	B	491/587 (84%)	473 (96%)	17 (4%)	1 (0%)	43	68
All	All	984/1174 (84%)	947 (96%)	35 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

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

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	440/532 (83%)	436 (99%)	4 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	430/532 (81%)	425 (99%)	5 (1%)	63	84
All	All	870/1064 (82%)	861 (99%)	9 (1%)	68	86

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	1450	ILE
1	A	1490	VAL
1	B	1396	TRP
1	B	1490	VAL
1	B	1745	GLU
1	B	1751	ARG
1	B	1916	ASN

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

Mol	Chain	Res	Type
1	A	1747	GLN
1	A	1843	GLN
1	B	1760	HIS
1	B	1841	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 oligosaccharides 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	505/587 (86%)	0.38	23 (4%) 37 34	42, 72, 114, 138	0
1	B	503/587 (85%)	0.47	31 (6%) 26 23	45, 80, 139, 160	0
All	All	1008/1174 (85%)	0.42	54 (5%) 31 27	42, 76, 128, 160	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1568	ASP	5.9
1	B	1674	PHE	5.7
1	B	1563	GLN	4.4
1	B	1677	VAL	4.4
1	B	1614	SER	4.3
1	B	1397	ASN	4.3
1	A	1389	THR	4.1
1	A	1590	ALA	3.9
1	A	1402	CYS	3.9
1	A	1361	PRO	3.6
1	B	1670	THR	3.5
1	A	1677	VAL	3.5
1	A	1671	GLU	3.3
1	A	1670	THR	3.2
1	A	1820	ASN	3.0
1	A	1563	GLN	3.0
1	B	1528	GLY	3.0
1	B	1345	GLY	3.0
1	B	1615	THR	3.0
1	B	1400	GLU	2.9
1	B	1628	VAL	2.9
1	B	1529	SER	2.8
1	B	1389	THR	2.8
1	B	1671	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1397	ASN	2.7
1	B	1390	HIS	2.7
1	B	1656	ASP	2.7
1	B	1562	PHE	2.6
1	B	1675	HIS	2.5
1	A	1923	SER	2.5
1	B	1568	ASP	2.5
1	B	1790	HIS	2.4
1	B	1630	GLU	2.4
1	A	1785	ILE	2.4
1	B	1527	LYS	2.3
1	A	1672	LYS	2.3
1	B	1919	TYR	2.3
1	B	1591	PHE	2.3
1	A	1922	TYR	2.3
1	A	1405	SER	2.2
1	A	1551	ILE	2.2
1	B	1398	ILE	2.2
1	B	1612	ALA	2.2
1	B	1922	TYR	2.2
1	A	1809	SER	2.2
1	A	1595	VAL	2.1
1	B	1572	VAL	2.1
1	B	1549	GLU	2.1
1	A	1655	THR	2.1
1	A	1345	GLY	2.1
1	A	1401	HIS	2.1
1	B	1360	PHE	2.1
1	A	1821	LYS	2.0
1	B	1636	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 oligosaccharides 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.