



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID : 4LNZ
Title : Crystal structure of human Myosin 5b globular domain
Authors : Velvarska, H.; Niessing, D.
Deposited on : 2013-07-12
Resolution : 3.11 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

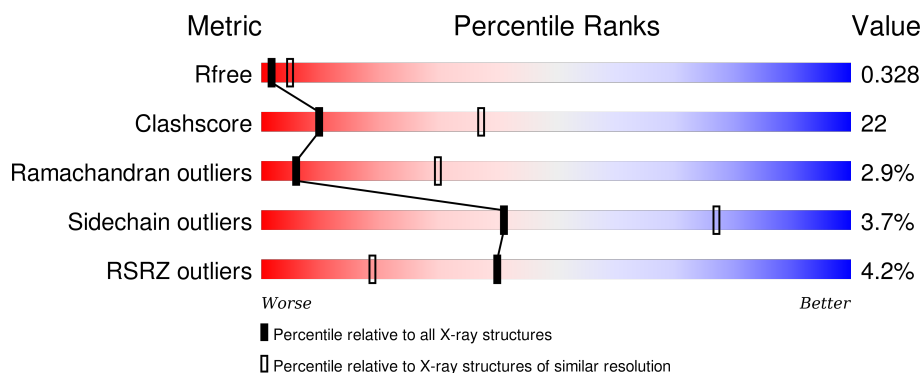
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	394	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5671 atoms, of which 2831 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 Unconventional myosin-Vb.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	H	N	O	S	40	0	0
			5671	1808	2831	477	530	25			

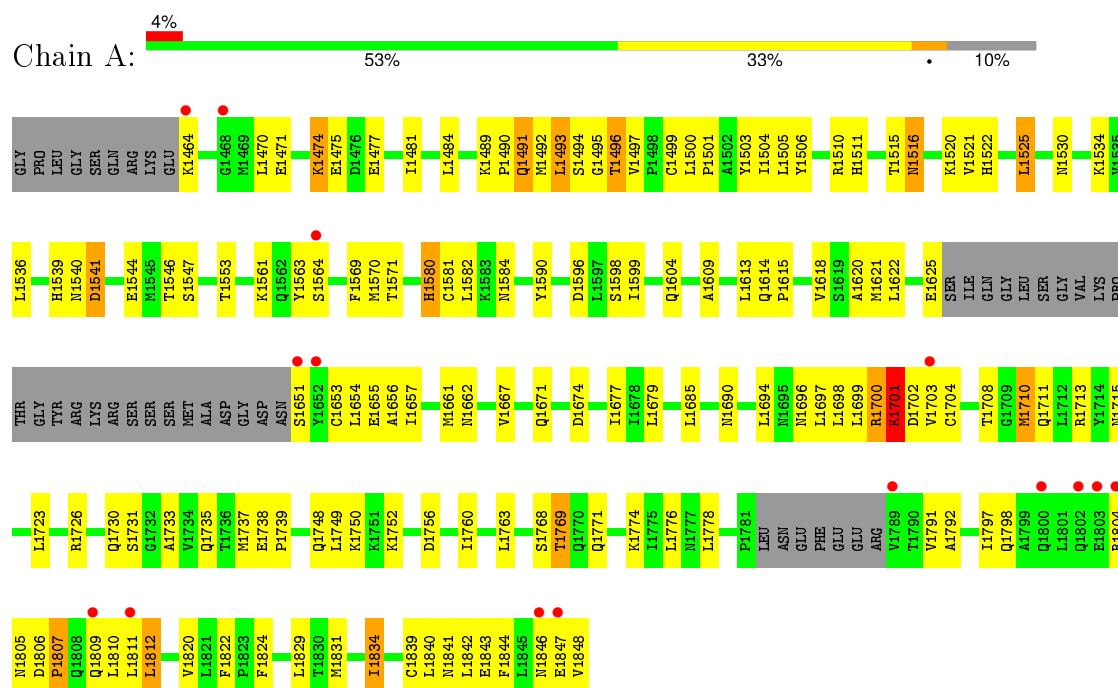
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1455	GLY	-	EXPRESSION TAG	UNP Q9ULV0
A	1456	PRO	-	EXPRESSION TAG	UNP Q9ULV0
A	1457	LEU	-	EXPRESSION TAG	UNP Q9ULV0
A	1458	GLY	-	EXPRESSION TAG	UNP Q9ULV0
A	1459	SER	-	EXPRESSION TAG	UNP Q9ULV0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Unconventional myosin-Vb



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.64Å 78.44Å 86.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.14 – 3.11 58.14 – 3.11	Depositor EDS
% Data completeness (in resolution range)	96.4 (58.14-3.11) 97.4 (58.14-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.253 , 0.312 0.259 , 0.328	Depositor DCC
R_{free} test set	350 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 78.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 7638 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5671	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.81	2/2889 (0.1%)	0.89	3/3909 (0.1%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1807	PRO	CB-CG	5.62	1.78	1.50
1	A	1807	PRO	CG-CD	5.22	1.67	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1701	LYS	N-CA-C	-6.32	93.94	111.00
1	A	1809	GLN	CB-CA-C	6.06	122.53	110.40
1	A	1621	MET	CA-CB-CG	-5.40	104.12	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1474	LYS	Peptide
1	A	1701	LYS	Peptide

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	2840	2831	2868	126	0
All	All	2840	2831	2868	126	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 22.

All (126) 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:A:1807:PRO:CB	1:A:1807:PRO:CG	1.78	1.49
1:A:1493:LEU:HA	1:A:1494:SER:HB2	1.37	1.05
1:A:1471:GLU:CB	1:A:1511:HIS:CD2	2.45	0.98
1:A:1697:LEU:O	1:A:1703:VAL:HG23	1.71	0.91
1:A:1471:GLU:HB2	1:A:1511:HIS:CD2	2.09	0.87
1:A:1471:GLU:HB3	1:A:1511:HIS:CD2	2.11	0.85
1:A:1471:GLU:HB3	1:A:1511:HIS:NE2	1.94	0.83
1:A:1471:GLU:CB	1:A:1511:HIS:NE2	2.46	0.79
1:A:1491:GLN:NE2	1:A:1544:GLU:OE1	2.18	0.75
1:A:1810:LEU:O	1:A:1811:LEU:HB3	1.87	0.75
1:A:1622:LEU:HA	1:A:1711:GLN:NE2	2.06	0.70
1:A:1516:ASN:OD1	1:A:1584:ASN:ND2	2.25	0.70
1:A:1700:ARG:HG3	1:A:1701:LYS:N	2.09	0.67
1:A:1540:ASN:O	1:A:1541:ASP:CB	2.42	0.67
1:A:1749:LEU:HD22	1:A:1760:ILE:CD1	2.24	0.67
1:A:1769:THR:HG22	1:A:1806:ASP:HB2	1.78	0.66
1:A:1497:VAL:HG12	1:A:1499:CYS:H	1.62	0.65
1:A:1769:THR:CG2	1:A:1806:ASP:HB2	2.27	0.65
1:A:1493:LEU:HA	1:A:1494:SER:CB	2.08	0.63
1:A:1697:LEU:HD12	1:A:1697:LEU:C	2.19	0.63
1:A:1496:THR:HG21	1:A:1500:LEU:HD22	1.82	0.62
1:A:1563:TYR:O	1:A:1581:CYS:HB2	1.99	0.62
1:A:1843:GLU:N	1:A:1843:GLU:OE2	2.32	0.62
1:A:1493:LEU:CA	1:A:1494:SER:HB2	2.24	0.61
1:A:1471:GLU:HB2	1:A:1511:HIS:NE2	2.15	0.60
1:A:1540:ASN:O	1:A:1541:ASP:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:THR:HG23	1:A:1711:GLN:HE21	1.67	0.59
1:A:1464:LYS:HG2	1:A:1464:LYS:O	2.03	0.58
1:A:1703:VAL:O	1:A:1704:CYS:HB2	2.02	0.58
1:A:1474:LYS:HG3	1:A:1520:LYS:HE3	1.87	0.57
1:A:1571:THR:O	1:A:1571:THR:HG22	2.03	0.57
1:A:1769:THR:CG2	1:A:1806:ASP:CB	2.82	0.57
1:A:1694:LEU:O	1:A:1698:LEU:HD12	2.05	0.56
1:A:1493:LEU:HD22	1:A:1494:SER:O	2.06	0.56
1:A:1564:SER:HB2	1:A:1582:LEU:HD12	1.87	0.56
1:A:1667:VAL:O	1:A:1671:GLN:HG2	2.06	0.56
1:A:1701:LYS:O	1:A:1701:LYS:HG3	2.04	0.56
1:A:1768:SER:O	1:A:1771:GLN:N	2.39	0.56
1:A:1477:GLU:O	1:A:1481:ILE:HG12	2.06	0.56
1:A:1563:TYR:O	1:A:1581:CYS:CB	2.54	0.55
1:A:1703:VAL:HG22	1:A:1703:VAL:O	2.08	0.54
1:A:1653:CYS:O	1:A:1656:ALA:N	2.40	0.54
1:A:1490:PRO:C	1:A:1492:MET:H	2.10	0.54
1:A:1749:LEU:CD1	1:A:1763:LEU:HD12	2.38	0.54
1:A:1490:PRO:O	1:A:1492:MET:N	2.34	0.54
1:A:1553:THR:CG2	1:A:1598:SER:HB3	2.38	0.53
1:A:1697:LEU:HD12	1:A:1697:LEU:O	2.08	0.53
1:A:1703:VAL:HB	1:A:1778:LEU:HB2	1.91	0.53
1:A:1703:VAL:HB	1:A:1778:LEU:CB	2.40	0.52
1:A:1750:LYS:O	1:A:1756:ASP:HB3	2.10	0.52
1:A:1710:MET:HG2	1:A:1748:GLN:OE1	2.10	0.52
1:A:1494:SER:HA	1:A:1496:THR:HG22	1.92	0.51
1:A:1497:VAL:HB	1:A:1500:LEU:HB2	1.92	0.51
1:A:1553:THR:HG21	1:A:1598:SER:HB3	1.92	0.51
1:A:1791:VAL:O	1:A:1792:ALA:HB3	2.10	0.51
1:A:1679:LEU:HG	1:A:1731:SER:HB3	1.93	0.51
1:A:1674:ASP:HB2	1:A:1677:ILE:HD12	1.92	0.51
1:A:1489:LYS:O	1:A:1492:MET:HB2	2.11	0.51
1:A:1506:TYR:CD1	1:A:1506:TYR:C	2.84	0.50
1:A:1521:VAL:HG23	1:A:1522:HIS:N	2.26	0.50
1:A:1690:ASN:HB2	1:A:1737:MET:HG2	1.93	0.50
1:A:1494:SER:N	1:A:1495:GLY:HA3	2.27	0.50
1:A:1620:ALA:HB3	1:A:1657:ILE:HD12	1.94	0.50
1:A:1662:ASN:OD1	1:A:1726:ARG:NH1	2.45	0.49
1:A:1496:THR:HG23	1:A:1497:VAL:N	2.27	0.49
1:A:1500:LEU:N	1:A:1501:PRO:CD	2.74	0.49
1:A:1654:LEU:CD1	1:A:1715:ASN:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:LEU:HD22	1:A:1760:ILE:HD11	1.93	0.48
1:A:1490:PRO:C	1:A:1492:MET:N	2.67	0.48
1:A:1829:LEU:HD23	1:A:1834:ILE:HD11	1.94	0.48
1:A:1702:ASP:HB3	1:A:1778:LEU:HD22	1.96	0.48
1:A:1774:LYS:HE3	1:A:1778:LEU:HD11	1.95	0.48
1:A:1546:THR:OG1	1:A:1547:SER:N	2.46	0.48
1:A:1596:ASP:HA	1:A:1599:ILE:HD12	1.96	0.47
1:A:1776:LEU:HD11	1:A:1797:ILE:CD1	2.44	0.47
1:A:1810:LEU:O	1:A:1811:LEU:CB	2.57	0.47
1:A:1713:ARG:HD2	1:A:1748:GLN:NE2	2.29	0.47
1:A:1561:LYS:HB2	1:A:1824:PHE:CE1	2.50	0.47
1:A:1806:ASP:CG	1:A:1807:PRO:HA	2.36	0.47
1:A:1846:ASN:O	1:A:1848:VAL:HG23	2.14	0.47
1:A:1500:LEU:HG	1:A:1504:ILE:CD1	2.45	0.46
1:A:1776:LEU:CD1	1:A:1797:ILE:CD1	2.94	0.46
1:A:1804:ARG:N	1:A:1805:ASN:HA	2.30	0.46
1:A:1774:LYS:CE	1:A:1778:LEU:HD11	2.46	0.46
1:A:1653:CYS:O	1:A:1655:GLU:N	2.49	0.46
1:A:1525:LEU:CD1	1:A:1590:TYR:CD1	2.98	0.46
1:A:1618:VAL:HG12	1:A:1618:VAL:O	2.15	0.45
1:A:1738:GLU:N	1:A:1739:PRO:CD	2.80	0.45
1:A:1497:VAL:HG11	1:A:1503:TYR:HD2	1.80	0.45
1:A:1501:PRO:O	1:A:1505:LEU:HG	2.17	0.45
1:A:1474:LYS:CG	1:A:1520:LYS:HE3	2.45	0.45
1:A:1703:VAL:HG13	1:A:1704:CYS:O	2.17	0.45
1:A:1700:ARG:HG3	1:A:1701:LYS:H	1.78	0.45
1:A:1539:HIS:O	1:A:1540:ASN:C	2.55	0.45
1:A:1679:LEU:HD21	1:A:1730:GLN:HG2	1.99	0.45
1:A:1614:GLN:HB3	1:A:1615:PRO:HD3	1.99	0.44
1:A:1844:PHE:CD1	1:A:1844:PHE:C	2.91	0.44
1:A:1484:LEU:HD23	1:A:1505:LEU:HD21	2.00	0.44
1:A:1493:LEU:CA	1:A:1494:SER:CB	2.90	0.44
1:A:1530:ASN:O	1:A:1534:LYS:HB2	2.18	0.44
1:A:1494:SER:HA	1:A:1496:THR:N	2.32	0.43
1:A:1723:LEU:HD11	1:A:1733:ALA:HB3	2.01	0.43
1:A:1497:VAL:HG12	1:A:1499:CYS:C	2.39	0.43
1:A:1546:THR:HG22	1:A:1604:GLN:OE1	2.17	0.43
1:A:1701:LYS:N	1:A:1702:ASP:HA	2.33	0.43
1:A:1569:PHE:N	1:A:1569:PHE:CD1	2.85	0.43
1:A:1497:VAL:HG12	1:A:1500:LEU:N	2.34	0.42
1:A:1657:ILE:O	1:A:1661:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1839:CYS:C	1:A:1840:LEU:HD12	2.40	0.42
1:A:1651:SER:OG	1:A:1651:SER:O	2.30	0.42
1:A:1609:ALA:HB1	1:A:1685:LEU:HD21	2.01	0.42
1:A:1735:GLN:N	1:A:1735:GLN:CD	2.73	0.41
1:A:1797:ILE:HG22	1:A:1798:GLN:N	2.33	0.41
1:A:1510:ARG:HH12	1:A:1580:HIS:CG	2.39	0.41
1:A:1749:LEU:HD22	1:A:1760:ILE:HD13	2.00	0.41
1:A:1708:THR:HG23	1:A:1711:GLN:NE2	2.33	0.41
1:A:1820:VAL:CG2	1:A:1822:PHE:CE1	3.04	0.41
1:A:1563:TYR:CZ	1:A:1831:MET:HE1	2.56	0.41
1:A:1470:LEU:HD23	1:A:1847:GLU:HA	2.02	0.41
1:A:1701:LYS:O	1:A:1704:CYS:SG	2.74	0.40
1:A:1622:LEU:HA	1:A:1711:GLN:HE22	1.85	0.40
1:A:1696:ASN:C	1:A:1698:LEU:H	2.25	0.40
1:A:1484:LEU:HD13	1:A:1842:LEU:HD11	2.04	0.40
1:A:1811:LEU:HG	1:A:1811:LEU:O	2.21	0.40
1:A:1500:LEU:N	1:A:1501:PRO:HD2	2.36	0.40
1:A:1613:LEU:HD12	1:A:1685:LEU:HD22	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	347/394 (88%)	307 (88%)	30 (9%)	10 (3%)	6 30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1475	GLU
1	A	1493	LEU
1	A	1700	ARG

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Mol	Chain	Res	Type
1	A	1541	ASP
1	A	1699	LEU
1	A	1752	LYS
1	A	1491	GLN
1	A	1812	LEU
1	A	1496	THR
1	A	1769	THR

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	325/359 (90%)	313 (96%)	12 (4%)	41	77

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

Mol	Chain	Res	Type
1	A	1515	THR
1	A	1516	ASN
1	A	1525	LEU
1	A	1536	LEU
1	A	1570	MET
1	A	1580	HIS
1	A	1625	GLU
1	A	1701	LYS
1	A	1710	MET
1	A	1812	LEU
1	A	1834	ILE
1	A	1841	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1584	ASN
1	A	1711	GLN

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Mol	Chain	Res	Type
1	A	1771	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	353/394 (89%)	0.35	15 (4%) 40 19	48, 71, 100, 117	5 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1651	SER	5.3
1	A	1703	VAL	4.1
1	A	1464	LYS	3.0
1	A	1800	GLN	3.0
1	A	1652	TYR	2.8
1	A	1811	LEU	2.7
1	A	1803	GLU	2.7
1	A	1789	VAL	2.6
1	A	1809	GLN	2.5
1	A	1468	GLY	2.5
1	A	1804	ARG	2.2
1	A	1802	GLN	2.2
1	A	1846	ASN	2.1
1	A	1564	SER	2.0
1	A	1847	GLU	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.