



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1IAJ
Title : CRYSTAL STRUCTURE OF THE ATYPICAL PROTEIN KINASE DOMAIN OF A TRP CA-CHANNEL, CHAK (APO)
Authors : Yamaguchi, H.; Matsushita, M.; Nairn, A.C.; Kuriyan, J.
Deposited on : 2001-03-22
Resolution : 2.80 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

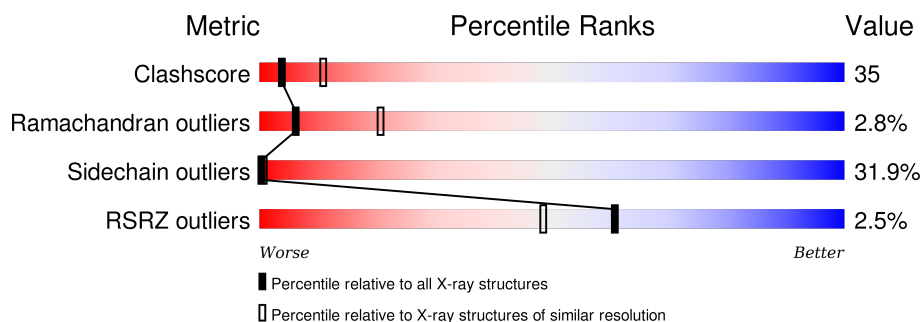
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	280	
1	B	280	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4134 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 TRANSIENT RECEPTOR POTENTIAL-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			2032	1297	346	375	14			
1	B	259	Total	C	N	O	S	0	0	0
			2100	1340	361	385	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

L1822	K1823	R1824	M1825	D1826	Y1827	T1828
-------	-------	-------	-------	-------	-------	-------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.27Å 138.20Å 113.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 97.4 (29.74-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	4.90	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.229 , 0.292 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20775 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4134	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.46	0/2080	0.62	0/2819
1	B	0.47	0/2148	0.64	0/2904
All	All	0.47	0/4228	0.63	0/5723

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	2032	0	1966	145	0
1	B	2100	0	2072	163	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4134	0	4038	286	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 35.

All (286) 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:1649:LEU:HD12	1:B:1649:LEU:H	1.18	1.08
1:B:1665:VAL:HG11	1:B:1713:GLN:HE22	1.14	1.06
1:A:1563:ARG:HH11	1:A:1563:ARG:HG3	1.25	1.00
1:B:1805:ARG:HG2	1:B:1822:LEU:HG	1.40	0.99
1:A:1605:LEU:H	1:A:1605:LEU:HD12	1.26	0.97
1:A:1602:GLN:HE21	1:A:1602:GLN:H	1.15	0.93
1:B:1665:VAL:HG11	1:B:1713:GLN:NE2	1.84	0.91
1:A:1645:ILE:HD11	1:A:1706:LEU:HD21	1.52	0.90
1:B:1568:ILE:HG23	1:B:1569:PRO:HD2	1.51	0.90
1:B:1605:LEU:HD12	1:B:1636:ILE:HG12	1.55	0.89
1:B:1820:PRO:HB2	1:B:1824:ARG:HH21	1.40	0.86
1:B:1667:HIS:HA	1:B:1670:LEU:HD12	1.58	0.85
1:A:1703:VAL:HG22	1:A:1718:GLU:HG3	1.57	0.84
1:A:1753:THR:O	1:A:1757:THR:HG23	1.79	0.81
1:A:1563:ARG:NH1	1:A:1563:ARG:HG3	1.94	0.81
1:A:1554:SER:OG	1:A:1556:VAL:HG23	1.80	0.81
1:B:1665:VAL:CG1	1:B:1713:GLN:HE22	1.95	0.79
1:B:1606:CYS:O	1:B:1633:GLU:HB2	1.81	0.79
1:A:1616:GLU:HG3	1:A:1623:ARG:CB	2.12	0.79
1:B:1626:LYS:HD3	1:B:1642:LEU:HD13	1.66	0.78
1:A:1602:GLN:N	1:A:1602:GLN:HE21	1.80	0.78
1:B:1587:GLU:HG3	1:B:1596:SER:OG	1.84	0.78
1:A:1713:GLN:HG3	1:A:1714:TRP:H	1.48	0.77
1:A:1578:GLU:OE2	1:A:1710:SER:HB3	1.84	0.76
1:A:1585:LEU:HB3	1:A:1677:ARG:HH21	1.51	0.76
1:A:1730:ASN:OD1	1:A:1734:ASP:HB2	1.86	0.75
1:A:1582:VAL:HG13	1:A:1636:ILE:HD13	1.69	0.74
1:A:1638:LYS:HE2	1:A:1719:GLU:OE1	1.89	0.73
1:B:1649:LEU:H	1:B:1649:LEU:CD1	1.95	0.72
1:A:1593:LEU:HD12	1:A:1681:LYS:HG2	1.72	0.72
1:A:1751:HIS:CD2	1:A:1822:LEU:HD13	2.25	0.72
1:B:1687:ASN:OD1	1:B:1697:SER:HB3	1.90	0.72
1:A:1751:HIS:NE2	1:A:1822:LEU:HD13	2.04	0.72
1:A:1758:ARG:HG3	1:B:1552:TYR:CD2	2.25	0.71
1:A:1553:TYR:HB3	1:B:1756:TYR:CZ	2.26	0.71
1:A:1622:ARG:N	1:A:1649:LEU:HD11	2.07	0.69
1:B:1817:LEU:HB3	1:B:1819:LEU:HD21	1.74	0.69
1:A:1553:TYR:HB3	1:B:1756:TYR:CE2	2.28	0.68
1:B:1645:ILE:HD13	1:B:1717:VAL:HG22	1.75	0.68
1:A:1666:LEU:O	1:A:1670:LEU:HD12	1.93	0.68
1:B:1677:ARG:O	1:B:1681:LYS:HG2	1.94	0.68
1:A:1646:LYS:HE3	1:A:1716:ALA:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1622:ARG:N	1:B:1649:LEU:HG	2.09	0.67
1:A:1713:GLN:HG3	1:A:1714:TRP:N	2.10	0.66
1:A:1820:PRO:HB2	1:A:1824:ARG:HH21	1.59	0.66
1:A:1587:GLU:O	1:A:1590:PRO:HD3	1.95	0.66
1:B:1649:LEU:N	1:B:1649:LEU:HD12	2.03	0.65
1:A:1758:ARG:HG3	1:B:1552:TYR:CE2	2.31	0.65
1:A:1765:ASP:HB2	1:A:1777:SER:HB2	1.79	0.65
1:A:1562:MET:CE	1:B:1780:LYS:HE2	2.27	0.65
1:B:1580:VAL:HG21	1:B:1706:LEU:HD21	1.78	0.65
1:B:1751:HIS:NE2	1:B:1822:LEU:HD13	2.11	0.64
1:A:1752:TRP:HB2	1:A:1819:LEU:HD11	1.78	0.64
1:A:1585:LEU:HD23	1:A:1677:ARG:HE	1.63	0.64
1:B:1727:LYS:HD3	1:B:1767:GLN:HB3	1.78	0.64
1:A:1552:TYR:HB3	1:B:1758:ARG:NH1	2.13	0.63
1:A:1757:THR:HG21	1:A:1761:LEU:HD12	1.80	0.63
1:B:1735:GLU:HB2	1:B:1747:LEU:HD21	1.79	0.63
1:A:1562:MET:HE1	1:B:1780:LYS:HE2	1.81	0.62
1:B:1585:LEU:HD23	1:B:1677:ARG:HE	1.64	0.62
1:A:1605:LEU:H	1:A:1605:LEU:CD1	2.03	0.62
1:A:1576:ARG:O	1:A:1608:LYS:HE2	2.00	0.62
1:A:1600:TRP:CE2	1:A:1670:LEU:HD23	2.33	0.62
1:B:1612:LEU:HG	1:B:1613:SER:N	2.15	0.62
1:B:1820:PRO:HB2	1:B:1824:ARG:NH2	2.12	0.61
1:B:1584:ARG:HG2	1:B:1585:LEU:N	2.15	0.61
1:A:1628:LEU:HD13	1:A:1642:LEU:HD13	1.81	0.61
1:B:1622:ARG:HH11	1:B:1622:ARG:HG2	1.64	0.61
1:A:1706:LEU:C	1:A:1706:LEU:HD12	2.21	0.60
1:A:1758:ARG:HB2	1:A:1758:ARG:HH11	1.66	0.60
1:A:1605:LEU:N	1:A:1605:LEU:HD12	2.08	0.60
1:A:1557:GLU:O	1:A:1561:LEU:HB2	2.00	0.60
1:A:1573:VAL:HG13	1:A:1574:PRO:HD2	1.84	0.60
1:B:1585:LEU:HB3	1:B:1677:ARG:HH21	1.66	0.60
1:B:1664:THR:HG22	1:B:1668:LEU:HD22	1.82	0.60
1:B:1684:PHE:O	1:B:1688:GLN:HB2	2.01	0.59
1:A:1725:PHE:HZ	1:A:1767:GLN:HE21	1.50	0.59
1:B:1655:THR:C	1:B:1656:TRP:CD1	2.76	0.59
1:A:1811:ASN:OD1	1:A:1813:CYS:HB2	2.03	0.59
1:B:1593:LEU:HD12	1:B:1681:LYS:HD3	1.84	0.59
1:B:1555:ALA:O	1:B:1559:ASN:HB2	2.02	0.58
1:A:1736:ILE:HD11	1:A:1743:GLU:HB3	1.85	0.58
1:A:1645:ILE:HG12	1:A:1717:VAL:HG13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1622:ARG:HG2	1:B:1622:ARG:NH1	2.18	0.58
1:A:1645:ILE:CD1	1:A:1706:LEU:HD21	2.30	0.57
1:B:1696:TYR:HB2	1:B:1745:ILE:HD13	1.86	0.57
1:A:1632:SER:HB2	1:A:1636:ILE:HG22	1.85	0.57
1:B:1568:ILE:HG23	1:B:1569:PRO:CD	2.30	0.57
1:B:1751:HIS:CD2	1:B:1822:LEU:HD13	2.39	0.57
1:A:1755:GLU:HG3	1:A:1819:LEU:HD22	1.87	0.57
1:A:1724:GLU:OE2	1:A:1726:ARG:HB3	2.05	0.56
1:B:1802:LYS:HG2	1:B:1803:ASN:N	2.20	0.56
1:B:1757:THR:O	1:B:1760:GLU:HB2	2.05	0.56
1:A:1582:VAL:CG1	1:A:1636:ILE:HD13	2.34	0.56
1:A:1699:ARG:NH2	1:A:1771:GLU:OE2	2.39	0.56
1:A:1803:ASN:HB3	1:A:1807:LYS:HE3	1.86	0.56
1:B:1580:VAL:HG22	1:B:1707:TYR:O	2.06	0.56
1:A:1552:TYR:CE1	1:B:1758:ARG:HG2	2.41	0.56
1:A:1589:SER:HB2	1:A:1592:ILE:HG13	1.88	0.56
1:A:1562:MET:HE1	1:B:1760:GLU:HG2	1.88	0.55
1:B:1644:ILE:HG12	1:B:1720:CYS:HB2	1.88	0.55
1:B:1622:ARG:N	1:B:1649:LEU:CG	2.69	0.55
1:A:1552:TYR:CD1	1:B:1758:ARG:CG	2.89	0.55
1:B:1765:ASP:HB2	1:B:1777:SER:HB2	1.88	0.55
1:B:1731:ASN:HD22	1:B:1731:ASN:C	2.09	0.55
1:A:1552:TYR:CD1	1:B:1758:ARG:HG2	2.42	0.55
1:A:1602:GLN:NE2	1:A:1602:GLN:H	1.97	0.55
1:B:1740:ASN:OD1	1:B:1743:GLU:HB2	2.06	0.55
1:B:1693:SER:HB2	1:B:1816:LYS:HD3	1.89	0.55
1:A:1563:ARG:HH11	1:A:1563:ARG:CG	2.08	0.54
1:A:1818:LYS:O	1:A:1820:PRO:HD3	2.07	0.54
1:A:1694:ILE:HG23	1:A:1745:ILE:HG12	1.89	0.54
1:B:1805:ARG:HG2	1:B:1822:LEU:CG	2.28	0.54
1:B:1593:LEU:HD12	1:B:1681:LYS:CD	2.37	0.54
1:B:1735:GLU:HB2	1:B:1747:LEU:CD2	2.38	0.54
1:B:1566:GLN:O	1:B:1568:ILE:HD13	2.08	0.54
1:B:1581:THR:CG2	1:B:1707:TYR:HB3	2.37	0.54
1:A:1576:ARG:NE	1:A:1576:ARG:HA	2.22	0.54
1:A:1568:ILE:HG23	1:A:1569:PRO:HD2	1.90	0.54
1:B:1578:GLU:OE2	1:B:1710:SER:HB2	2.09	0.53
1:A:1681:LYS:HE3	1:B:1564:LEU:HD11	1.89	0.53
1:A:1710:SER:OG	1:A:1711:ALA:N	2.40	0.53
1:A:1558:ARG:O	1:A:1562:MET:HB2	2.08	0.53
1:B:1651:GLU:HA	1:B:1654:ASN:ND2	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:PHE:CD2	1:A:1725:PHE:C	2.82	0.53
1:A:1696:TYR:CD2	1:A:1742:LEU:HD23	2.44	0.53
1:B:1600:TRP:CE2	1:B:1670:LEU:HD23	2.44	0.53
1:A:1757:THR:CG2	1:A:1761:LEU:HD12	2.38	0.53
1:B:1761:LEU:HA	1:B:1779:ILE:O	2.09	0.52
1:B:1683:THR:HG22	1:B:1684:PHE:N	2.25	0.52
1:B:1690:LYS:HG3	1:B:1690:LYS:O	2.09	0.52
1:A:1633:GLU:HG2	1:A:1634:HIS:CD2	2.44	0.52
1:A:1721:MET:HE3	1:A:1769:VAL:HG23	1.92	0.52
1:A:1648:PHE:CE2	1:A:1668:LEU:HB3	2.44	0.52
1:B:1758:ARG:NH1	1:B:1758:ARG:HG3	2.25	0.51
1:B:1826:ASP:N	1:B:1826:ASP:OD1	2.41	0.51
1:B:1608:LYS:HB2	1:B:1631:TRP:CE2	2.45	0.51
1:B:1627:VAL:O	1:B:1642:LEU:HD23	2.10	0.51
1:A:1553:TYR:H	1:A:1553:TYR:HD2	1.58	0.51
1:A:1756:TYR:CE2	1:B:1553:TYR:HB3	2.46	0.51
1:B:1580:VAL:HG23	1:B:1708:CYS:HA	1.92	0.51
1:A:1586:GLU:HG3	1:A:1599:SER:O	2.11	0.51
1:B:1633:GLU:O	1:B:1634:HIS:HB2	2.10	0.51
1:B:1568:ILE:CG2	1:B:1569:PRO:HD2	2.33	0.50
1:B:1820:PRO:CB	1:B:1824:ARG:HH21	2.19	0.50
1:B:1622:ARG:N	1:B:1649:LEU:HD11	2.26	0.50
1:A:1632:SER:OG	1:A:1635:ASP:HA	2.11	0.50
1:B:1626:LYS:HG2	1:B:1642:LEU:HD22	1.92	0.50
1:A:1622:ARG:HA	1:A:1649:LEU:HG	1.92	0.50
1:B:1666:LEU:HD13	1:B:1714:TRP:CE2	2.46	0.50
1:A:1597:MET:HA	1:B:1560:ASN:OD1	2.10	0.50
1:B:1690:LYS:CD	1:B:1694:ILE:HB	2.42	0.50
1:A:1707:TYR:CD1	1:A:1713:GLN:O	2.65	0.50
1:A:1782:GLU:OE1	1:A:1782:GLU:HA	2.11	0.50
1:A:1656:TRP:N	1:A:1656:TRP:CD1	2.80	0.50
1:A:1758:ARG:CB	1:A:1758:ARG:HH11	2.25	0.49
1:A:1687:ASN:HA	1:A:1690:LYS:HE3	1.93	0.49
1:A:1780:LYS:HD2	1:B:1562:MET:CE	2.42	0.49
1:B:1664:THR:HG23	1:B:1668:LEU:HD13	1.94	0.49
1:B:1732:ASN:HB3	1:B:1734:ASP:OD1	2.11	0.49
1:A:1750:SER:OG	1:A:1763:VAL:O	2.23	0.49
1:B:1563:ARG:HH11	1:B:1563:ARG:CG	2.24	0.49
1:A:1706:LEU:O	1:A:1706:LEU:HD12	2.12	0.49
1:B:1816:LYS:NZ	1:B:1816:LYS:HB2	2.27	0.49
1:A:1576:ARG:HB2	1:B:1603:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1754:TYR:HB2	1:A:1762:LEU:HD13	1.94	0.49
1:A:1677:ARG:HH12	1:A:1702:GLU:HG2	1.78	0.48
1:B:1798:GLU:O	1:B:1801:ILE:HG22	2.12	0.48
1:A:1615:GLU:O	1:A:1624:ALA:O	2.31	0.48
1:A:1552:TYR:HB3	1:B:1758:ARG:HH11	1.77	0.48
1:B:1622:ARG:NH2	1:B:1646:LYS:HE3	2.29	0.48
1:A:1588:SER:OG	1:A:1597:MET:N	2.46	0.48
1:A:1588:SER:HG	1:A:1597:MET:H	1.60	0.48
1:A:1562:MET:CE	1:B:1760:GLU:HG2	2.44	0.47
1:B:1581:THR:HG23	1:B:1707:TYR:HB3	1.95	0.47
1:B:1742:LEU:O	1:B:1746:MET:HG2	2.15	0.47
1:A:1581:THR:O	1:A:1706:LEU:HA	2.14	0.47
1:A:1574:PRO:O	1:A:1575:PRO:C	2.52	0.47
1:B:1805:ARG:CG	1:B:1822:LEU:HG	2.29	0.47
1:A:1573:VAL:HG23	1:B:1602:GLN:HG2	1.96	0.47
1:A:1566:GLN:O	1:A:1568:ILE:N	2.48	0.47
1:A:1593:LEU:O	1:A:1681:LYS:HD3	2.15	0.47
1:A:1751:HIS:CE1	1:A:1819:LEU:HB3	2.50	0.47
1:B:1817:LEU:CB	1:B:1819:LEU:HD21	2.44	0.47
1:A:1611:PHE:HA	1:A:1627:VAL:HG22	1.97	0.47
1:B:1622:ARG:N	1:B:1649:LEU:CD1	2.78	0.47
1:A:1803:ASN:HD22	1:A:1803:ASN:N	2.13	0.47
1:A:1798:GLU:HA	1:A:1801:ILE:HB	1.97	0.47
1:B:1609:ILE:HG22	1:B:1629:CYS:HA	1.97	0.47
1:A:1622:ARG:N	1:A:1649:LEU:CD1	2.78	0.46
1:A:1694:ILE:HG13	1:A:1817:LEU:HD21	1.97	0.46
1:B:1644:ILE:CG1	1:B:1720:CYS:HB2	2.46	0.46
1:B:1662:GLU:HG2	1:B:1663:ASP:N	2.30	0.46
1:B:1622:ARG:HH22	1:B:1646:LYS:HE3	1.81	0.46
1:B:1649:LEU:HB2	1:B:1651:GLU:OE2	2.16	0.46
1:B:1645:ILE:CD1	1:B:1717:VAL:HG22	2.42	0.46
1:B:1662:GLU:OE2	1:B:1663:ASP:HB2	2.15	0.45
1:B:1625:VAL:HG12	1:B:1626:LYS:N	2.31	0.45
1:A:1553:TYR:CE2	1:B:1757:THR:HA	2.51	0.45
1:B:1706:LEU:HD13	1:B:1717:VAL:HG21	1.97	0.45
1:A:1593:LEU:HD11	1:A:1677:ARG:HD2	1.97	0.45
1:B:1774:THR:OG1	1:B:1775:ASP:N	2.50	0.45
1:A:1600:TRP:NE1	1:A:1670:LEU:HD23	2.32	0.45
1:B:1736:ILE:HD11	1:B:1743:GLU:HG2	1.99	0.45
1:A:1566:GLN:HA	1:A:1566:GLN:OE1	2.14	0.45
1:A:1764:LEU:HD12	1:A:1779:ILE:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1652:VAL:O	1:B:1656:TRP:NE1	2.44	0.45
1:B:1563:ARG:CG	1:B:1563:ARG:NH1	2.80	0.45
1:B:1626:LYS:HD3	1:B:1642:LEU:CD1	2.41	0.45
1:A:1655:THR:C	1:A:1656:TRP:CG	2.90	0.45
1:B:1626:LYS:HB2	1:B:1626:LYS:HZ3	1.82	0.45
1:A:1706:LEU:CD1	1:A:1706:LEU:C	2.86	0.44
1:B:1625:VAL:CG1	1:B:1626:LYS:N	2.80	0.44
1:B:1580:VAL:HG11	1:B:1706:LEU:HD11	2.00	0.44
1:B:1697:SER:O	1:B:1771:GLU:HG2	2.16	0.44
1:B:1804:PHE:CE2	1:B:1822:LEU:HD21	2.52	0.44
1:A:1674:GLN:HG2	1:B:1564:LEU:HD23	2.00	0.44
1:B:1693:SER:O	1:B:1695:PRO:HD3	2.17	0.44
1:B:1693:SER:CB	1:B:1816:LYS:HD3	2.48	0.44
1:B:1608:LYS:HB2	1:B:1631:TRP:NE1	2.33	0.44
1:A:1693:SER:O	1:A:1695:PRO:HD3	2.18	0.44
1:B:1593:LEU:O	1:B:1681:LYS:HE2	2.18	0.44
1:A:1696:TYR:CG	1:A:1742:LEU:HD23	2.52	0.44
1:B:1664:THR:CG2	1:B:1668:LEU:HD13	2.48	0.43
1:B:1749:PHE:O	1:B:1752:TRP:HB3	2.17	0.43
1:A:1587:GLU:OE2	1:A:1681:LYS:NZ	2.51	0.43
1:B:1607:ALA:HA	1:B:1631:TRP:CZ3	2.52	0.43
1:A:1677:ARG:O	1:A:1681:LYS:HG3	2.18	0.43
1:A:1585:LEU:HD12	1:A:1600:TRP:CD2	2.53	0.43
1:B:1600:TRP:HE1	1:B:1674:GLN:HE21	1.66	0.43
1:B:1817:LEU:O	1:B:1818:LYS:HB2	2.18	0.43
1:B:1691:PRO:C	1:B:1693:SER:H	2.21	0.43
1:A:1741:THR:O	1:A:1742:LEU:C	2.56	0.43
1:A:1782:GLU:H	1:A:1798:GLU:CB	2.32	0.43
1:B:1648:PHE:CD1	1:B:1648:PHE:N	2.87	0.42
1:B:1664:THR:O	1:B:1665:VAL:C	2.56	0.42
1:B:1566:GLN:HB2	1:B:1566:GLN:HE21	1.72	0.42
1:B:1605:LEU:HB3	1:B:1633:GLU:HB3	2.01	0.42
1:B:1651:GLU:C	1:B:1653:ILE:H	2.21	0.42
1:A:1822:LEU:HA	1:A:1822:LEU:HD12	1.77	0.42
1:B:1802:LYS:O	1:B:1803:ASN:C	2.56	0.42
1:B:1724:GLU:N	1:B:1769:VAL:HG13	2.34	0.42
1:B:1805:ARG:HA	1:B:1822:LEU:HD23	2.01	0.42
1:A:1749:PHE:O	1:A:1753:THR:HG23	2.19	0.42
1:B:1587:GLU:HG2	1:B:1593:LEU:HD13	2.02	0.42
1:A:1710:SER:C	1:A:1712:GLY:H	2.22	0.42
1:A:1573:VAL:CG1	1:A:1574:PRO:HD2	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1690:LYS:HD2	1:B:1694:ILE:HB	2.01	0.42
1:A:1729:ASN:HA	1:A:1734:ASP:O	2.19	0.42
1:A:1696:TYR:HB2	1:A:1745:ILE:HD13	2.02	0.42
1:A:1697:SER:HA	1:A:1698:PRO:HD2	1.87	0.42
1:B:1636:ILE:HD12	1:B:1636:ILE:HA	1.75	0.42
1:A:1671:ARG:HH11	1:A:1671:ARG:HG3	1.85	0.42
1:B:1649:LEU:HD22	1:B:1651:GLU:OE2	2.20	0.42
1:B:1622:ARG:HG2	1:B:1622:ARG:O	2.19	0.42
1:B:1764:LEU:HA	1:B:1764:LEU:HD23	1.84	0.42
1:B:1651:GLU:C	1:B:1653:ILE:N	2.73	0.41
1:A:1701:LEU:HB2	1:A:1718:GLU:CD	2.40	0.41
1:A:1824:ARG:HH11	1:A:1824:ARG:CG	2.33	0.41
1:B:1690:LYS:HA	1:B:1691:PRO:HD2	1.87	0.41
1:A:1628:LEU:HB2	1:A:1642:LEU:CD1	2.49	0.41
1:A:1557:GLU:HG3	1:A:1557:GLU:H	1.51	0.41
1:A:1579:PRO:O	1:A:1709:HIS:HD2	2.04	0.41
1:B:1667:HIS:CA	1:B:1670:LEU:HD12	2.41	0.41
1:B:1700:PHE:CE2	1:B:1776:PRO:HG3	2.54	0.41
1:B:1701:LEU:HD22	1:B:1719:GLU:HB3	2.03	0.41
1:B:1551:TYR:N	1:B:1551:TYR:CD2	2.89	0.41
1:B:1725:PHE:HZ	1:B:1767:GLN:HE21	1.68	0.41
1:A:1804:PHE:CE1	1:A:1808:HIS:HB2	2.54	0.41
1:B:1673:ILE:HG12	1:B:1703:VAL:HG12	2.02	0.41
1:B:1622:ARG:HH11	1:B:1622:ARG:CG	2.33	0.41
1:B:1713:GLN:HB3	1:B:1715:PHE:CE1	2.55	0.41
1:A:1655:THR:O	1:A:1655:THR:HG22	2.21	0.41
1:B:1707:TYR:HB2	1:B:1714:TRP:CZ3	2.55	0.41
1:A:1552:TYR:CB	1:B:1758:ARG:HH11	2.33	0.41
1:B:1656:TRP:HB2	1:B:1661:LYS:O	2.20	0.41
1:B:1626:LYS:HZ3	1:B:1626:LYS:CB	2.34	0.41
1:B:1779:ILE:HD12	1:B:1779:ILE:N	2.35	0.41
1:A:1615:GLU:H	1:A:1615:GLU:HG3	1.59	0.41
1:A:1624:ALA:HA	1:A:1646:LYS:HA	2.02	0.40
1:A:1782:GLU:OE1	1:A:1782:GLU:CA	2.68	0.40
1:B:1735:GLU:OE2	1:B:1747:LEU:HD22	2.21	0.40
1:B:1589:SER:OG	1:B:1592:ILE:HD12	2.21	0.40
1:B:1651:GLU:CD	1:B:1652:VAL:N	2.75	0.40
1:A:1710:SER:C	1:A:1712:GLY:N	2.75	0.40
1:A:1744:GLU:OE1	1:A:1811:ASN:HB2	2.21	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	245/280 (88%)	216 (88%)	22 (9%)	7 (3%)	6	19
1	B	251/280 (90%)	219 (87%)	25 (10%)	7 (3%)	6	21
All	All	496/560 (89%)	435 (88%)	47 (10%)	14 (3%)	6	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1567	SER
1	B	1612	LEU
1	B	1823	LYS
1	B	1575	PRO
1	B	1588	SER
1	A	1593	LEU
1	A	1732	ASN
1	B	1665	VAL
1	A	1592	ILE
1	A	1712	GLY
1	A	1822	LEU
1	B	1639	SER
1	A	1695	PRO
1	B	1797	GLY

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	223/253 (88%)	143 (64%)	80 (36%)	0	0
1	B	234/253 (92%)	168 (72%)	66 (28%)	0	1
All	All	457/506 (90%)	311 (68%)	146 (32%)	0	1

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1553	TYR
1	A	1556	VAL
1	A	1557	GLU
1	A	1558	ARG
1	A	1562	MET
1	A	1563	ARG
1	A	1564	LEU
1	A	1565	SER
1	A	1566	GLN
1	A	1567	SER
1	A	1571	VAL
1	A	1576	ARG
1	A	1578	GLU
1	A	1584	ARG
1	A	1586	GLU
1	A	1588	SER
1	A	1589	SER
1	A	1591	SER
1	A	1592	ILE
1	A	1593	LEU
1	A	1596	SER
1	A	1597	MET
1	A	1598	SER
1	A	1599	SER
1	A	1602	GLN
1	A	1603	LEU
1	A	1605	LEU
1	A	1608	LYS
1	A	1610	GLU
1	A	1613	SER
1	A	1615	GLU
1	A	1616	GLU
1	A	1622	ARG
1	A	1626	LYS
1	A	1627	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1635	ASP
1	A	1638	LYS
1	A	1642	LEU
1	A	1645	ILE
1	A	1646	LYS
1	A	1647	SER
1	A	1649	LEU
1	A	1656	TRP
1	A	1665	VAL
1	A	1666	LEU
1	A	1670	LEU
1	A	1671	ARG
1	A	1672	GLU
1	A	1674	GLN
1	A	1675	GLN
1	A	1683	THR
1	A	1689	MET
1	A	1693	SER
1	A	1699	ARG
1	A	1702	GLU
1	A	1706	LEU
1	A	1710	SER
1	A	1713	GLN
1	A	1717	VAL
1	A	1718	GLU
1	A	1720	CYS
1	A	1721	MET
1	A	1725	PHE
1	A	1726	ARG
1	A	1731	ASN
1	A	1732	ASN
1	A	1739	THR
1	A	1750	SER
1	A	1758	ARG
1	A	1761	LEU
1	A	1777	SER
1	A	1779	ILE
1	A	1780	LYS
1	A	1782	GLU
1	A	1801	ILE
1	A	1811	ASN
1	A	1812	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1818	LYS
1	A	1823	LYS
1	A	1824	ARG
1	B	1553	TYR
1	B	1558	ARG
1	B	1559	ASN
1	B	1562	MET
1	B	1563	ARG
1	B	1568	ILE
1	B	1571	VAL
1	B	1578	GLU
1	B	1580	VAL
1	B	1582	VAL
1	B	1588	SER
1	B	1591	SER
1	B	1592	ILE
1	B	1593	LEU
1	B	1602	GLN
1	B	1603	LEU
1	B	1608	LYS
1	B	1609	ILE
1	B	1617	MET
1	B	1623	ARG
1	B	1628	LEU
1	B	1630	THR
1	B	1633	GLU
1	B	1636	ILE
1	B	1638	LYS
1	B	1644	ILE
1	B	1647	SER
1	B	1649	LEU
1	B	1652	VAL
1	B	1653	ILE
1	B	1655	THR
1	B	1662	GLU
1	B	1668	LEU
1	B	1671	ARG
1	B	1672	GLU
1	B	1681	LYS
1	B	1682	LEU
1	B	1683	THR
1	B	1688	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1690	LYS
1	B	1693	SER
1	B	1697	SER
1	B	1699	ARG
1	B	1701	LEU
1	B	1713	GLN
1	B	1724	GLU
1	B	1726	ARG
1	B	1727	LYS
1	B	1731	ASN
1	B	1743	GLU
1	B	1744	GLU
1	B	1760	GLU
1	B	1774	THR
1	B	1777	SER
1	B	1801	ILE
1	B	1802	LYS
1	B	1812	SER
1	B	1815	ARG
1	B	1816	LYS
1	B	1818	LYS
1	B	1819	LEU
1	B	1822	LEU
1	B	1823	LYS
1	B	1824	ARG
1	B	1826	ASP
1	B	1828	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1602	GLN
1	A	1634	HIS
1	A	1688	GLN
1	A	1709	HIS
1	A	1713	GLN
1	A	1767	GLN
1	A	1803	ASN
1	A	1825	ASN
1	B	1566	GLN
1	B	1674	GLN
1	B	1713	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1731	ASN
1	B	1767	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	253/280 (90%)	-0.12	7 (2%) 56 44	29, 59, 95, 100	0
1	B	259/280 (92%)	0.07	6 (2%) 64 52	32, 67, 96, 100	0
All	All	512/560 (91%)	-0.02	13 (2%) 61 48	29, 63, 96, 100	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1795	ASN	4.4
1	A	1551	TYR	3.6
1	A	1616	GLU	3.1
1	A	1614	LYS	3.0
1	A	1615	GLU	2.9
1	B	1654	ASN	2.9
1	A	1613	SER	2.7
1	B	1649	LEU	2.5
1	B	1595	ASN	2.3
1	A	1617	MET	2.2
1	B	1650	PRO	2.2
1	A	1826	ASP	2.2
1	B	1592	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	2001	1/1	0.98	0.17	0.20	59,59,59,59	0
2	ZN	B	2001	1/1	0.98	0.12	-1.12	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.