



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 1UX5 / pdb_00001ux5
Title : Crystal Structures of a Formin Homology-2 domain reveal a flexibly tethered dimer architecture
Authors : Xu, Y.; Moseley, J.B.; Sagot, I.; Poy, F.; Pellman, D.; Goode, B.L.; Eck, M.J.
Deposited on : 2004-02-19
Resolution : 2.50 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

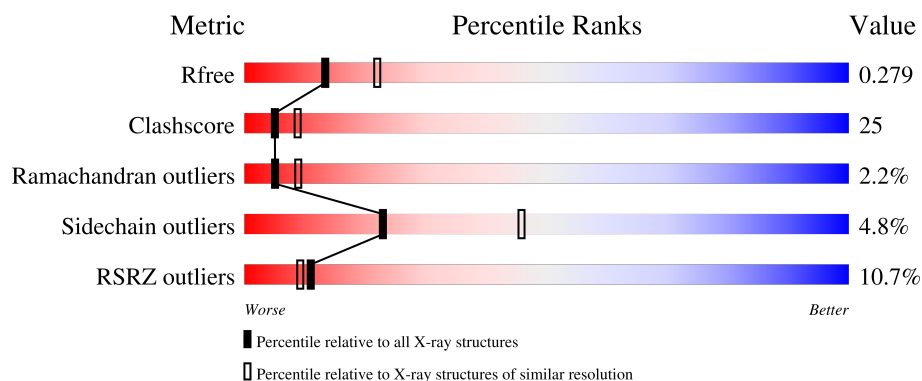
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	411	11% 55% 41% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3366 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 BNI1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	7	0	0
			3335	2124	560	641	10			

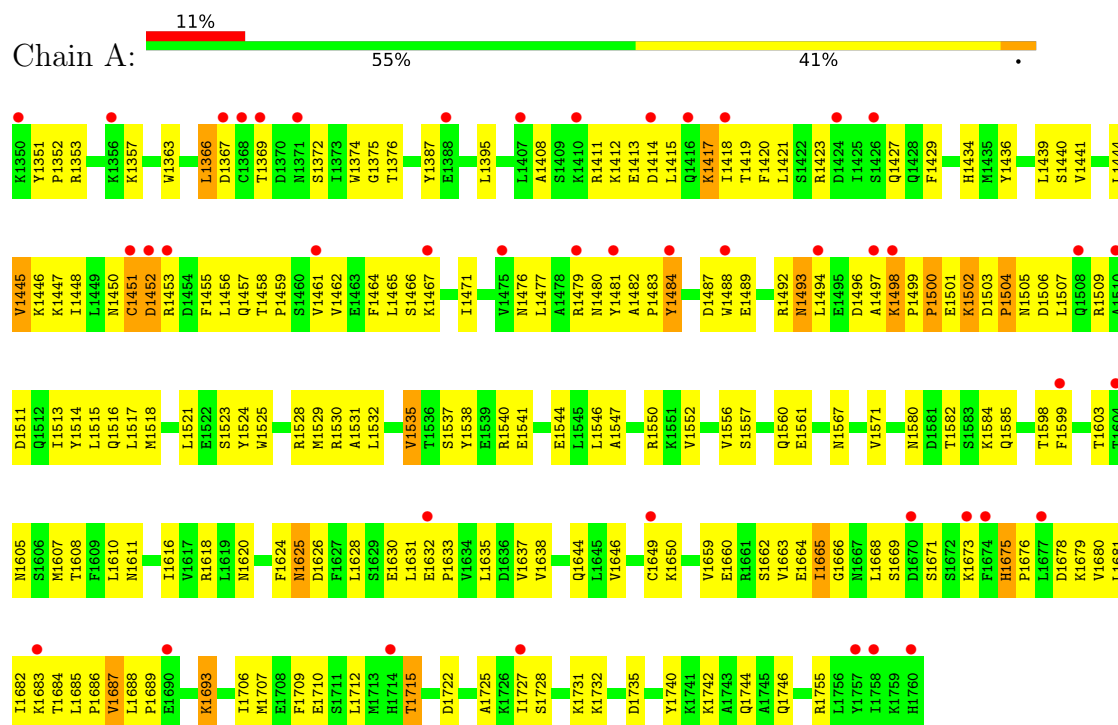
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		

3 Residue-property plots [i](#)

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: BNI1 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.40Å 101.40Å 265.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	65.5 (30.00-2.50) 67.5 (30.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.251 0.241 , 0.279	Depositor DCC
R_{free} test set	2337 reflections (6.75%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3366	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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, 0.333 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	0.45	0/3395	0.95	11/4577 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	LEU	N-CA-C	-8.77	95.81	109.76
1	A	1687	VAL	N-CA-C	6.70	118.68	111.58
1	A	1684	THR	N-CA-C	6.50	118.05	110.97
1	A	1571	VAL	N-CA-C	-6.23	104.67	110.53
1	A	1367	ASP	N-CA-C	5.93	118.50	111.33
1	A	1631	LEU	N-CA-C	5.69	119.00	112.57
1	A	1675	HIS	N-CA-C	-5.57	103.02	109.93
1	A	1372	SER	N-CA-C	5.52	115.57	108.34
1	A	1727	ILE	N-CA-C	5.47	116.20	110.62
1	A	1376	THR	N-CA-C	-5.41	106.35	113.17
1	A	1669	SER	N-CA-C	-5.11	106.21	112.90

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	3335	0	3349	166	0
2	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3366	0	3349	166	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 25.

All (166) 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:1528:ARG:HG3	1:A:1680:VAL:HG11	1.39	1.02
1:A:1646:VAL:O	1:A:1649:CYS:SG	2.22	0.97
1:A:1448:ILE:HD13	1:A:1465:LEU:HD11	1.54	0.87
1:A:1498:LYS:O	1:A:1500:PRO:HD3	1.78	0.84
1:A:1514:TYR:HA	1:A:1518:MET:HE2	1.59	0.83
1:A:1369:THR:HG21	1:A:1375:GLY:HA3	1.60	0.82
1:A:1693:LYS:HB2	1:A:1693:LYS:NZ	1.97	0.80
1:A:1369:THR:CG2	1:A:1375:GLY:HA3	2.13	0.78
1:A:1447:LYS:HD2	1:A:1452:ASP:OD2	1.85	0.77
1:A:1528:ARG:HG3	1:A:1680:VAL:CG1	2.19	0.72
1:A:1662:SER:HA	1:A:1666:GLY:HA3	1.71	0.72
1:A:1625:ASN:ND2	1:A:1744:GLN:HE22	1.88	0.71
1:A:1517:LEU:HA	1:A:1521:LEU:HD12	1.71	0.71
1:A:1557:SER:O	1:A:1561:GLU:HG2	1.91	0.70
1:A:1608:THR:HG22	1:A:1611:ASN:H	1.56	0.70
1:A:1466:SER:HA	1:A:1471:ILE:HD11	1.74	0.70
1:A:1444:LEU:O	1:A:1447:LYS:HB3	1.93	0.69
1:A:1679:LYS:HB2	1:A:1682:ILE:HG22	1.75	0.68
1:A:1679:LYS:HB2	1:A:1682:ILE:CG2	2.24	0.68
1:A:1608:THR:HG22	1:A:1611:ASN:OD1	1.94	0.67
1:A:1456:LEU:HD13	1:A:1683:LYS:HE3	1.75	0.67
1:A:1493:ASN:HD21	1:A:1496:ASP:HB2	1.58	0.67
1:A:1625:ASN:HD21	1:A:1744:GLN:HE22	1.40	0.67
1:A:1487:ASP:OD1	1:A:1489:GLU:HB2	1.95	0.67
1:A:1608:THR:HG23	1:A:1610:LEU:N	2.08	0.67
1:A:1535:VAL:HG13	1:A:1687:VAL:HG11	1.77	0.66
1:A:1679:LYS:O	1:A:1682:ILE:HG22	1.96	0.66
1:A:1625:ASN:HD21	1:A:1744:GLN:NE2	1.95	0.65
1:A:1608:THR:CG2	1:A:1611:ASN:H	2.09	0.65
1:A:1531:ALA:O	1:A:1535:VAL:HG23	1.96	0.65
1:A:1742:LYS:O	1:A:1746:GLN:HG3	1.99	0.63
1:A:1626:ASP:O	1:A:1630:GLU:HG3	1.99	0.62
1:A:1632:GLU:N	1:A:1633:PRO:HD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:GLN:HE21	1:A:1644:GLN:HA	1.63	0.61
1:A:1493:ASN:ND2	1:A:1496:ASP:HB2	2.15	0.61
1:A:1582:THR:HA	1:A:1585:GLN:HG2	1.83	0.61
1:A:1423:ARG:O	1:A:1427:GLN:HB2	2.00	0.61
1:A:1418:ILE:HG23	1:A:1507:LEU:HD13	1.83	0.60
1:A:1453:ARG:HG2	1:A:1457:GLN:NE2	2.15	0.60
1:A:1644:GLN:HA	1:A:1644:GLN:NE2	2.18	0.59
1:A:1556:VAL:O	1:A:1560:GLN:HB2	2.03	0.59
1:A:1681:LEU:HD22	1:A:1685:LEU:HD21	1.84	0.59
1:A:1441:VAL:HG22	1:A:1513:ILE:HD11	1.84	0.59
1:A:1419:THR:HG23	1:A:1511:ASP:OD2	2.04	0.58
1:A:1458:THR:O	1:A:1461:VAL:HG22	2.04	0.58
1:A:1369:THR:HG23	1:A:1374:TRP:O	2.05	0.56
1:A:1528:ARG:HH11	1:A:1529:MET:CE	2.18	0.56
1:A:1482:ALA:HB3	1:A:1483:PRO:HD3	1.86	0.56
1:A:1497:ALA:C	1:A:1499:PRO:CD	2.78	0.56
1:A:1464:PHE:HA	1:A:1467:LYS:HG3	1.87	0.55
1:A:1660:GLU:HG2	1:A:1688:LEU:HD22	1.89	0.54
1:A:1680:VAL:HG23	1:A:1681:LEU:N	2.23	0.54
1:A:1681:LEU:HB3	1:A:1685:LEU:HD23	1.89	0.54
1:A:1659:VAL:O	1:A:1663:VAL:HG23	2.08	0.54
1:A:1693:LYS:HB2	1:A:1693:LYS:HZ3	1.71	0.54
1:A:1608:THR:HG23	1:A:1610:LEU:H	1.71	0.53
1:A:1451:CYS:SG	1:A:1679:LYS:HG3	2.49	0.53
1:A:1706:ILE:O	1:A:1710:GLU:HG3	2.08	0.53
1:A:1420:PHE:CD2	1:A:1480:ASN:HB3	2.44	0.53
1:A:1476:ASN:O	1:A:1479:ARG:HB2	2.09	0.52
1:A:1461:VAL:HG23	1:A:1462:VAL:N	2.24	0.52
1:A:1452:ASP:O	1:A:1455:PHE:HB3	2.09	0.52
1:A:1693:LYS:HB2	1:A:1693:LYS:HZ2	1.69	0.52
1:A:1712:LEU:O	1:A:1715:THR:HB	2.09	0.52
1:A:1369:THR:HG22	1:A:1369:THR:O	2.10	0.52
1:A:1481:TYR:HD2	1:A:1515:LEU:HD13	1.74	0.52
1:A:1532:LEU:HA	1:A:1535:VAL:HG23	1.91	0.52
1:A:1580:ASN:HB3	1:A:1584:LYS:HB2	1.92	0.52
1:A:1411:ARG:O	1:A:1415:LEU:HB2	2.10	0.51
1:A:1503:ASP:OD1	1:A:1504:PRO:HD2	2.10	0.51
1:A:1421:LEU:HG	1:A:1481:TYR:OH	2.11	0.51
1:A:1521:LEU:HD21	1:A:1675:HIS:HB2	1.92	0.51
1:A:1450:ASN:C	1:A:1451:CYS:SG	2.94	0.51
1:A:1453:ARG:HG2	1:A:1457:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:LYS:HE2	1:A:1357:LYS:N	2.27	0.50
1:A:1497:ALA:O	1:A:1498:LYS:HB2	2.12	0.49
1:A:1646:VAL:CG2	1:A:1706:ILE:HD11	2.42	0.49
1:A:1626:ASP:C	1:A:1630:GLU:HG3	2.38	0.49
1:A:1487:ASP:O	1:A:1488:TRP:HB2	2.12	0.49
1:A:1414:ASP:O	1:A:1414:ASP:OD1	2.31	0.49
1:A:1446:LYS:O	1:A:1446:LYS:HG2	2.13	0.49
1:A:1523:SER:HB2	1:A:1673:LYS:HE2	1.95	0.49
1:A:1457:GLN:O	1:A:1459:PRO:HD3	2.13	0.48
1:A:1447:LYS:HA	1:A:1452:ASP:OD2	2.14	0.48
1:A:1451:CYS:O	1:A:1452:ASP:C	2.56	0.48
1:A:1498:LYS:O	1:A:1500:PRO:CD	2.57	0.48
1:A:1419:THR:HG23	1:A:1511:ASP:CG	2.38	0.48
1:A:1436:TYR:CB	1:A:1444:LEU:HD13	2.44	0.48
1:A:1419:THR:HG22	1:A:1421:LEU:H	1.78	0.48
1:A:1504:PRO:HA	1:A:1507:LEU:HD23	1.95	0.48
1:A:1513:ILE:O	1:A:1514:TYR:C	2.57	0.48
1:A:1413:GLU:C	1:A:1415:LEU:H	2.21	0.48
1:A:1408:ALA:O	1:A:1412:LYS:HG3	2.13	0.47
1:A:1504:PRO:O	1:A:1507:LEU:HB2	2.14	0.47
1:A:1755:ARG:HH11	1:A:1755:ARG:HG3	1.78	0.47
1:A:1477:LEU:O	1:A:1481:TYR:HD1	1.97	0.47
1:A:1528:ARG:NH1	1:A:1529:MET:CE	2.77	0.47
1:A:1535:VAL:HG13	1:A:1687:VAL:CG1	2.45	0.47
1:A:1441:VAL:HG22	1:A:1513:ILE:CD1	2.43	0.46
1:A:1417:LYS:HE2	1:A:1505:ASN:O	2.15	0.46
1:A:1497:ALA:C	1:A:1499:PRO:HD3	2.40	0.46
1:A:1632:GLU:N	1:A:1633:PRO:CD	2.79	0.46
1:A:1509:ARG:O	1:A:1513:ILE:HD13	2.16	0.46
1:A:1525:TRP:CZ3	1:A:1528:ARG:HD3	2.51	0.45
1:A:1411:ARG:O	1:A:1411:ARG:HG2	2.16	0.45
1:A:1497:ALA:O	1:A:1499:PRO:HD3	2.16	0.45
1:A:1436:TYR:HB3	1:A:1444:LEU:HD13	1.97	0.45
1:A:1484:TYR:HD2	1:A:1503:ASP:O	1.99	0.45
1:A:1664:GLU:C	1:A:1665:ILE:HG23	2.42	0.45
1:A:1492:ARG:O	1:A:1493:ASN:HB3	2.17	0.45
1:A:1500:PRO:HG2	1:A:1501:GLU:H	1.81	0.45
1:A:1529:MET:O	1:A:1530:ARG:C	2.60	0.45
1:A:1679:LYS:HB2	1:A:1682:ILE:HG21	1.97	0.45
1:A:1448:ILE:HD13	1:A:1465:LEU:CD1	2.34	0.45
1:A:1628:LEU:HD21	1:A:1740:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:LEU:N	1:A:1439:LEU:HD12	2.31	0.44
1:A:1685:LEU:N	1:A:1685:LEU:HD22	2.32	0.44
1:A:1419:THR:HG23	1:A:1511:ASP:OD1	2.18	0.44
1:A:1728:SER:O	1:A:1732:LYS:HG3	2.16	0.44
1:A:1683:LYS:O	1:A:1686:PRO:HD2	2.17	0.44
1:A:1646:VAL:HG22	1:A:1706:ILE:HD11	1.99	0.44
1:A:1525:TRP:O	1:A:1528:ARG:HB3	2.18	0.44
1:A:1479:ARG:O	1:A:1482:ALA:HB3	2.18	0.43
1:A:1500:PRO:O	1:A:1501:GLU:HB2	2.18	0.43
1:A:1560:GLN:HA	1:A:1560:GLN:OE1	2.18	0.43
1:A:1646:VAL:HG12	1:A:1650:LYS:HE3	1.99	0.43
1:A:1352:PRO:HB3	1:A:1387:TYR:CD1	2.53	0.43
1:A:1440:SER:O	1:A:1441:VAL:C	2.62	0.43
1:A:1535:VAL:CG1	1:A:1687:VAL:HG11	2.47	0.43
1:A:1503:ASP:HB3	1:A:1506:ASP:OD2	2.19	0.43
1:A:1546:LEU:O	1:A:1550:ARG:HG2	2.17	0.43
1:A:1649:CYS:SG	1:A:1650:LYS:N	2.91	0.43
1:A:1466:SER:OG	1:A:1529:MET:HB3	2.18	0.43
1:A:1688:LEU:N	1:A:1689:PRO:HD2	2.33	0.43
1:A:1722:ASP:HB3	1:A:1725:ALA:HB3	2.01	0.43
1:A:1471:ILE:HG12	1:A:1525:TRP:HD1	1.85	0.42
1:A:1537:SER:O	1:A:1538:TYR:C	2.62	0.42
1:A:1436:TYR:HE2	1:A:1447:LYS:HE2	1.83	0.42
1:A:1497:ALA:C	1:A:1499:PRO:HD2	2.44	0.42
1:A:1632:GLU:HA	1:A:1635:LEU:HD12	2.02	0.42
1:A:1709:PHE:O	1:A:1712:LEU:HB3	2.19	0.42
1:A:1441:VAL:O	1:A:1445:VAL:HB	2.20	0.41
1:A:1544:GLU:O	1:A:1547:ALA:HB3	2.19	0.41
1:A:1598:THR:O	1:A:1598:THR:HG22	2.19	0.41
1:A:1493:ASN:HA	1:A:1676:PRO:HB3	2.02	0.41
1:A:1501:GLU:O	1:A:1502:LYS:HB2	2.20	0.41
1:A:1603:THR:C	1:A:1605:ASN:H	2.27	0.41
1:A:1731:LYS:HG2	1:A:1735:ASP:OD2	2.20	0.41
1:A:1666:GLY:C	1:A:1668:LEU:H	2.28	0.41
1:A:1471:ILE:HG12	1:A:1525:TRP:CD1	2.54	0.41
1:A:1603:THR:C	1:A:1605:ASN:N	2.78	0.41
1:A:1678:ASP:OD2	1:A:1679:LYS:N	2.53	0.41
1:A:1497:ALA:HB1	1:A:1499:PRO:HD2	2.02	0.41
1:A:1552:VAL:HA	1:A:1637:VAL:HG21	2.02	0.41
1:A:1599:PHE:CD1	1:A:1599:PHE:N	2.86	0.41
1:A:1434:HIS:C	1:A:1436:TYR:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:HIS:C	1:A:1436:TYR:H	2.28	0.41
1:A:1363:TRP:HD1	1:A:1363:TRP:O	2.04	0.40
1:A:1567:ASN:HB3	1:A:1624:PHE:CE2	2.56	0.40
1:A:1366:LEU:HD23	1:A:1366:LEU:HA	1.88	0.40
1:A:1660:GLU:CG	1:A:1688:LEU:HD22	2.50	0.40
1:A:1353:ARG:HA	1:A:1353:ARG:HD3	1.84	0.40
1:A:1498:LYS:N	1:A:1499:PRO:CD	2.84	0.40
1:A:1616:ILE:O	1:A:1620:ASN:HB2	2.21	0.40
1:A:1618:ARG:HH11	1:A:1618:ARG:HG2	1.86	0.40
1:A:1663:VAL:HG11	1:A:1685:LEU:HD11	2.03	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	409/411 (100%)	357 (87%)	43 (10%)	9 (2%)	5 9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1498	LYS
1	A	1417	LYS
1	A	1452	ASP
1	A	1502	LYS
1	A	1493	ASN
1	A	1524	TYR
1	A	1665	ILE
1	A	1500	PRO
1	A	1504	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	374/374 (100%)	356 (95%)	18 (5%)	23 46

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1351	TYR
1	A	1395	LEU
1	A	1429	PHE
1	A	1445	VAL
1	A	1451	CYS
1	A	1484	TYR
1	A	1494	LEU
1	A	1516	GLN
1	A	1535	VAL
1	A	1540	ARG
1	A	1541	GLU
1	A	1607	MET
1	A	1625	ASN
1	A	1638	VAL
1	A	1671	SER
1	A	1693	LYS
1	A	1707	MET
1	A	1715	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1450	ASN
1	A	1457	GLN
1	A	1480	ASN
1	A	1516	GLN
1	A	1543	ASN
1	A	1605	ASN
1	A	1625	ASN

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Mol	Chain	Res	Type
1	A	1644	GLN
1	A	1654	GLN
1	A	1667	ASN
1	A	1714	HIS

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 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	411/411 (100%)	0.60	44 (10%) 11 9	33, 70, 130, 160	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1649	CYS	11.2
1	A	1451	CYS	7.8
1	A	1369	THR	4.4
1	A	1683	LYS	4.0
1	A	1757	TYR	4.0
1	A	1368	CYS	3.8
1	A	1452	ASP	3.6
1	A	1475	VAL	3.4
1	A	1414	ASP	3.4
1	A	1424	ASP	3.4
1	A	1416	GLN	3.4
1	A	1494	LEU	3.3
1	A	1371	ASN	3.2
1	A	1690	GLU	3.1
1	A	1670	ASP	3.1
1	A	1350	LYS	3.0
1	A	1410	LYS	2.8
1	A	1510	ALA	2.8
1	A	1677	LEU	2.7
1	A	1673	LYS	2.7
1	A	1498	LYS	2.6
1	A	1479	ARG	2.5
1	A	1632	GLU	2.4
1	A	1484	TYR	2.4
1	A	1467	LYS	2.4
1	A	1367	ASP	2.4
1	A	1356	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1481	TYR	2.4
1	A	1604	THR	2.3
1	A	1418	ILE	2.3
1	A	1758	ILE	2.3
1	A	1508	GLN	2.3
1	A	1599	PHE	2.3
1	A	1461	VAL	2.3
1	A	1453	ARG	2.3
1	A	1727	ILE	2.2
1	A	1674	PHE	2.2
1	A	1426	SER	2.2
1	A	1497	ALA	2.2
1	A	1388	GLU	2.2
1	A	1407	LEU	2.1
1	A	1714	HIS	2.1
1	A	1488	TRP	2.0
1	A	1760	HIS	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 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.