



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LAR  
Title : CRYSTAL STRUCTURE OF THE TANDEM PHOSPHATASE DOMAINS  
OF RPTP LAR  
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Deposited on : 1999-04-20  
Resolution : 2.00 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

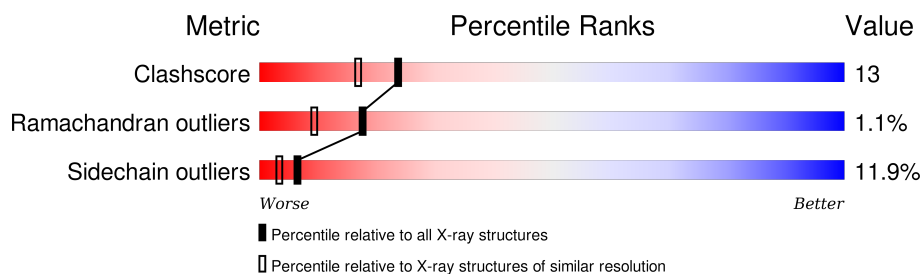
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	575	 72% 22% 5%
1	B	575	 64% 24% 5% 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9338 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 PROTEIN (LAR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4565	2889	796	847	33			
1	B	533	Total	C	N	O	S	0	0	0
			4300	2724	753	791	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1307	MET	PRO	MUTATION	UNP P10586
B	1307	MET	PRO	MUTATION	UNP P10586

- Molecule 2 is water.

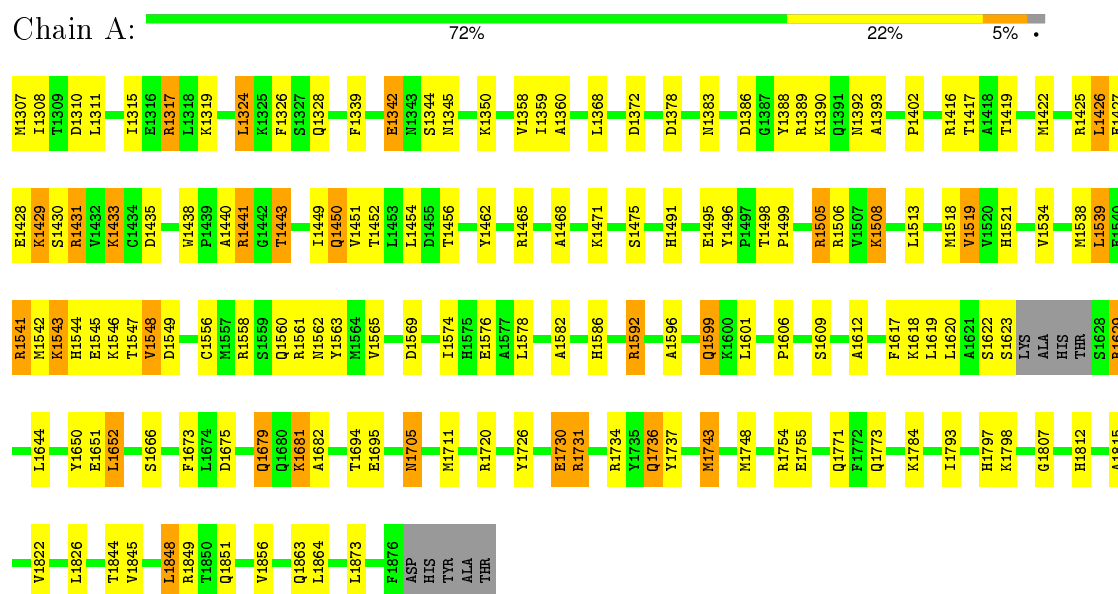
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	286	Total	O	0	0
			286	286		
2	B	187	Total	O	0	0
			187	187		

### 3 Residue-property plots

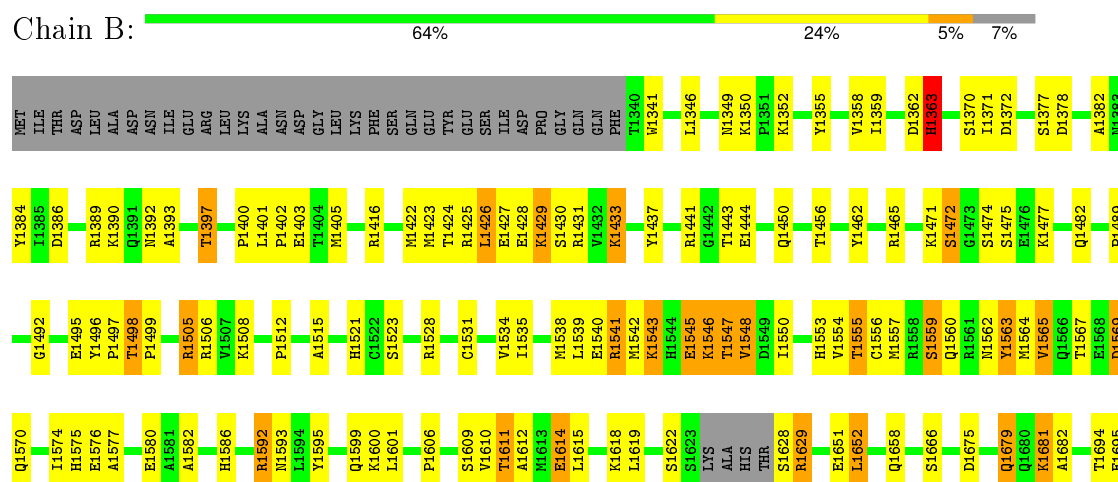
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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.

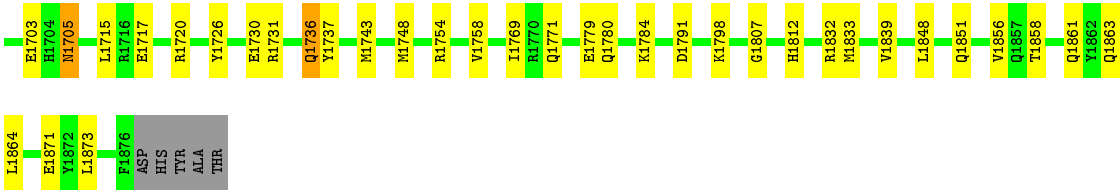
Note EDS was not executed.

#### • Molecule 1: PROTEIN (LAR)



#### • Molecule 1: PROTEIN (LAR)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.92Å 62.73Å 161.59Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.7 (50.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.222 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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	0.38	0/4671	0.62	0/6326
1	B	0.39	0/4402	0.63	1/5964 (0.0%)
All	All	0.38	0/9073	0.63	1/12290 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1363	HIS	N-CA-C	-5.93	94.99	111.00

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	4565	0	4470	109	0
1	B	4300	0	4219	122	0
2	A	286	0	0	9	1
2	B	187	0	0	9	4
All	All	9338	0	8689	231	4

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 13.

All (231) 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:1629:ARG:HH22	1:B:1652:LEU:HB2	1.02	1.15
1:B:1592:ARG:HH11	1:B:1592:ARG:HG3	1.11	1.15
1:B:1629:ARG:HG3	1:B:1629:ARG:HH11	1.08	1.11
1:B:1382:ALA:HB2	1:B:1397:THR:HG23	1.29	1.09
1:B:1498:THR:HG23	1:B:1499:PRO:HD3	1.45	0.98
1:B:1629:ARG:HH12	1:B:1652:LEU:H	1.01	0.97
1:B:1629:ARG:NH2	1:B:1652:LEU:HB2	1.77	0.97
1:B:1791:ASP:HB2	2:B:2358:HOH:O	1.64	0.96
1:B:1675:ASP:H	1:B:1851:GLN:HE22	1.04	0.95
1:A:1386:ASP:H	1:A:1560:GLN:HE22	1.09	0.92
1:B:1675:ASP:H	1:B:1851:GLN:NE2	1.66	0.91
1:B:1610:VAL:HG12	1:B:1611:THR:H	1.37	0.89
1:A:1592:ARG:HB3	1:A:1592:ARG:HH11	1.39	0.87
1:B:1681:LYS:N	1:B:1681:LYS:HD2	1.91	0.86
1:A:1629:ARG:HD3	1:A:1652:LEU:H	1.40	0.86
1:B:1629:ARG:HG3	1:B:1629:ARG:NH1	1.83	0.85
1:B:1541:ARG:HH21	1:B:1548:VAL:H	1.21	0.83
1:A:1383:ASN:HD22	1:A:1561:ARG:HD2	1.43	0.83
1:B:1610:VAL:HG11	1:B:1614:GLU:OE1	1.80	0.81
1:B:1592:ARG:HG3	1:B:1592:ARG:NH1	1.84	0.81
1:B:1592:ARG:HH11	1:B:1592:ARG:CG	1.91	0.78
1:B:1382:ALA:CB	1:B:1397:THR:HG23	2.11	0.78
1:B:1382:ALA:HB2	1:B:1397:THR:CG2	2.12	0.78
1:B:1541:ARG:HH21	1:B:1548:VAL:N	1.80	0.77
1:A:1629:ARG:NE	1:A:1652:LEU:HB2	1.99	0.77
1:A:1629:ARG:HD2	1:A:1650:TYR:HB3	1.67	0.76
1:B:1471:LYS:HG3	1:B:1472:SER:N	1.98	0.76
1:A:1317:ARG:HH11	1:A:1317:ARG:HB2	1.50	0.75
1:B:1390:LYS:HG3	1:B:1393:ALA:HB2	1.67	0.75
1:A:1417:THR:HG21	1:A:1519:VAL:HG13	1.68	0.74
1:B:1611:THR:HG23	1:B:1614:GLU:HB3	1.69	0.74
1:B:1569:ASP:N	1:B:1569:ASP:OD1	2.21	0.72
1:B:1705:ASN:O	1:B:1807:GLY:HA3	1.90	0.72
1:A:1508:LYS:N	1:A:1508:LYS:HD2	2.05	0.71
1:A:1450:GLN:HB2	2:A:2218:HOH:O	1.90	0.71
1:A:1358:VAL:HA	1:A:1562:ASN:HD22	1.55	0.71
1:B:1508:LYS:HE3	1:B:1540:GLU:OE1	1.90	0.71
1:B:1754:ARG:HH11	1:B:1771:GLN:NE2	1.88	0.71
1:B:1471:LYS:HG3	1:B:1472:SER:H	1.53	0.70
1:A:1541:ARG:HH21	1:A:1548:VAL:C	1.94	0.70
1:A:1449:ILE:HD13	1:A:1471:LYS:HG3	1.73	0.70
1:B:1512:PRO:HG2	1:B:1515:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1717:GLU:HB3	1:B:1779:GLU:HG2	1.75	0.69
1:B:1462:TYR:OH	1:B:1506:ARG:NH1	2.25	0.69
1:B:1498:THR:CG2	1:B:1499:PRO:HD3	2.21	0.69
1:B:1681:LYS:HD2	1:B:1681:LYS:H	1.56	0.69
1:A:1462:TYR:OH	1:A:1506:ARG:NH1	2.25	0.69
1:A:1629:ARG:HG2	1:A:1651:GLU:HB2	1.77	0.67
1:B:1629:ARG:HH12	1:B:1652:LEU:N	1.83	0.67
1:A:1543:LYS:HG2	1:A:1544:HIS:ND1	2.09	0.67
1:B:1629:ARG:NH1	1:B:1652:LEU:H	1.85	0.67
1:A:1383:ASN:ND2	1:A:1561:ARG:HH11	1.94	0.66
1:A:1538:MET:O	1:A:1542:MET:HG2	1.96	0.66
1:A:1844:THR:O	1:A:1848:LEU:HD22	1.95	0.65
1:B:1666:SER:O	2:B:2208:HOH:O	2.14	0.64
1:A:1619:LEU:HA	1:A:1622:SER:OG	1.97	0.64
1:B:1505:ARG:HG2	1:B:1586:HIS:CE1	2.33	0.63
1:B:1679:GLN:HG2	1:B:1682:ALA:HB2	1.78	0.63
1:A:1383:ASN:HD22	1:A:1561:ARG:HH11	1.45	0.62
1:B:1341:TRP:CG	1:B:1359:ILE:HD13	2.34	0.62
1:A:1644:LEU:HD12	1:A:1815:ALA:HB2	1.79	0.62
1:B:1541:ARG:NH2	1:B:1548:VAL:H	1.95	0.62
1:A:1454:LEU:HD11	1:A:1468:ALA:HB2	1.81	0.62
1:A:1730:GLU:H	1:A:1730:GLU:CD	2.01	0.62
1:A:1681:LYS:N	1:A:1681:LYS:HD2	2.15	0.62
1:B:1614:GLU:OE2	1:B:1618:LYS:HE2	2.00	0.61
1:A:1372:ASP:HB3	2:B:2199:HOH:O	2.00	0.61
1:B:1543:LYS:HG3	1:B:1543:LYS:O	2.01	0.60
1:A:1498:THR:HB	1:A:1499:PRO:HD3	1.83	0.60
1:A:1359:ILE:H	1:A:1562:ASN:ND2	2.00	0.60
1:A:1558:ARG:NH2	2:A:2036:HOH:O	2.29	0.60
1:A:1679:GLN:HG2	1:A:1682:ALA:HB2	1.84	0.60
1:A:1675:ASP:H	1:A:1851:GLN:HE22	1.48	0.60
1:A:1754:ARG:HH11	1:A:1771:GLN:NE2	1.99	0.60
1:A:1545:GLU:O	1:A:1546:LYS:HG2	2.02	0.59
1:A:1845:VAL:O	1:A:1849:ARG:HG3	2.02	0.59
1:A:1863:GLN:HG3	2:A:2311:HOH:O	2.02	0.59
1:A:1629:ARG:HE	1:A:1652:LEU:HB2	1.67	0.58
1:B:1754:ARG:HH11	1:B:1771:GLN:HE22	1.49	0.58
1:A:1422:MET:HG3	1:A:1521:HIS:CE1	2.37	0.58
1:B:1610:VAL:HG12	1:B:1611:THR:N	2.13	0.58
1:B:1610:VAL:HG12	1:B:1611:THR:HG22	1.85	0.58
1:A:1541:ARG:HH21	1:A:1549:ASP:N	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:ARG:HG2	1:A:1586:HIS:CE1	2.38	0.58
1:A:1317:ARG:NH1	1:A:1317:ARG:HB2	2.19	0.57
1:B:1570:GLN:O	1:B:1574:ILE:HG12	2.04	0.57
1:B:1541:ARG:HE	1:B:1548:VAL:HA	1.69	0.57
1:A:1506:ARG:NH2	2:A:2473:HOH:O	2.32	0.57
1:B:1523:SER:HB3	2:B:2344:HOH:O	2.04	0.57
1:B:1362:ASP:O	1:B:1363:HIS:HB3	2.04	0.57
1:A:1345:ASN:O	1:A:1350:LYS:HE3	2.06	0.56
1:A:1754:ARG:HD2	1:A:1771:GLN:HE22	1.70	0.56
1:B:1545:GLU:O	1:B:1546:LYS:C	2.44	0.56
1:A:1705:ASN:O	1:A:1807:GLY:HA3	2.04	0.56
1:A:1592:ARG:CB	1:A:1592:ARG:HH11	2.15	0.56
1:A:1734:ARG:HD2	1:A:1736:GLN:O	2.05	0.55
1:A:1673:PHE:HB3	1:A:1681:LYS:HG3	1.88	0.55
1:A:1443:THR:HB	1:A:1452:THR:OG1	2.07	0.55
1:A:1609:SER:HA	2:A:2454:HOH:O	2.06	0.55
1:A:1754:ARG:HH11	1:A:1771:GLN:HE22	1.54	0.55
1:B:1675:ASP:N	1:B:1851:GLN:NE2	2.46	0.54
1:A:1629:ARG:CD	1:A:1650:TYR:HB3	2.37	0.54
1:B:1531:CYS:SG	1:B:1574:ILE:HD11	2.46	0.54
1:A:1426:LEU:HD21	1:A:1438:TRP:CH2	2.43	0.54
1:B:1675:ASP:N	1:B:1851:GLN:HE22	1.88	0.53
1:B:1563:TYR:N	1:B:1563:TYR:CD1	2.75	0.53
1:A:1822:VAL:HG12	1:A:1826:LEU:HD12	1.90	0.53
1:B:1550:ILE:HG21	1:B:1575:HIS:CE1	2.44	0.53
1:A:1601:LEU:HA	1:A:1612:ALA:HB3	1.91	0.53
1:A:1754:ARG:HD2	1:A:1771:GLN:NE2	2.24	0.52
1:B:1346:LEU:O	1:B:1350:LYS:HG3	2.09	0.52
1:A:1629:ARG:HD3	1:A:1651:GLU:N	2.24	0.52
1:B:1402:PRO:HD2	1:B:1403:GLU:OE2	2.09	0.52
1:B:1743:MET:HA	1:B:1743:MET:HE2	1.92	0.51
1:B:1593:ASN:HD22	1:B:1593:ASN:N	2.08	0.51
1:A:1541:ARG:NH2	1:A:1549:ASP:HB2	2.26	0.51
1:B:1619:LEU:HA	1:B:1622:SER:OG	2.10	0.51
1:B:1541:ARG:NH2	1:B:1548:VAL:N	2.55	0.50
1:A:1360:ALA:HA	1:A:1383:ASN:HD21	1.77	0.50
1:B:1450:GLN:HG2	2:B:2304:HOH:O	2.11	0.50
1:A:1755:GLU:HB2	2:A:2245:HOH:O	2.10	0.50
1:A:1743:MET:HA	1:A:1743:MET:CE	2.41	0.50
1:B:1629:ARG:CG	1:B:1629:ARG:O	2.59	0.50
1:B:1400:PRO:HG2	1:B:1437:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:GLN:HG2	2:A:2078:HOH:O	2.12	0.49
1:B:1541:ARG:NH2	1:B:1547:THR:HB	2.27	0.49
1:B:1593:ASN:N	1:B:1593:ASN:ND2	2.61	0.49
1:B:1758:VAL:CG2	1:B:1769:ILE:HD13	2.43	0.49
1:A:1315:ILE:O	1:A:1319:LYS:HB2	2.12	0.49
1:B:1833:MET:HG3	1:B:1839:VAL:HG22	1.95	0.49
1:B:1595:TYR:HB3	2:B:2321:HOH:O	2.13	0.49
1:A:1711:MET:HG2	1:A:1773:GLN:HG3	1.94	0.49
1:A:1617:PHE:O	1:A:1620:LEU:HB2	2.13	0.49
1:A:1358:VAL:HA	1:A:1562:ASN:ND2	2.25	0.49
1:B:1547:THR:O	1:B:1548:VAL:HB	2.13	0.48
1:B:1401:LEU:O	1:B:1405:MET:HG3	2.13	0.48
1:B:1629:ARG:CG	1:B:1629:ARG:NH1	2.63	0.48
1:A:1599:GLN:NE2	2:A:2416:HOH:O	2.43	0.48
1:A:1429:LYS:HD2	1:A:1491:HIS:CE1	2.49	0.48
1:A:1428:GLU:O	1:A:1429:LYS:HB2	2.13	0.48
1:B:1423:MET:O	1:B:1528:ARG:HD3	2.14	0.48
1:B:1541:ARG:HH21	1:B:1548:VAL:CA	2.27	0.47
1:A:1675:ASP:N	1:A:1851:GLN:HE22	2.12	0.47
1:B:1422:MET:CE	1:B:1426:LEU:HD13	2.44	0.47
1:B:1694:THR:HG23	1:B:1726:TYR:HB2	1.96	0.47
1:A:1390:LYS:HG3	1:A:1393:ALA:HB2	1.96	0.47
1:B:1550:ILE:HD12	1:B:1575:HIS:CD2	2.49	0.47
1:A:1429:LYS:O	1:A:1430:SER:HB2	2.15	0.47
1:A:1534:VAL:HG11	1:A:1574:ILE:HD13	1.95	0.47
1:B:1389:ARG:O	1:B:1389:ARG:HG2	2.14	0.47
1:B:1465:ARG:HD2	1:B:1482:GLN:HE22	1.80	0.47
1:B:1557:MET:C	1:B:1559:SER:N	2.68	0.47
1:B:1833:MET:HG3	1:B:1839:VAL:CG2	2.45	0.47
1:B:1858:THR:H	1:B:1861:GLN:NE2	2.12	0.46
1:A:1449:ILE:CD1	1:A:1471:LYS:HG3	2.44	0.46
1:B:1424:THR:HA	1:B:1528:ARG:NH1	2.30	0.46
1:B:1541:ARG:HE	1:B:1548:VAL:CA	2.29	0.46
1:A:1539:LEU:HD13	1:A:1578:LEU:CD2	2.46	0.46
1:A:1386:ASP:N	1:A:1560:GLN:HE22	1.93	0.46
1:B:1743:MET:CE	1:B:1743:MET:HA	2.46	0.46
1:B:1384:TYR:HB3	1:B:1392:ASN:HB3	1.97	0.45
1:B:1629:ARG:NH1	1:B:1651:GLU:N	2.63	0.45
1:B:1497:PRO:CB	1:B:1577:ALA:HA	2.46	0.45
1:B:1541:ARG:HH21	1:B:1548:VAL:C	2.19	0.45
1:A:1419:THR:HB	1:A:1518:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1736:GLN:HB3	1:A:1737:TYR:H	1.57	0.45
1:A:1456:THR:HG23	1:A:1465:ARG:HG2	1.99	0.45
1:B:1362:ASP:OD1	1:B:1363:HIS:N	2.50	0.45
1:A:1443:THR:HA	1:A:1451:VAL:O	2.17	0.45
1:B:1422:MET:HG3	1:B:1521:HIS:CE1	2.52	0.45
1:B:1736:GLN:HB3	1:B:1737:TYR:H	1.61	0.45
1:B:1378:ASP:C	1:B:1378:ASP:OD1	2.54	0.45
1:B:1371:ILE:HG13	1:B:1377:SER:HB2	1.99	0.45
1:A:1596:ALA:O	1:A:1599:GLN:HB2	2.17	0.44
1:A:1543:LYS:HD3	1:A:1544:HIS:CE1	2.53	0.44
1:B:1422:MET:HE1	1:B:1426:LEU:HD13	1.99	0.44
1:A:1433:LYS:HB3	1:A:1433:LYS:HZ2	1.83	0.44
1:B:1498:THR:HB	1:B:1580:GLU:OE2	2.17	0.44
1:A:1388:TYR:CD1	1:A:1541:ARG:HB2	2.52	0.44
1:A:1428:GLU:O	1:A:1431:ARG:HG2	2.16	0.44
1:B:1601:LEU:HA	1:B:1612:ALA:HB3	2.00	0.44
1:B:1726:TYR:OH	1:B:1812:HIS:HE1	2.00	0.43
1:B:1428:GLU:HB2	1:B:1433:LYS:HD3	1.99	0.43
1:B:1489:PRO:HG2	1:B:1492:GLY:O	2.17	0.43
1:A:1392:ASN:N	1:A:1392:ASN:HD22	2.15	0.43
1:A:1392:ASN:N	1:A:1392:ASN:ND2	2.66	0.43
1:B:1658:GLN:HG2	1:B:1703:GLU:OE2	2.18	0.43
1:A:1629:ARG:CD	1:A:1652:LEU:H	2.23	0.43
1:A:1592:ARG:HB3	1:A:1592:ARG:NH1	2.19	0.43
1:B:1384:TYR:CD1	1:B:1392:ASN:HB3	2.53	0.43
1:B:1386:ASP:H	1:B:1560:GLN:HE22	1.67	0.43
1:A:1629:ARG:HD3	1:A:1652:LEU:N	2.20	0.43
1:A:1311:LEU:O	1:A:1315:ILE:HG13	2.19	0.43
1:B:1629:ARG:O	1:B:1629:ARG:HG2	2.18	0.43
1:B:1564:MET:O	1:B:1565:VAL:HB	2.19	0.43
1:A:1378:ASP:C	1:A:1378:ASP:OD1	2.57	0.43
1:B:1534:VAL:HG13	1:B:1535:ILE:N	2.34	0.43
1:B:1610:VAL:HG11	1:B:1614:GLU:CD	2.39	0.42
1:B:1531:CYS:CB	1:B:1574:ILE:HD11	2.48	0.42
1:B:1812:HIS:HD2	2:B:2102:HOH:O	2.02	0.42
1:A:1793:ILE:O	1:A:1797:HIS:HD2	2.01	0.42
1:A:1730:GLU:OE1	1:A:1731:ARG:HG2	2.19	0.42
1:A:1508:LYS:HD2	1:A:1508:LYS:H	1.82	0.42
1:A:1545:GLU:O	1:A:1547:THR:HG23	2.19	0.42
1:B:1495:GLU:HB3	1:B:1496:TYR:CE1	2.55	0.42
1:B:1456:THR:HG21	2:B:2282:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1349:ASN:O	1:B:1352:LYS:HB2	2.20	0.42
1:B:1542:MET:HE3	1:B:1582:ALA:HA	2.01	0.42
1:A:1429:LYS:HE3	1:A:1491:HIS:NE2	2.35	0.42
1:A:1324:LEU:O	1:A:1328:GLN:HG3	2.19	0.42
1:A:1694:THR:HG23	1:A:1726:TYR:HB2	2.01	0.42
1:A:1342:GLU:H	1:A:1342:GLU:HG2	1.52	0.41
1:B:1614:GLU:HG3	1:B:1615:LEU:N	2.34	0.41
1:A:1539:LEU:HD12	1:A:1539:LEU:HA	1.90	0.41
1:B:1433:LYS:HE3	1:B:1433:LYS:HB3	1.70	0.41
1:A:1422:MET:CE	1:A:1426:LEU:HD13	2.50	0.41
1:B:1554:VAL:HG12	1:B:1554:VAL:O	2.20	0.41
1:A:1592:ARG:NH1	1:A:1592:ARG:CB	2.82	0.41
1:A:1402:PRO:HD3	1:A:1435:ASP:OD2	2.20	0.41
1:B:1538:MET:HA	1:B:1538:MET:CE	2.51	0.40
1:B:1610:VAL:HG12	1:B:1611:THR:CG2	2.49	0.40
1:A:1812:HIS:HD2	2:A:2150:HOH:O	2.04	0.40
1:A:1539:LEU:HD13	1:A:1578:LEU:HD23	2.03	0.40
1:A:1726:TYR:OH	1:A:1812:HIS:HE1	2.04	0.40
1:B:1429:LYS:N	2:B:2267:HOH:O	2.54	0.40
1:B:1355:TYR:HB2	1:B:1358:VAL:HB	2.03	0.40
1:A:1543:LYS:HG2	1:A:1544:HIS:HD1	1.84	0.40
1:B:1748:MET:HB2	1:B:1748:MET:HE2	1.96	0.40
1:A:1307:MET:HE2	1:A:1582:ALA:HB1	2.02	0.40
1:A:1440:ALA:C	1:A:1441:ARG:HG3	2.41	0.40
1:B:1553:HIS:C	1:B:1555:THR:N	2.75	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2470:HOH:O	2:B:2094:HOH:O[1_565]	1.24	0.96
2:B:2117:HOH:O	2:B:2356:HOH:O[2_657]	1.54	0.66
2:B:2115:HOH:O	2:B:2212:HOH:O[2_657]	1.64	0.56
2:B:2108:HOH:O	2:B:2207:HOH:O[2_657]	2.15	0.05

## 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	562/575 (98%)	531 (94%)	27 (5%)	4 (1%)	26	19
1	B	529/575 (92%)	494 (93%)	27 (5%)	8 (2%)	13	5
All	All	1091/1150 (95%)	1025 (94%)	54 (5%)	12 (1%)	17	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1472	SER
1	B	1548	VAL
1	B	1562	ASN
1	B	1606	PRO
1	B	1363	HIS
1	B	1546	LYS
1	A	1606	PRO
1	A	1565	VAL
1	A	1856	VAL
1	B	1856	VAL
1	A	1548	VAL
1	B	1565	VAL

### 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	493/500 (99%)	437 (89%)	56 (11%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	464/500 (93%)	406 (88%)	58 (12%)	6	3
All	All	957/1000 (96%)	843 (88%)	114 (12%)	6	3

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1308	ILE
1	A	1310	ASP
1	A	1317	ARG
1	A	1324	LEU
1	A	1326	PHE
1	A	1339	PHE
1	A	1342	GLU
1	A	1344	SER
1	A	1368	LEU
1	A	1389	ARG
1	A	1416	ARG
1	A	1425	ARG
1	A	1426	LEU
1	A	1427	GLU
1	A	1429	LYS
1	A	1431	ARG
1	A	1433	LYS
1	A	1441	ARG
1	A	1443	THR
1	A	1450	GLN
1	A	1475	SER
1	A	1495	GLU
1	A	1496	TYR
1	A	1505	ARG
1	A	1508	LYS
1	A	1513	LEU
1	A	1519	VAL
1	A	1539	LEU
1	A	1541	ARG
1	A	1543	LYS
1	A	1556	CYS
1	A	1563	TYR
1	A	1569	ASP
1	A	1576	GLU
1	A	1592	ARG
1	A	1599	GLN

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Mol	Chain	Res	Type
1	A	1618	LYS
1	A	1623	SER
1	A	1629	ARG
1	A	1652	LEU
1	A	1666	SER
1	A	1679	GLN
1	A	1681	LYS
1	A	1695	GLU
1	A	1705	ASN
1	A	1720	ARG
1	A	1730	GLU
1	A	1731	ARG
1	A	1736	GLN
1	A	1743	MET
1	A	1748	MET
1	A	1784	LYS
1	A	1798	LYS
1	A	1848	LEU
1	A	1864	LEU
1	A	1873	LEU
1	B	1370	SER
1	B	1372	ASP
1	B	1397	THR
1	B	1416	ARG
1	B	1425	ARG
1	B	1426	LEU
1	B	1427	GLU
1	B	1429	LYS
1	B	1430	SER
1	B	1431	ARG
1	B	1433	LYS
1	B	1441	ARG
1	B	1443	THR
1	B	1444	GLU
1	B	1474	SER
1	B	1475	SER
1	B	1477	LYS
1	B	1498	THR
1	B	1505	ARG
1	B	1539	LEU
1	B	1541	ARG
1	B	1543	LYS

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Mol	Chain	Res	Type
1	B	1545	GLU
1	B	1547	THR
1	B	1555	THR
1	B	1556	CYS
1	B	1559	SER
1	B	1563	TYR
1	B	1567	THR
1	B	1569	ASP
1	B	1576	GLU
1	B	1592	ARG
1	B	1599	GLN
1	B	1600	LYS
1	B	1609	SER
1	B	1611	THR
1	B	1614	GLU
1	B	1628	SER
1	B	1629	ARG
1	B	1652	LEU
1	B	1679	GLN
1	B	1681	LYS
1	B	1695	GLU
1	B	1705	ASN
1	B	1715	LEU
1	B	1720	ARG
1	B	1730	GLU
1	B	1731	ARG
1	B	1736	GLN
1	B	1780	GLN
1	B	1784	LYS
1	B	1798	LYS
1	B	1832	ARG
1	B	1848	LEU
1	B	1863	GLN
1	B	1864	LEU
1	B	1871	GLU
1	B	1873	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1383	ASN
1	A	1391	GLN

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Mol	Chain	Res	Type
1	A	1392	ASN
1	A	1415	GLN
1	A	1450	GLN
1	A	1511	ASN
1	A	1560	GLN
1	A	1562	ASN
1	A	1586	HIS
1	A	1679	GLN
1	A	1771	GLN
1	A	1797	HIS
1	A	1802	GLN
1	A	1812	HIS
1	A	1851	GLN
1	A	1857	GLN
1	A	1861	GLN
1	B	1391	GLN
1	B	1415	GLN
1	B	1450	GLN
1	B	1482	GLN
1	B	1511	ASN
1	B	1560	GLN
1	B	1566	GLN
1	B	1586	HIS
1	B	1593	ASN
1	B	1634	ASN
1	B	1705	ASN
1	B	1750	GLN
1	B	1771	GLN
1	B	1812	HIS
1	B	1843	GLN
1	B	1851	GLN
1	B	1857	GLN
1	B	1861	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 [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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.