Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2024 – 03:21 AM EST

PDB ID	:	4R04
Title	:	Clostridium difficile Toxin A (TcdA)
Authors	:	Lacy, D.B.; Spiller, B.W.; Rutherford, S.A.
Deposited on	:	2014-07-29
Resolution	:	3.26 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 (i) 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 (1)) were used in the production of this report:

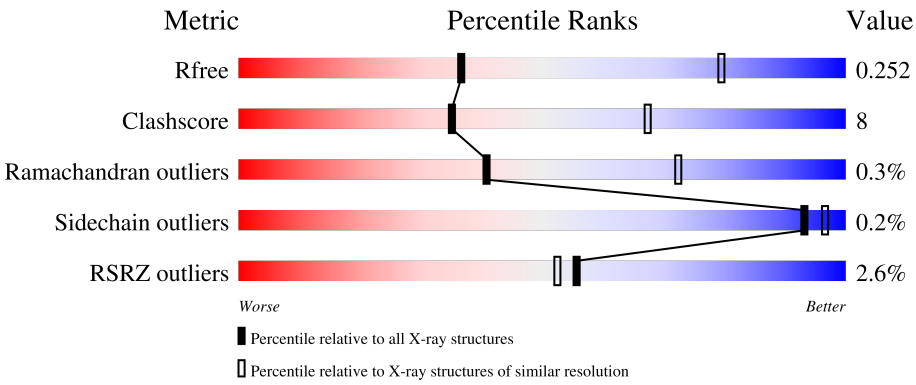
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	1838	3% 76% 21% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14410 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 Toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1793	14409	9199	2332	2852	26	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	HIS	-	expression tag	UNP P16154
A	1834	HIS	-	expression tag	UNP P16154
A	1835	HIS	-	expression tag	UNP P16154
A	1836	HIS	-	expression tag	UNP P16154
A	1837	HIS	-	expression tag	UNP P16154
A	1838	HIS	-	expression tag	UNP P16154

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

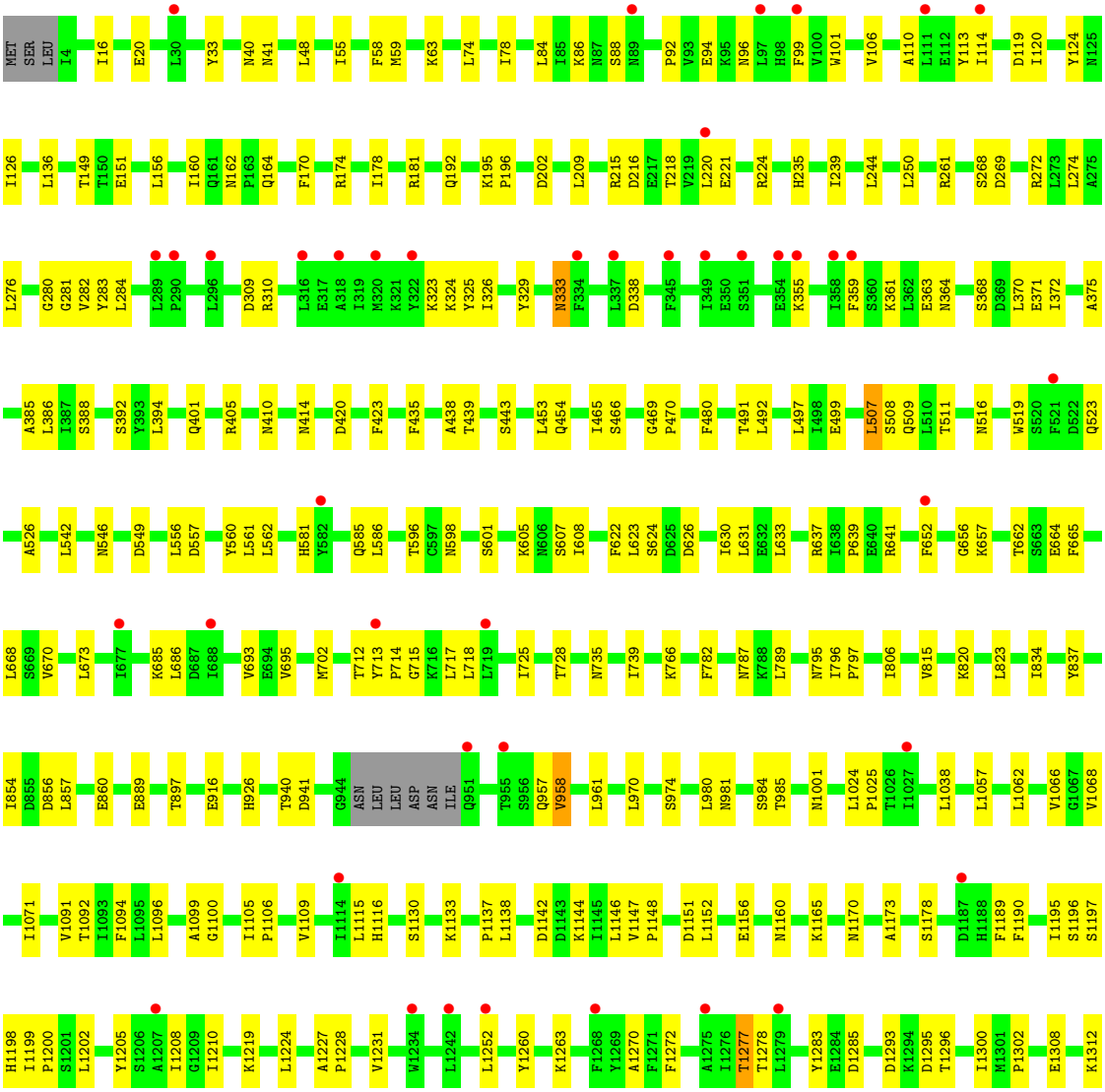
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

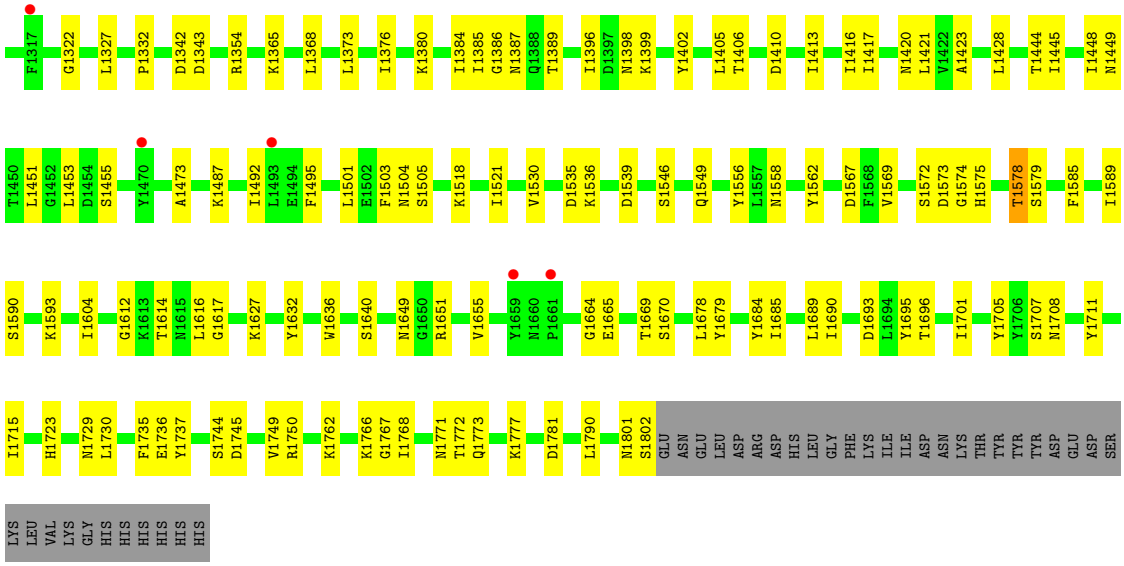
3 Residue-property plots (i)

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: Toxin A

Chain A: 3% 76% 21%




F1317
G1322
L1327
P1332
D1342
D1343
R1354
K1365
L1368
L1373
I1376
K1380
I1384
I1385
G1386
N1387
Q1388
T1389
I1396
D1397
N1398
K1399
Y1402
L1405
T1406
D1410
I1413
I1416
I1417
N1420
L1421
Y1422
A1423
L1428
T1444
I1445
I1448
N1449
T1450
L1451
G1452
L1453
D1454
S1455
Y1470
A1473
K1487
I1492
L1493
E1494
F1495
L1501
E1502
F1503
N1504
S1505
K1518
I1521
V1530
D1535
K1536
D1539
S1546
Q1549
Y1556
L1557
N1558
Y1562
D1567
F1568
V1569
S1572
D1573
G1574
H1575
T1578
S1579
F1585
I1589
S1590
K1593
I1604
G1612
K1613
T1614
N1615
L1616
G1617
K1627
Y1632
W1636
S1640
N1649
G1650
R1651
V1655
Y1659
N1660
P1661
G1664
E1665
T1669
S1670
L1678
Y1679
Y1684
I1685
L1689
I1690
D1693
L1694
Y1695
T1696
I1701
Y1705
Y1706
S1707
N1708
Y1711
I1715
H1723
N1729
L1730
F1735
E1736
Y1737
S1744
D1745
V1749
R1750
K1762
K1766
G1767
I1768
N1771
T1772
Q1773
K1777
D1781
L1790
N1801
S1802
GLU ASN GLU LEU ASP ARG ASP HIS LEU GLY PHE LYS ILE ILE ASP ASN LYS THR TYR TYR TYR ASP GLU ASP SER
LYS LEU VAL LYS GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	303.49Å 124.54Å 75.95Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	61.62 – 3.26 62.27 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.62-3.26) 94.3 (62.27-3.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1565)	Depositor
R, R_{free}	0.221 , 0.249 0.223 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14410	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.22	0/14671	0.39	1/19845 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	507	LEU	CA-CB-CG	5.04	126.88	115.30

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	14409	0	14349	235	0
2	A	1	0	0	0	0
All	All	14410	0	14349	235	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 8.

All (235) 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:371:GLU:HA	1:A:394:LEU:HD13	1.61	0.81
1:A:1495:PHE:HB3	1:A:1503:PHE:HB3	1.63	0.78
1:A:1156:GLU:HB3	1:A:1165:LYS:HB2	1.65	0.78
1:A:1178:SER:HB2	1:A:1190:PHE:HB3	1.74	0.69
1:A:239:ILE:HG23	1:A:244:LEU:HD12	1.74	0.68
1:A:1195:ILE:HG21	1:A:1199:ILE:HB	1.75	0.68
1:A:1224:LEU:HB2	1:A:1302:PRO:HD3	1.76	0.67
1:A:94:GLU:HB2	1:A:280:GLY:HA3	1.77	0.66
1:A:1380:LYS:HA	1:A:1421:LEU:HB3	1.78	0.65
1:A:361:LYS:HE3	1:A:363:GLU:HG2	1.79	0.64
1:A:16:ILE:HG13	1:A:1664:GLY:HA3	1.79	0.64
1:A:16:ILE:HD12	1:A:1665:GLU:HG3	1.81	0.63
1:A:1546:SER:HB3	1:A:1549:GLN:HG2	1.79	0.63
1:A:586:LEU:HD11	1:A:652:PHE:HD1	1.64	0.63
1:A:1384:ILE:HG12	1:A:1389:THR:HG23	1.81	0.63
1:A:970:LEU:O	1:A:984:SER:OG	2.17	0.62
1:A:1428:LEU:HD22	1:A:1455:SER:HB2	1.81	0.62
1:A:492:LEU:HB2	1:A:497:LEU:HD11	1.83	0.61
1:A:491:THR:HG21	1:A:1771:ASN:HB2	1.82	0.61
1:A:796:ILE:HD11	1:A:837:TYR:HD2	1.66	0.61
1:A:1130:SER:HB3	1:A:1252:LEU:HD22	1.81	0.61
1:A:1410:ASP:HB3	1:A:1413:ILE:HB	1.83	0.60
1:A:1208:ILE:HG12	1:A:1252:LEU:HD11	1.84	0.60
1:A:250:LEU:HD13	1:A:274:LEU:HD21	1.83	0.60
1:A:269:ASP:HA	1:A:272:ARG:HD2	1.85	0.59
1:A:209:LEU:HB3	1:A:215:ARG:HG3	1.82	0.59
1:A:585:GLN:HB2	1:A:596:THR:HG21	1.84	0.59
1:A:1578:THR:HG22	1:A:1579:SER:HA	1.85	0.59
1:A:283:TYR:HB3	1:A:386:LEU:HB2	1.85	0.58
1:A:276:LEU:HD23	1:A:388:SER:HB3	1.84	0.58
1:A:657:LYS:HB3	1:A:662:THR:HG23	1.86	0.57
1:A:1332:PRO:HG3	1:A:1387:ASN:HB3	1.86	0.57
1:A:405:ARG:NH1	1:A:466:SER:O	2.36	0.57
1:A:1539:ASP:HB2	1:A:1556:TYR:HB3	1.87	0.57
1:A:20:GLU:HG3	1:A:58:PHE:HE1	1.70	0.57
1:A:1285:ASP:HA	1:A:1312:LYS:HB3	1.87	0.57
1:A:1092:THR:OG1	1:A:1365:LYS:NZ	2.36	0.57
1:A:55:ILE:HD11	1:A:74:LEU:HD23	1.85	0.56
1:A:465:ILE:HG23	1:A:470:PRO:HD2	1.86	0.56
1:A:124:TYR:OH	1:A:363:GLU:O	2.17	0.56
1:A:1137:PRO:HB2	1:A:1138:LEU:HD12	1.87	0.56
1:A:1406:THR:HG22	1:A:1416:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ILE:HG12	1:A:1715:ILE:HD12	1.87	0.55
1:A:326:ILE:HB	1:A:329:TYR:HB2	1.89	0.55
1:A:860:GLU:OE1	1:A:926:HIS:NE2	2.40	0.55
1:A:1745:ASP:HB3	1:A:1766:LYS:HA	1.87	0.55
1:A:637:ARG:HD2	1:A:686:LEU:HD11	1.89	0.55
1:A:670:VAL:HG22	1:A:713:TYR:HD2	1.72	0.55
1:A:557:ASP:HB3	1:A:560:TYR:HB3	1.89	0.54
1:A:84:LEU:O	1:A:88:SER:OG	2.21	0.54
1:A:796:ILE:HD12	1:A:834:ILE:HG23	1.89	0.54
1:A:221:GLU:HG3	1:A:224:ARG:HH21	1.72	0.54
1:A:86:LYS:HZ1	1:A:499:GLU:HB3	1.72	0.54
1:A:1405:LEU:HB2	1:A:1417:ILE:HB	1.90	0.53
1:A:1448:ILE:HG23	1:A:1453:LEU:HD12	1.90	0.53
1:A:113:TYR:HE2	1:A:511:THR:HG21	1.74	0.53
1:A:712:THR:O	1:A:715:GLY:N	2.41	0.53
1:A:1744:SER:HB3	1:A:1767:GLY:HA2	1.89	0.53
1:A:940:THR:OG1	1:A:941:ASP:N	2.41	0.53
1:A:1170:ASN:HB2	1:A:1231:VAL:HG22	1.89	0.53
1:A:136:LEU:HD21	1:A:220:LEU:HB3	1.91	0.53
1:A:1092:THR:O	1:A:1365:LYS:NZ	2.42	0.52
1:A:439:THR:O	1:A:443:SER:OG	2.28	0.52
1:A:1420:ASN:HB3	1:A:1423:ALA:HB3	1.91	0.52
1:A:92:PRO:HB3	1:A:364:ASN:HB3	1.91	0.52
1:A:1115:LEU:O	1:A:1116:HIS:ND1	2.43	0.52
1:A:1640:SER:OG	1:A:1670:SER:O	2.27	0.51
1:A:136:LEU:HD13	1:A:202:ASP:HB2	1.92	0.51
1:A:695:VAL:HB	1:A:739:ILE:HG12	1.91	0.51
1:A:1616:LEU:HB3	1:A:1636:TRP:HB2	1.91	0.51
1:A:1604:ILE:HB	1:A:1627:LYS:HE2	1.93	0.51
1:A:119:ASP:OD2	1:A:355:LYS:NZ	2.34	0.51
1:A:735:ASN:HB2	1:A:782:PHE:O	2.11	0.51
1:A:1504:ASN:OD1	1:A:1505:SER:N	2.43	0.51
1:A:507:LEU:HD12	1:A:508:SER:H	1.76	0.51
1:A:815:VAL:HG13	1:A:820:LYS:HE2	1.92	0.51
1:A:854:ILE:HD11	1:A:1689:LEU:HB2	1.93	0.51
1:A:99:PHE:CE1	1:A:284:LEU:HB2	2.47	0.50
1:A:889:GLU:OE2	1:A:1001:ASN:ND2	2.40	0.50
1:A:1071:ILE:HG22	1:A:1473:ALA:HB2	1.93	0.50
1:A:491:THR:HB	1:A:1772:THR:H	1.76	0.50
1:A:624:SER:HB3	1:A:631:LEU:HD13	1.93	0.50
1:A:516:ASN:HA	1:A:519:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:LEU:HD11	1:A:1649:ASN:HD22	1.76	0.50
1:A:63:LYS:HD2	1:A:1723:HIS:ND1	2.27	0.49
1:A:375:ALA:HB2	1:A:385:ALA:HB3	1.94	0.49
1:A:1368:LEU:HD22	1:A:1451:LEU:HD11	1.94	0.49
1:A:1445:ILE:O	1:A:1449:ASN:ND2	2.45	0.49
1:A:1708:ASN:HB2	1:A:1711:TYR:CE1	2.47	0.49
1:A:120:ILE:HD13	1:A:359:PHE:HB2	1.94	0.49
1:A:1343:ASP:OD1	1:A:1343:ASP:N	2.45	0.49
1:A:1678:LEU:HG	1:A:1685:ILE:HD12	1.95	0.49
1:A:1569:VAL:HA	1:A:1572:SER:HB3	1.94	0.49
1:A:507:LEU:HB2	1:A:509:GLN:HG3	1.95	0.49
1:A:624:SER:O	1:A:641:ARG:NH2	2.46	0.49
1:A:368:SER:HB3	1:A:371:GLU:HG2	1.95	0.49
1:A:1300:ILE:HG23	1:A:1327:LEU:HD22	1.95	0.49
1:A:718:LEU:HD23	1:A:789:LEU:HD22	1.95	0.48
1:A:370:LEU:O	1:A:392:SER:OG	2.32	0.48
1:A:261:ARG:HE	1:A:453:LEU:HD22	1.79	0.48
1:A:1160:ASN:HB3	1:A:1293:ASP:HB3	1.95	0.48
1:A:507:LEU:HD13	1:A:509:GLN:HG3	1.94	0.48
1:A:516:ASN:HA	1:A:519:TRP:HD1	1.79	0.48
1:A:974:SER:HB2	1:A:985:THR:HG22	1.96	0.48
1:A:1354:ARG:HG2	1:A:1368:LEU:HD23	1.96	0.48
1:A:401:GLN:O	1:A:405:ARG:HG2	2.13	0.47
1:A:1146:LEU:HG	1:A:1219:LYS:HB2	1.95	0.47
1:A:1285:ASP:OD1	1:A:1285:ASP:N	2.45	0.47
1:A:980:LEU:HG	1:A:981:ASN:HA	1.96	0.47
1:A:1024:LEU:HD12	1:A:1025:PRO:HD2	1.96	0.47
1:A:162:ASN:OD1	1:A:164:GLN:HG2	2.15	0.47
1:A:507:LEU:HD12	1:A:508:SER:N	2.29	0.47
1:A:608:ILE:HG22	1:A:622:PHE:HB3	1.97	0.46
1:A:110:ALA:O	1:A:114:ILE:HG12	2.15	0.46
1:A:164:GLN:HB2	1:A:766:LYS:HD2	1.98	0.46
1:A:1614:THR:HG23	1:A:1617:GLY:H	1.81	0.46
1:A:149:THR:HG23	1:A:170:PHE:HZ	1.80	0.46
1:A:523:GLN:HA	1:A:526:ALA:HB3	1.98	0.46
1:A:1801:ASN:OD1	1:A:1802:SER:N	2.41	0.46
1:A:1295:ASP:OD1	1:A:1296:THR:N	2.49	0.46
1:A:1091:VAL:HG12	1:A:1327:LEU:HD13	1.98	0.46
1:A:633:LEU:HD21	1:A:637:ARG:HB2	1.98	0.46
1:A:435:PHE:HA	1:A:438:ALA:HB2	1.98	0.45
1:A:1768:ILE:HG21	1:A:1790:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:THR:HG22	1:A:916:GLU:HG2	1.98	0.45
1:A:1099:ALA:HA	1:A:1100:GLY:HA2	1.56	0.45
1:A:1729:ASN:HA	1:A:1781:ASP:HB2	1.98	0.45
1:A:1590:SER:HB2	1:A:1593:LYS:HG3	1.97	0.45
1:A:656:GLY:HA3	1:A:702:MET:HE3	1.99	0.45
1:A:1038:LEU:HD22	1:A:1521:ILE:HD13	1.98	0.45
1:A:1562:TYR:CD1	1:A:1612:GLY:HA3	2.51	0.45
1:A:1530:VAL:HB	1:A:1536:LYS:HB3	1.99	0.45
1:A:1385:ILE:HD13	1:A:1405:LEU:HD21	1.99	0.45
1:A:40:ASN:HB3	1:A:41:ASN:H	1.59	0.45
1:A:693:VAL:HG11	1:A:725:ILE:HD13	1.98	0.45
1:A:1173:ALA:HB2	1:A:1202:LEU:HG	1.99	0.45
1:A:1573:ASP:HB2	1:A:1575:HIS:ND1	2.32	0.45
1:A:216:ASP:OD2	1:A:218:THR:OG1	2.35	0.44
1:A:276:LEU:HG	1:A:281:GLY:HA2	1.99	0.44
1:A:1057:LEU:HD21	1:A:1399:LYS:O	2.17	0.44
1:A:1106:PRO:HG3	1:A:1115:LEU:HD13	1.99	0.44
1:A:1270:ALA:C	1:A:1272:PHE:H	2.20	0.44
1:A:1669:THR:HA	1:A:1695:TYR:O	2.17	0.44
1:A:323:LYS:HB3	1:A:325:TYR:CE1	2.53	0.44
1:A:151:GLU:OE2	1:A:181:ARG:NH2	2.50	0.44
1:A:1655:VAL:HB	1:A:1690:ILE:HA	1.99	0.44
1:A:372:ILE:HG22	1:A:394:LEU:HB3	1.99	0.44
1:A:1737:TYR:CE1	1:A:1750:ARG:HB2	2.52	0.44
1:A:1189:PHE:HB3	1:A:1190:PHE:H	1.65	0.44
1:A:1535:ASP:O	1:A:1558:ASN:ND2	2.38	0.44
1:A:74:LEU:O	1:A:78:ILE:HG13	2.17	0.44
1:A:192:GLN:HA	1:A:195:LYS:HE3	1.98	0.44
1:A:1151:ASP:HA	1:A:1227:ALA:HB2	1.99	0.44
1:A:624:SER:OG	1:A:626:ASP:O	2.19	0.44
1:A:622:PHE:CE1	1:A:639:PRO:HG3	2.53	0.43
1:A:1386:GLY:HA2	1:A:1387:ASN:HA	1.64	0.43
1:A:1773:GLN:O	1:A:1777:LYS:HG3	2.18	0.43
1:A:324:LYS:C	1:A:326:ILE:H	2.22	0.43
1:A:1396:ILE:HD12	1:A:1398:ASN:HB2	2.00	0.43
1:A:323:LYS:HB3	1:A:325:TYR:HE1	1.84	0.43
1:A:556:LEU:HD23	1:A:561:LEU:HD13	2.00	0.43
1:A:86:LYS:NZ	1:A:499:GLU:HB3	2.34	0.43
1:A:423:PHE:HZ	1:A:454:GLN:HG2	1.83	0.43
1:A:59:MET:O	1:A:63:LYS:HD3	2.19	0.43
1:A:1068:VAL:HG22	1:A:1518:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:PRO:HG2	1:A:1283:TYR:CD1	2.54	0.43
1:A:1100:GLY:H	1:A:1105:ILE:HG12	1.84	0.43
1:A:1133:LYS:HZ1	1:A:1210:ILE:HG23	1.83	0.43
1:A:1701:ILE:HB	1:A:1730:LEU:HD23	2.00	0.43
1:A:465:ILE:HA	1:A:469:GLY:HA3	2.00	0.43
1:A:1094:PHE:HE2	1:A:1096:LEU:HD11	1.84	0.43
1:A:1195:ILE:HD12	1:A:1195:ILE:HA	1.92	0.43
1:A:101:TRP:CD1	1:A:106:VAL:HG22	2.54	0.42
1:A:662:THR:HG22	1:A:664:GLU:H	1.84	0.42
1:A:961:LEU:HD11	1:A:1632:TYR:CE2	2.54	0.42
1:A:272:ARG:NE	1:A:283:TYR:OH	2.52	0.42
1:A:1322:GLY:O	1:A:1343:ASP:HB2	2.19	0.42
1:A:1396:ILE:O	1:A:1398:ASN:N	2.48	0.42
1:A:1402:TYR:CD1	1:A:1420:ASN:HB2	2.54	0.42
1:A:491:THR:N	1:A:1772:THR:OG1	2.44	0.42
1:A:562:LEU:HB2	1:A:630:ILE:HD11	2.02	0.42
1:A:713:TYR:HA	1:A:714:PRO:HA	1.87	0.42
1:A:1260:TYR:HB3	1:A:1263:LYS:HB2	1.99	0.42
1:A:806:ILE:HG23	1:A:823:LEU:HB3	2.02	0.42
1:A:795:ASN:OD1	1:A:797:PRO:HD2	2.19	0.42
1:A:1308:GLU:O	1:A:1312:LYS:HG2	2.19	0.42
1:A:1196:SER:N	1:A:1197:SER:HA	2.35	0.42
1:A:605:LYS:HG2	1:A:623:LEU:HD23	2.02	0.42
1:A:673:LEU:HD23	1:A:717:LEU:HD11	2.02	0.42
1:A:957:GLN:HG2	1:A:958:VAL:HG23	2.02	0.42
1:A:1585:PHE:O	1:A:1589:ILE:HG12	2.20	0.42
1:A:1693:ASP:O	1:A:1696:THR:OG1	2.36	0.42
1:A:507:LEU:HD22	1:A:509:GLN:OE1	2.20	0.42
1:A:1651:ARG:HB3	1:A:1684:TYR:O	2.19	0.42
1:A:20:GLU:HG3	1:A:58:PHE:CE1	2.53	0.41
1:A:96:ASN:O	1:A:282:VAL:HB	2.19	0.41
1:A:598:ASN:O	1:A:601:SER:OG	2.27	0.41
1:A:1749:VAL:HG22	1:A:1762:LYS:HG3	2.01	0.41
1:A:1152:LEU:HD12	1:A:1205:TYR:CZ	2.55	0.41
1:A:410:ASN:HB3	1:A:414:ASN:ND2	2.35	0.41
1:A:581:HIS:HB3	1:A:607:SER:HB3	2.00	0.41
1:A:1396:ILE:O	1:A:1396:ILE:HG13	2.20	0.41
1:A:1487:LYS:HB3	1:A:1492:ILE:HD12	2.02	0.41
1:A:126:ILE:HG13	1:A:235:HIS:CG	2.55	0.41
1:A:1062:LEU:O	1:A:1066:VAL:HG22	2.20	0.41
1:A:33:TYR:CZ	1:A:48:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:ASP:O	1:A:860:GLU:HG2	2.21	0.41
1:A:665:PHE:O	1:A:668:LEU:HB2	2.20	0.41
1:A:1735:PHE:CD1	1:A:1736:GLU:HG3	2.55	0.41
1:A:156:LEU:O	1:A:160:ILE:HG13	2.21	0.41
1:A:174:ARG:O	1:A:178:ILE:HG13	2.21	0.41
1:A:195:LYS:HA	1:A:196:PRO:HD3	1.89	0.41
1:A:333:ASN:N	1:A:333:ASN:HD22	2.17	0.41
1:A:1277:THR:HG23	1:A:1278:THR:H	1.86	0.41
1:A:1501:LEU:HD21	1:A:1504:ASN:HB2	2.03	0.41
1:A:1705:TYR:CE2	1:A:1707:SER:HB2	2.56	0.41
1:A:806:ILE:HD12	1:A:823:LEU:HD22	2.02	0.41
1:A:1413:ILE:HD12	1:A:1444:THR:HG21	2.03	0.41
1:A:1578:THR:CG2	1:A:1579:SER:HA	2.49	0.41
1:A:542:LEU:HB3	1:A:546:ASN:OD1	2.21	0.41
1:A:685:LYS:HE2	1:A:728:THR:HG23	2.02	0.41
1:A:1142:ASP:O	1:A:1144:LYS:HG3	2.22	0.41
1:A:1373:LEU:HB3	1:A:1376:ILE:HD11	2.03	0.41
1:A:1574:GLY:N	1:A:1575:HIS:HA	2.36	0.41
1:A:309:ASP:OD1	1:A:310:ARG:N	2.55	0.40
1:A:394:LEU:HD11	1:A:480:PHE:CG	2.56	0.40
1:A:1195:ILE:HG13	1:A:1198:HIS:H	1.86	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.90	0.40
1:A:1293:ASP:OD1	1:A:1293:ASP:N	2.55	0.40
1:A:20:GLU:H	1:A:20:GLU:HG2	1.75	0.40
1:A:970:LEU:HD23	1:A:970:LEU:HA	1.94	0.40
1:A:1342:ASP:HB2	1:A:1396:ILE:HD11	2.03	0.40
1:A:1567:ASP:OD1	1:A:1679:TYR:OH	2.29	0.40
1:A:268:SER:O	1:A:272:ARG:HG3	2.20	0.40
1:A:1147:VAL:HA	1:A:1148:PRO:HD3	1.95	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	1789/1838 (97%)	1656 (93%)	127 (7%)	6 (0%)	41 72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ASP
1	A	549	ASP
1	A	787	ASN
1	A	338	ASP
1	A	958	VAL
1	A	1200	PRO

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	1652/1696 (97%)	1648 (100%)	4 (0%)	93 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ASN
1	A	1109	VAL
1	A	1277	THR
1	A	1578	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 (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	1793/1838 (97%)	0.26	47 (2%) 56 52	58, 115, 195, 286	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	4.6
1	A	354	GLU	4.6
1	A	290	PRO	4.1
1	A	337	LEU	4.0
1	A	322	TYR	3.6
1	A	951	GLN	3.4
1	A	359	PHE	3.2
1	A	345	PHE	3.1
1	A	318	ALA	3.0
1	A	97	LEU	2.9
1	A	220	LEU	2.9
1	A	652	PHE	2.9
1	A	316	LEU	2.9
1	A	334	PHE	2.8
1	A	355	LYS	2.7
1	A	320	MET	2.7
1	A	1659	TYR	2.6
1	A	296	LEU	2.6
1	A	1242	LEU	2.6
1	A	688	ILE	2.5
1	A	1275	ALA	2.5
1	A	1252	LEU	2.5
1	A	1234	TRP	2.4
1	A	582	TYR	2.4
1	A	111	LEU	2.3
1	A	955	THR	2.3
1	A	1279	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1470	TYR	2.3
1	A	30	LEU	2.2
1	A	1207	ALA	2.2
1	A	351	SER	2.2
1	A	289	LEU	2.2
1	A	114	ILE	2.2
1	A	358	ILE	2.2
1	A	521	PHE	2.2
1	A	713	TYR	2.2
1	A	99	PHE	2.1
1	A	1317	PHE	2.1
1	A	1114	ILE	2.1
1	A	89	ASN	2.1
1	A	677	ILE	2.1
1	A	1493	LEU	2.1
1	A	1027	ILE	2.1
1	A	1268	PHE	2.1
1	A	1187	ASP	2.1
1	A	1661	PRO	2.0
1	A	719	LEU	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	ZN	A	1901	1/1	0.96	0.12	132,132,132,132	0

6.5 Other polymers (i)

There are no such residues in this entry.