



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:33 PM UTC

PDB ID : 4R04 / pdb_00004r04
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 ⓘ 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

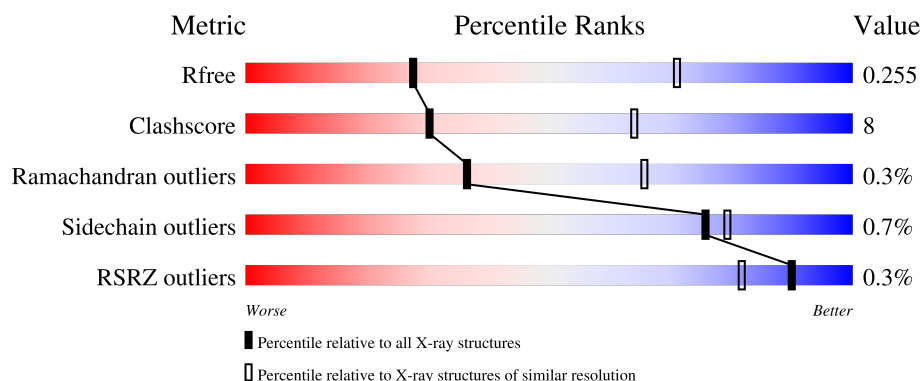
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 $\leq 5\%$. 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	1838	 75% 22% .

2 Entry composition

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
1	A	1793	Total	C	N	O	S	0	0	0
			14409	9199	2332	2852	26			

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 (CCD ID: ZN) (formula: Zn).

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

D1535	K1536	D1539	S1546	Q1549	Y1556	L1557	N1558	Y1562	D1567	F1568	V1569	S1572	D1573	G1574	H1575	T1578	S1579	F1585	I1589	S1590	K1593	I1604	V1611	G1612	K1613	T1614	N1615	L1616	G1617	K1627	Y1632	V1636	S1640	G1648	N1649	G1650	R1651	V1655	G1664	
E1665	T1669	S1670	L1678	Y1679	Y1684	I1685	L1689	I1690	D1693	L1694	Y1695	T1696	I1701	Y1705	Y1706	S1707	N1708	Y1711	I1715	H1723	I1728	N1729	L1730	F1735	E1736	Y1737	S1744	D1745	V1749	R1750	K1762	K1766	G1767	I1768	N1771	T1772	Q1773	K1777	M1778	D1781
L1790	N1801	S1802	GLU	ASN	GLU	LEU	ASP	ARG	ASP	ASP	HIS	LEU	GLY	PHE	LYS	ILE	ILE	ASP	ASN	ASN	LYS	THR	TYR	TYR	ASP	GLU	ASP	SER	LYS	LEU	VAL	LYS	GLY	HIS	HIS	HIS	HIS	HIS	HIS	

4 Data and refinement statistics

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 61.62 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.62-3.26) 94.3 (61.62-3.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1565)	Depositor
R, R_{free}	0.221 , 0.249 0.228 , 0.255	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)	0.31 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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](#)

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	0.27	0/14671	0.71	8/19845 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1574	GLY	N-CA-C	5.37	124.81	115.62
1	A	1519	ASP	CB-CA-C	-5.32	109.99	117.23
1	A	336	LYS	N-CA-C	5.32	117.42	108.96
1	A	363	GLU	CB-CA-C	-5.17	110.20	117.23
1	A	1498	ASP	CB-CA-C	-5.16	110.64	116.63
1	A	469	GLY	CA-C-N	5.02	125.30	119.47
1	A	469	GLY	C-N-CA	5.02	125.30	119.47
1	A	1189	PHE	N-CA-C	5.02	115.00	108.07

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	242	0
2	A	1	0	0	0	0
All	All	14410	0	14349	242	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 (242) 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:1071:ILE:HD11	1:A:1073:MET:HE2	1.82	0.60
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:84:LEU:O	1:A:88:SER:OG	2.21	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:MET:HE1	1:A:459:PRO:HG2	1.87	0.56
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
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: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: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:598:ASN:O	1:A:601:SER:OG	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:999:GLY:O	1:A:1002:THR:OG1	2.28	0.49
1:A:1678:LEU:HG	1:A:1685:ILE:HD12	1.95	0.49
1:A:1270:ALA:C	1:A:1272:PHE:H	2.20	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:662:THR:HG21	1:A:702:MET:HE1	1.95	0.49
1:A:368:SER:HB3	1:A:371:GLU:HG2	1.95	0.49
1:A:624:SER:OG	1:A:626:ASP:O	2.19	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:324:LYS:C	1:A:326:ILE:H	2.22	0.48
1:A:1160:ASN:HB3	1:A:1293:ASP:HB3	1.95	0.48
1:A:1343:ASP:OD1	1:A:1343:ASP:N	2.45	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:1728:ILE:HG13	1:A:1778:MET:HE1	1.96	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:119:ASP:OD2	1:A:355:LYS:NZ	2.34	0.47
1:A:162:ASN:OD1	1:A:164:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:ASN:O	1:A:1500:THR:OG1	2.30	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:1133:LYS:HZ1	1:A:1210:ILE:HG23	1.81	0.45
1:A:1768:ILE:HG21	1:A:1790:LEU:HD12	1.98	0.45
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:ASP:HA	1:A:1227:ALA:HB2	1.99	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: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:1174:MET:HE2	1:A:1174:MET:HB3	1.86	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:O	1:A:282:VAL:HB	2.19	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:1477:THR:C	1:A:1479:GLN:H	2.28	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
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:1648:GLY:C	1:A:1650:GLY:H	2.30	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%)	36 66

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%)	1641 (99%)	11 (1%)	76 79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	LEU
1	A	507	LEU

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Mol	Chain	Res	Type
1	A	815	VAL
1	A	843	LEU
1	A	958	VAL
1	A	979	VAL
1	A	1071	ILE
1	A	1109	VAL
1	A	1277	THR
1	A	1578	THR
1	A	1611	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	182	GLN
1	A	256	GLN
1	A	278	ASN
1	A	366	ASN
1	A	410	ASN
1	A	414	ASN
1	A	482	ASN
1	A	506	ASN
1	A	529	GLN
1	A	570	ASN
1	A	661	ASN
1	A	696	ASN
1	A	701	ASN
1	A	765	ASN
1	A	787	ASN
1	A	866	ASN
1	A	957	GLN
1	A	1440	ASN
1	A	1553	ASN
1	A	1583	ASN
1	A	1588	ASN
1	A	1660	ASN
1	A	1796	ASN

5.3.3 RNA ⓘ

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](#)

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%)	-0.23	6 (0%)	90 82	58, 115, 195, 286	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	3.5
1	A	1190	PHE	2.5
1	A	1342	ASP	2.1
1	A	958	VAL	2.1
1	A	812	ASP	2.1
1	A	309	ASP	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](#)

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	0.06	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.