



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 AM UTC

PDB ID : 4YOC / pdb_00004yoc
Title : Crystal Structure of human DNMT1 and USP7/HAUSP complex
Authors : Cheng, J.; Yang, H.; Fang, J.; Gong, R.; Wang, P.; Li, Z.; Xu, Y.
Deposited on : 2015-03-11
Resolution : 2.92 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

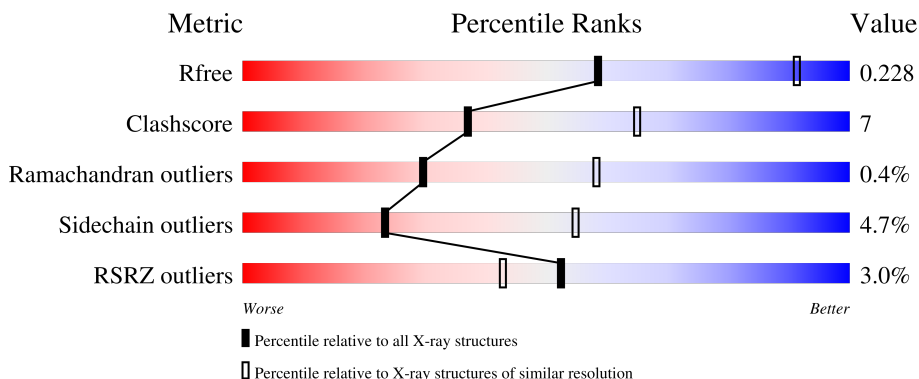
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	1004	3% 69% 17% • 12%
2	C	548	2% 76% 18% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11386 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	882	Total	C	N	O	S	0	1	0
			7033	4453	1240	1296	44			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	SER	-	expression tag	UNP P26358
A	598	GLU	-	expression tag	UNP P26358
A	599	PHE	-	expression tag	UNP P26358

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	529	Total	C	N	O	S	0	0	0
			4340	2762	733	818	27			

There are 5 discrepancies between the modelled and reference sequences:

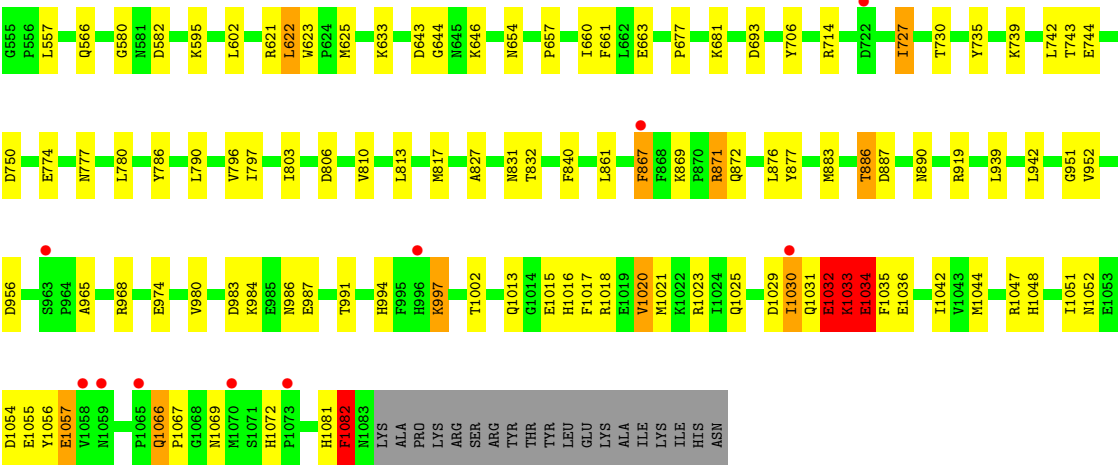
Chain	Residue	Modelled	Actual	Comment	Reference
C	555	GLY	-	expression tag	UNP Q93009
C	556	PRO	-	expression tag	UNP Q93009
C	557	LEU	-	expression tag	UNP Q93009
C	558	GLY	-	expression tag	UNP Q93009
C	559	SER	-	expression tag	UNP Q93009

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total 9	O 9	0	0
4	C	2	Total 2	O 2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.23Å 111.62Å 163.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 2.92 49.42 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.42-2.92) 99.1 (49.42-2.92)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.258 0.213 , 0.228	Depositor DCC
R_{free} test set	2248 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11386	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

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	0.30	0/7214	0.83	11/9755 (0.1%)
2	C	0.28	0/4440	0.78	9/5995 (0.2%)
All	All	0.30	0/11654	0.81	20/15750 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	C	0	2
All	All	0	7

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	709	ILE	N-CA-C	9.14	117.86	107.89
2	C	951	GLY	N-CA-C	6.94	121.00	110.18
2	C	1082	PHE	CB-CA-C	-6.78	106.85	116.34
1	A	1079	GLY	CA-C-N	6.50	125.72	118.97
1	A	1079	GLY	C-N-CA	6.50	125.72	118.97
2	C	1032	GLU	N-CA-C	6.49	119.84	112.97
2	C	693	ASP	CA-C-N	5.93	125.63	119.05
2	C	693	ASP	C-N-CA	5.93	125.63	119.05
1	A	1031	THR	CA-C-N	-5.82	113.81	119.87
1	A	1031	THR	C-N-CA	-5.82	113.81	119.87
1	A	1539	VAL	N-CA-C	5.42	118.10	112.90
2	C	1034	GLU	N-CA-C	-5.27	106.11	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	582	ASP	CB-CA-C	-5.20	109.02	115.89
1	A	715	PRO	N-CA-C	5.20	123.19	112.47
1	A	1537	GLY	CA-C-N	-5.11	114.16	122.34
1	A	1537	GLY	C-N-CA	-5.11	114.16	122.34
1	A	1335	ALA	CA-C-N	5.09	124.70	119.05
1	A	1335	ALA	C-N-CA	5.09	124.70	119.05
2	C	1072	HIS	CA-C-N	5.03	125.03	119.90
2	C	1072	HIS	C-N-CA	5.03	125.03	119.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1536	GLN	Peptide
1	A	707	ASP	Peptide
1	A	708	ASN	Peptide
1	A	714	SER	Peptide
1	A	715	PRO	Peptide
2	C	1032	GLU	Peptide
2	C	1033	LYS	Peptide

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	7033	0	6901	98	0
2	C	4340	0	4252	62	0
3	A	2	0	0	0	0
4	A	9	0	0	0	0
4	C	2	0	0	0	0
All	All	11386	0	11153	159	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 7.

All (159) 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:1036:HIS:O	1:A:1398:ARG:NH2	2.20	0.74
2:C:1033:LYS:HE3	2:C:1036:GLU:HB2	1.76	0.67
2:C:867:PHE:H	2:C:867:PHE:HD1	1.42	0.67
2:C:625:MET:HG3	2:C:633:LYS:HG2	1.79	0.65
2:C:919:ARG:NH2	2:C:956:ASP:OD1	2.31	0.64
2:C:1016:HIS:HA	2:C:1056:TYR:HB3	1.79	0.64
1:A:622:LYS:HD2	1:A:850:ASP:HB3	1.82	0.62
1:A:1038:ASP:OD1	1:A:1398:ARG:NH1	2.32	0.62
1:A:886:GLU:HA	1:A:889:LYS:HG3	1.82	0.61
2:C:965:ALA:HB3	2:C:968:ARG:HG3	1.83	0.61
1:A:884:PRO:HB3	1:A:892:PHE:CG	2.35	0.61
1:A:1219:MET:HE1	1:A:1592:ILE:HD13	1.82	0.60
1:A:1368:ARG:NH2	1:A:1520:ASP:OD1	2.31	0.60
2:C:1017:PHE:O	2:C:1020:VAL:HG12	2.01	0.60
2:C:797:ILE:HG12	2:C:810:VAL:HG22	1.83	0.59
2:C:1015:GLU:HG2	2:C:1020:VAL:HB	1.84	0.59
1:A:703:GLU:HG3	1:A:705:VAL:H	1.68	0.58
1:A:997:LYS:NZ	1:A:1048:GLU:OE1	2.33	0.58
1:A:818:ASP:OD2	1:A:898:ARG:NH1	2.37	0.57
2:C:1031:GLN:HB3	2:C:1034:GLU:HB3	1.87	0.57
1:A:928:LYS:NZ	1:A:1053:PHE:O	2.36	0.57
2:C:869:LYS:HB2	2:C:872:GLN:HG3	1.85	0.57
2:C:1052:ASN:ND2	2:C:1055:GLU:OE2	2.33	0.57
1:A:1400:LEU:HD23	1:A:1555:ARG:HD3	1.87	0.56
1:A:1461:ASP:OD2	1:A:1464:ASN:ND2	2.40	0.55
2:C:625:MET:HE1	2:C:661:PHE:HB2	1.89	0.55
1:A:707:ASP:N	1:A:707:ASP:OD1	2.40	0.55
1:A:1109:LYS:NZ	2:C:744:GLU:OE1	2.40	0.55
2:C:983:ASP:HB3	2:C:986:ASN:HB2	1.88	0.54
2:C:1044:MET:HG3	2:C:1047:ARG:HG2	1.89	0.54
1:A:1281:LYS:NZ	1:A:1346:ASP:OD2	2.36	0.54
1:A:998:GLU:HB2	1:A:1017:ARG:HB3	1.89	0.54
1:A:877:GLU:HA	1:A:1293:GLN:HB3	1.89	0.53
1:A:1472:LEU:H	1:A:1472:LEU:HD12	1.73	0.53
1:A:714:SER:CB	1:A:1349:LYS:HB3	2.38	0.53
2:C:643:ASP:OD1	2:C:646:LYS:NZ	2.41	0.53
2:C:727:ILE:O	2:C:730:THR:OG1	2.23	0.53
1:A:1519:TRP:NE1	1:A:1543:GLU:OE2	2.36	0.53
1:A:785:ASP:O	1:A:789:GLY:N	2.35	0.52
2:C:1082:PHE:N	2:C:1082:PHE:HD1	2.07	0.52
1:A:796:TRP:HE1	1:A:821:GLU:HG2	1.73	0.52
1:A:1462:ARG:HH12	1:A:1480:GLU:CD	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LYS:HD3	1:A:758:GLU:HG2	1.91	0.52
2:C:883:MET:HE2	2:C:887:ASP:HB3	1.90	0.52
1:A:714:SER:HB2	1:A:1349:LYS:HB3	1.92	0.52
1:A:917:LEU:O	1:A:1003:LYS:NZ	2.39	0.52
2:C:1066:GLN:NE2	2:C:1069:ASN:OD1	2.43	0.51
1:A:1235:PHE:CE1	1:A:1275:LYS:HG3	2.45	0.51
2:C:774:GLU:OE2	2:C:777:ASN:ND2	2.42	0.51
2:C:1020:VAL:HG23	2:C:1023:ARG:NH1	2.26	0.51
1:A:1030:SER:OG	1:A:1031:THR:N	2.43	0.51
2:C:840:PHE:HB2	2:C:877:TYR:HB2	1.91	0.51
2:C:663:GLU:OE1	2:C:706:TYR:OH	2.29	0.51
1:A:1022:TYR:OH	1:A:1047:GLU:OE2	2.27	0.51
2:C:1082:PHE:N	2:C:1082:PHE:CD1	2.79	0.51
1:A:1446:LEU:HD12	1:A:1450:THR:HB	1.93	0.51
2:C:1031:GLN:OE1	2:C:1032:GLU:N	2.44	0.50
2:C:869:LYS:HB3	2:C:871:ARG:HE	1.77	0.50
1:A:1263:PHE:HB3	1:A:1317:ALA:HB3	1.93	0.50
2:C:1057:GLU:OE1	2:C:1057:GLU:N	2.35	0.50
1:A:913:GLN:HA	1:A:923:TYR:HA	1.94	0.50
1:A:1329:GLU:OE2	1:A:1355:THR:N	2.45	0.49
1:A:1516:ARG:HA	1:A:1540:LEU:HB2	1.94	0.49
1:A:1224:PRO:O	1:A:1267:ASN:ND2	2.45	0.49
2:C:566:GLN:HB2	2:C:657:PRO:HB3	1.93	0.49
1:A:631:PHE:CZ	1:A:1278:MET:HE2	2.47	0.49
1:A:928:LYS:O	1:A:931:ILE:HG12	2.13	0.49
1:A:1528:THR:O	1:A:1573:HIS:HB3	2.12	0.49
1:A:874:ALA:HB2	1:A:1350:PHE:CD1	2.48	0.48
1:A:1008:ARG:HG3	1:A:1009:PRO:HD2	1.95	0.48
1:A:1075:TYR:CZ	1:A:1082:ARG:HB3	2.48	0.48
2:C:942:LEU:HD13	2:C:952:VAL:HG22	1.96	0.48
1:A:709:ILE:HD12	1:A:710:PRO:HD2	1.95	0.48
1:A:1411:ASP:OD1	1:A:1572:LYS:NZ	2.34	0.48
1:A:1445:ARG:HG2	1:A:1451:MET:SD	2.54	0.48
1:A:1414:CYS:SG	1:A:1546:ARG:HD2	2.54	0.47
1:A:1500:LEU:HB2	1:A:1501:PRO:HD3	1.96	0.47
1:A:1395:TRP:O	1:A:1399:GLN:HG2	2.13	0.47
1:A:765:VAL:HG13	1:A:827:TYR:O	2.15	0.47
1:A:1527:VAL:HG22	1:A:1528:THR:H	1.80	0.47
2:C:983:ASP:O	2:C:987:GLU:N	2.46	0.47
1:A:885:THR:OG1	1:A:886:GLU:N	2.48	0.47
1:A:1409:LEU:HD11	1:A:1551:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1025:GLN:HG3	2:C:1035:PHE:CE2	2.50	0.47
2:C:1018:ARG:HA	2:C:1021:MET:HG2	1.97	0.46
2:C:780:LEU:HD13	2:C:786:TYR:HA	1.97	0.46
1:A:1031:THR:O	1:A:1034:SER:OG	2.31	0.46
1:A:1141:THR:HG23	1:A:1219:MET:HG2	1.98	0.46
2:C:997:LYS:HG3	2:C:1082:PHE:CZ	2.51	0.46
2:C:1042:ILE:O	2:C:1048:HIS:HA	2.15	0.46
2:C:939:LEU:HD23	2:C:974:GLU:HA	1.97	0.45
1:A:713:PRO:HG2	1:A:714:SER:H	1.82	0.45
1:A:1093:SER:OG	1:A:1095:SER:OG	2.31	0.45
2:C:735:TYR:HB3	2:C:743:THR:HG22	1.98	0.45
1:A:1139:LEU:HD21	1:A:1261:ARG:HH21	1.81	0.45
2:C:714:ARG:NH1	2:C:750:ASP:OD1	2.48	0.45
1:A:1330:PRO:HD2	1:A:1356:ARG:HB2	1.98	0.45
2:C:621:ARG:HG2	2:C:623:TRP:NE1	2.32	0.45
2:C:621:ARG:NH2	2:C:677:PRO:O	2.40	0.45
1:A:624:VAL:HG22	1:A:1286:CYS:SG	2.57	0.45
1:A:971:GLU:OE1	1:A:974:ARG:HD2	2.16	0.44
2:C:739:LYS:HG2	2:C:742:LEU:HB3	1.99	0.44
2:C:803:ILE:HB	2:C:806:ASP:HB2	1.99	0.44
2:C:1030:ILE:HG13	2:C:1031:GLN:H	1.82	0.44
1:A:709:ILE:HA	1:A:710:PRO:HD2	1.78	0.44
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.52	0.44
2:C:602:LEU:HB3	2:C:644:GLY:HA2	1.99	0.44
2:C:867:PHE:CD1	2:C:867:PHE:N	2.84	0.44
1:A:714:SER:HB3	1:A:715:PRO:HD3	1.99	0.44
2:C:1066:GLN:HB2	2:C:1067:PRO:HD2	1.98	0.44
1:A:1568:ASN:ND2	1:A:1571:ASP:OD2	2.51	0.44
1:A:1269:ARG:O	1:A:1272:VAL:HG22	2.17	0.44
1:A:767:PRO:HB3	1:A:775:TYR:HE1	1.82	0.43
2:C:1020:VAL:HG23	2:C:1023:ARG:HH12	1.83	0.43
1:A:1224:PRO:HA	1:A:1225:PRO:HD3	1.88	0.43
1:A:1435:ASP:HA	1:A:1515:GLY:HA2	2.00	0.43
2:C:1015:GLU:O	2:C:1016:HIS:HB3	2.18	0.43
1:A:1335:ALA:HA	1:A:1336:PRO:HD3	1.85	0.43
1:A:1515:GLY:C	1:A:1538:ARG:HG3	2.43	0.43
2:C:796:VAL:HG21	2:C:861:LEU:HD21	2.00	0.43
2:C:1033:LYS:HD2	2:C:1033:LYS:HA	1.68	0.43
1:A:1324:LEU:HD12	1:A:1325:PRO:HD2	2.00	0.43
1:A:723:LYS:HA	1:A:768:ASP:HB3	2.01	0.43
1:A:931:ILE:HG13	1:A:933:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:827:ALA:HB1	2:C:832:THR:O	2.18	0.43
1:A:719:HIS:CE1	1:A:796:TRP:HB3	2.53	0.42
1:A:1064:TYR:CE1	1:A:1099:PRO:HG2	2.54	0.42
1:A:757:LEU:HD23	1:A:831:LYS:HD2	2.01	0.42
1:A:1303:GLN:HB3	1:A:1330:PRO:HB3	2.01	0.42
2:C:580:GLY:HA2	2:C:790:LEU:HD21	2.00	0.42
1:A:973:TYR:CZ	1:A:1473:ARG:HD3	2.55	0.42
1:A:722:LYS:O	1:A:723:LYS:HG3	2.20	0.42
1:A:941:LEU:HB2	1:A:992:ARG:HB2	2.01	0.42
2:C:986:ASN:HB3	2:C:1013:GLN:CD	2.45	0.42
1:A:1003:LYS:HA	1:A:1009:PRO:HA	2.01	0.42
1:A:1141:THR:OG1	1:A:1161:SER:HB2	2.20	0.42
2:C:1031:GLN:OE1	2:C:1034:GLU:N	2.45	0.42
2:C:622:LEU:HG	2:C:660:ILE:HG21	2.02	0.42
2:C:813:LEU:HB3	2:C:817:MET:SD	2.60	0.42
1:A:631:PHE:O	1:A:631:PHE:CG	2.73	0.41
1:A:1514:TYR:CE2	1:A:1533:MET:HG3	2.55	0.41
1:A:1406:GLN:HA	1:A:1407:PRO:HD2	1.91	0.41
1:A:723:LYS:HG2	1:A:767:PRO:HA	2.02	0.41
1:A:995:ARG:HB2	1:A:1021:PHE:HE2	1.84	0.41
1:A:1566:PHE:O	1:A:1575:GLN:NE2	2.53	0.41
1:A:1219:MET:HE3	1:A:1262:PHE:HB2	2.02	0.41
1:A:1226:CYS:HA	1:A:1229:PHE:CZ	2.56	0.41
2:C:566:GLN:OE1	2:C:595:LYS:HE2	2.20	0.41
2:C:886:THR:O	2:C:890:ASN:ND2	2.52	0.41
2:C:1029:ASP:HA	2:C:1035:PHE:HZ	1.86	0.41
2:C:869:LYS:HB3	2:C:871:ARG:NE	2.36	0.41
1:A:1114:GLY:C	1:A:1115:LYS:HD3	2.45	0.40
1:A:1142:LEU:HD13	1:A:1165:TRP:HB2	2.03	0.40
1:A:739:LYS:HD2	1:A:739:LYS:HA	1.79	0.40
1:A:744:LYS:HB3	1:A:783:TRP:CD1	2.57	0.40
1:A:783:TRP:CE2	1:A:791:MET:HB2	2.55	0.40
1:A:817:VAL:HG23	1:A:819:GLU:HB2	2.03	0.40
1:A:850:ASP:OD1	1:A:850:ASP:N	2.39	0.40
1:A:951:LYS:HB3	1:A:951:LYS:HE3	1.80	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	871/1004 (87%)	830 (95%)	39 (4%)	2 (0%)	43	71
2	C	527/548 (96%)	499 (95%)	25 (5%)	3 (1%)	21	50
All	All	1398/1552 (90%)	1329 (95%)	64 (5%)	5 (0%)	30	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1033	LYS
2	C	1081	HIS
1	A	819	GLU
2	C	980	VAL
1	A	705	VAL

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	764/869 (88%)	730 (96%)	34 (4%)	24	56
2	C	484/501 (97%)	460 (95%)	24 (5%)	22	52
All	All	1248/1370 (91%)	1190 (95%)	58 (5%)	23	56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	630	THR

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Mol	Chain	Res	Type
1	A	703	GLU
1	A	714	SER
1	A	716	LYS
1	A	718	MET
1	A	756	THR
1	A	757	LEU
1	A	786	SER
1	A	804	VAL
1	A	805	LEU
1	A	840	SER
1	A	850	ASP
1	A	861	LYS
1	A	862	THR
1	A	871	GLN
1	A	885	THR
1	A	889	LYS
1	A	899	LEU
1	A	903	ARG
1	A	913	GLN
1	A	931	ILE
1	A	939	VAL
1	A	950	ILE
1	A	952	LEU
1	A	1097	GLU
1	A	1101	ASN
1	A	1115	LYS
1	A	1203	THR
1	A	1207	ARG
1	A	1337	ARG
1	A	1378	ARG
1	A	1445	ARG
1	A	1493	ASN
1	A	1547	VAL
2	C	557	LEU
2	C	622	LEU
2	C	654	ASN
2	C	681	LYS
2	C	727	ILE
2	C	831	ASN
2	C	867	PHE
2	C	871	ARG
2	C	876	LEU

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Mol	Chain	Res	Type
2	C	886	THR
2	C	984	LYS
2	C	991	THR
2	C	994	HIS
2	C	997	LYS
2	C	1002	THR
2	C	1020	VAL
2	C	1030	ILE
2	C	1032	GLU
2	C	1034	GLU
2	C	1051	ILE
2	C	1054	ASP
2	C	1057	GLU
2	C	1066	GLN
2	C	1082	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	726	GLN
1	A	1101	ASN
1	A	1573	HIS
2	C	581	ASN
2	C	700	ASN
2	C	851	ASN
2	C	1013	GLN
2	C	1081	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

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

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	882/1004 (87%)	0.01	32 (3%)	46 37	23, 54, 116, 158	1 (0%)
2	C	529/548 (96%)	0.09	10 (1%)	66 58	31, 61, 136, 173	0
All	All	1411/1552 (90%)	0.04	42 (2%)	52 43	23, 58, 127, 173	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1483	LYS	5.4
1	A	633	ALA	5.3
1	A	709	ILE	5.0
2	C	996	HIS	4.6
1	A	715	PRO	4.2
1	A	721	GLY	3.8
1	A	710	PRO	3.5
2	C	963	SER	3.4
2	C	1059	ASN	3.3
2	C	1030	ILE	3.3
1	A	712	MET	3.2
1	A	1484	ALA	3.1
1	A	615	PRO	3.1
1	A	713	PRO	3.0
1	A	952	LEU	3.0
1	A	978	ASP	2.9
1	A	853	SER	2.9
1	A	1600	ALA	2.9
1	A	705	VAL	2.8
2	C	867	PHE	2.8
1	A	861	LYS	2.7
1	A	1537	GLY	2.7
1	A	756	THR	2.7
2	C	1058	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	1070	MET	2.5
1	A	860	GLY	2.5
1	A	714	SER	2.4
1	A	1480	GLU	2.4
1	A	1536	GLN	2.4
1	A	1508	ASN	2.4
2	C	722	ASP	2.4
2	C	1065	PRO	2.2
1	A	738	VAL	2.2
1	A	632	PHE	2.2
1	A	1482	GLY	2.2
1	A	1524	SER	2.1
2	C	1073	PRO	2.1
1	A	1115	LYS	2.1
1	A	979	TYR	2.1
1	A	1106	PRO	2.0
1	A	977	SER	2.0
1	A	716	LYS	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($\text{\AA}^2$)	Q<0.9
3	ZN	A	1701	1/1	0.99	0.03	76,76,76,76	0
3	ZN	A	1702	1/1	0.99	0.03	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.