



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:58 PM UTC

PDB ID : 3AV4 / pdb_00003av4
Title : Crystal structure of mouse DNA methyltransferase 1
Authors : Takeshita, K.; Suetake, I.; Yamashita, E.; Suga, M.; Narita, H.; Nakagawa, A.; Tajima, S.
Deposited on : 2011-02-22
Resolution : 2.75 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

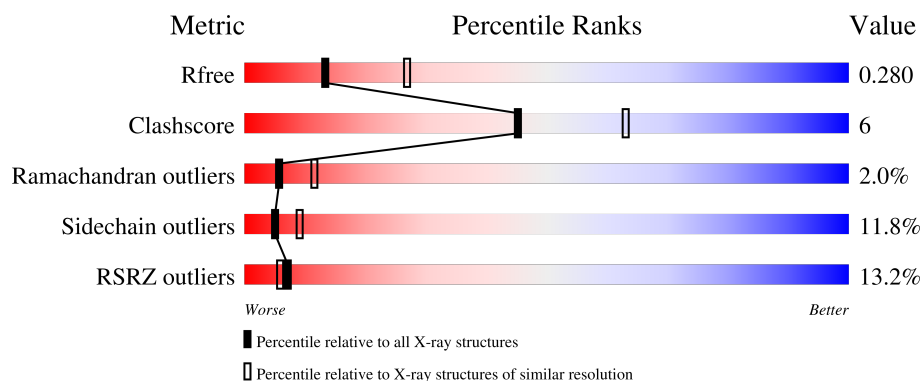
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	1330	11% 61% 21% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9156 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	1140	Total	C	N	O	S	0	0	0
			9110	5766	1586	1699	59			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		

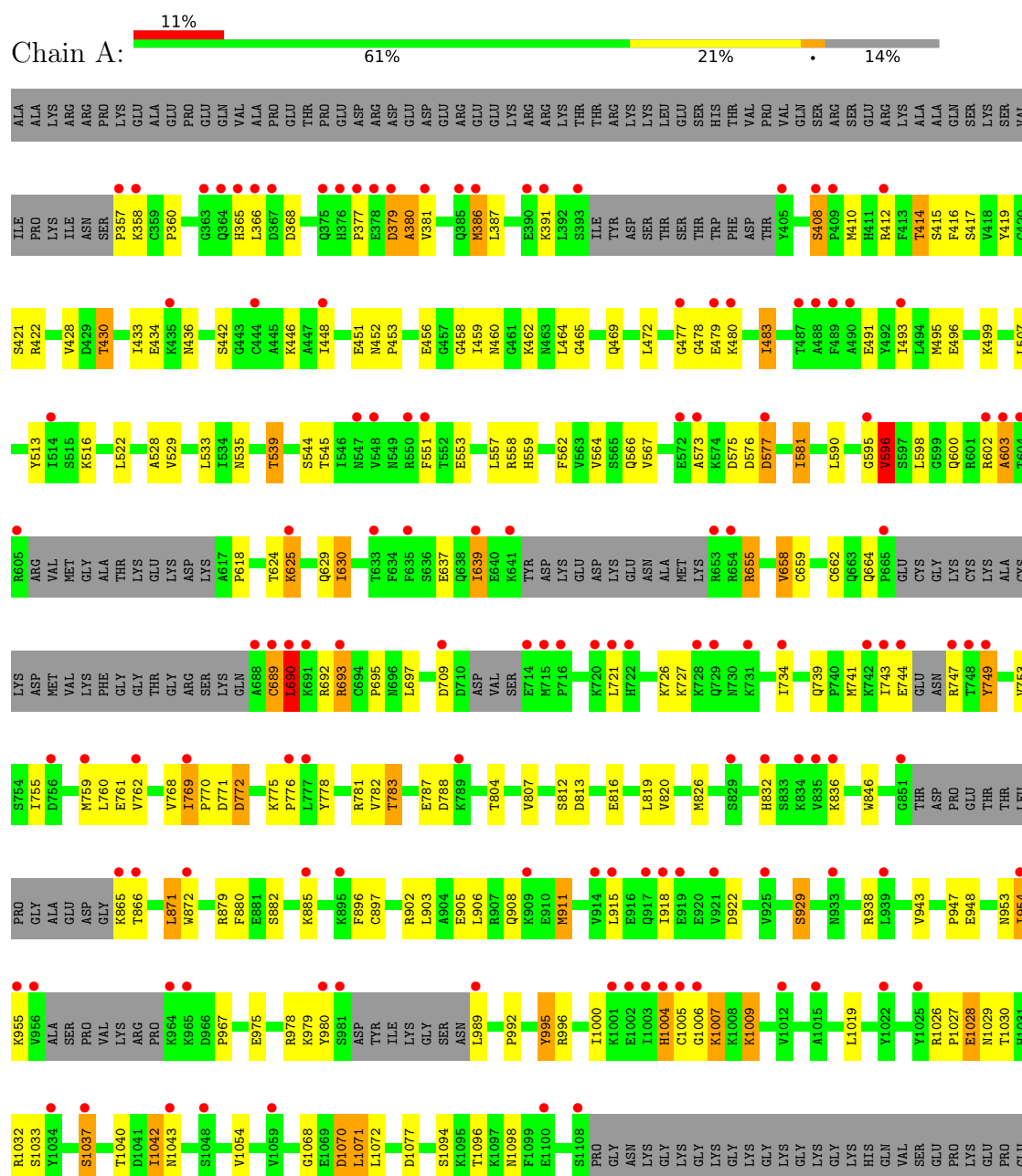
- Molecule 3 is water.

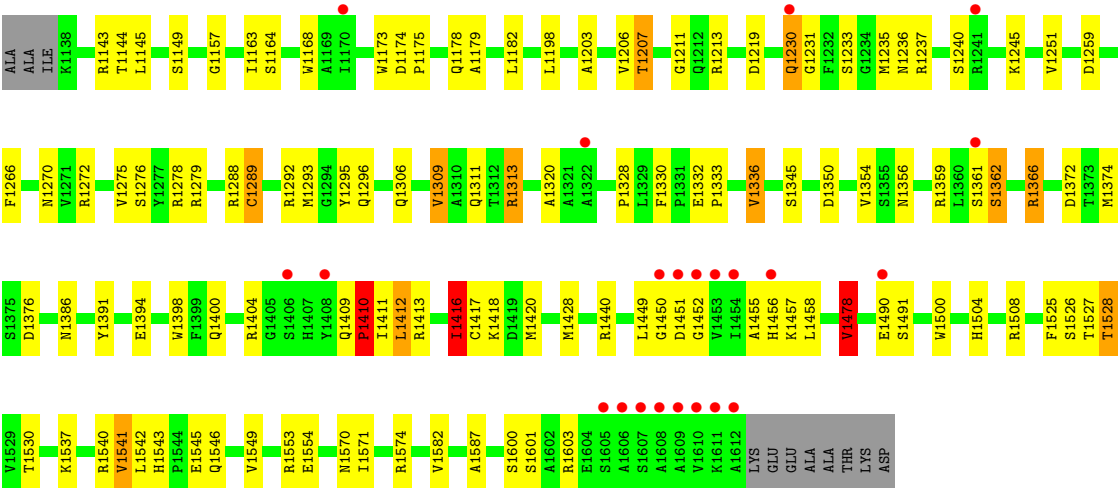
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		

3 Residue-property plots

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: DNA (cytosine-5)-methyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.78Å 97.86Å 130.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.42 – 2.75 43.42 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.42-2.75) 99.7 (43.42-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.230 , 0.267 0.237 , 0.280	Depositor DCC
R_{free} test set	2315 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9156	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	0.87	1/9330 (0.0%)	1.44	102/12615 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1541	VAL	CA-C	5.19	1.59	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1491	SER	N-CA-C	-10.72	98.34	114.64
1	A	1582	VAL	N-CA-C	-10.00	100.03	108.63
1	A	1070	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	1042	ILE	CA-C-N	8.24	134.69	120.68
1	A	1042	ILE	C-N-CA	8.24	134.69	120.68
1	A	1004	HIS	N-CA-C	8.04	120.12	111.36
1	A	1490	GLU	CA-C-N	7.82	135.73	121.41
1	A	1490	GLU	C-N-CA	7.82	135.73	121.41
1	A	1372	ASP	CA-C-N	7.82	130.60	120.44
1	A	1372	ASP	C-N-CA	7.82	130.60	120.44
1	A	1240	SER	N-CA-C	-7.41	102.58	111.69
1	A	379	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	689	CYS	CA-C-N	6.83	134.59	121.54
1	A	689	CYS	C-N-CA	6.83	134.59	121.54
1	A	596	VAL	N-CA-C	6.81	118.47	109.21
1	A	1164	SER	N-CA-C	6.64	118.85	108.96
1	A	575	ASP	N-CA-C	6.59	119.26	108.52
1	A	1362	SER	N-CA-C	6.52	118.28	110.19
1	A	1410	PRO	CA-C-N	6.47	129.90	120.91
1	A	1410	PRO	C-N-CA	6.47	129.90	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1026	ARG	N-CA-C	-6.13	101.83	110.29
1	A	419	TYR	N-CA-C	6.11	118.35	109.07
1	A	1251	VAL	N-CA-C	-6.08	104.81	110.53
1	A	1029	ASN	CA-C-N	6.07	131.12	120.87
1	A	1029	ASN	C-N-CA	6.07	131.12	120.87
1	A	1235	MET	N-CA-C	6.07	120.75	113.23
1	A	1149	SER	N-CA-C	6.05	118.65	111.33
1	A	1416	ILE	CA-CB-CG2	6.00	120.70	110.50
1	A	1398	TRP	CA-C-N	5.96	128.59	120.54
1	A	1398	TRP	C-N-CA	5.96	128.59	120.54
1	A	602	ARG	CA-C-N	5.94	132.88	121.54
1	A	602	ARG	C-N-CA	5.94	132.88	121.54
1	A	788	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	528	ALA	CA-C-N	5.88	129.35	120.95
1	A	528	ALA	C-N-CA	5.88	129.35	120.95
1	A	577	ASP	N-CA-C	-5.85	106.18	113.38
1	A	954	ILE	N-CA-C	5.85	121.51	109.34
1	A	391	LYS	N-CA-C	-5.81	106.04	113.01
1	A	1528	THR	CB-CA-C	5.78	119.45	110.67
1	A	1491	SER	CA-C-N	5.76	130.57	121.99
1	A	1491	SER	C-N-CA	5.76	130.57	121.99
1	A	846	TRP	CA-C-N	5.69	128.48	120.28
1	A	846	TRP	C-N-CA	5.69	128.48	120.28
1	A	458	GLY	N-CA-C	5.67	120.50	110.80
1	A	782	VAL	CA-C-N	5.61	128.26	120.63
1	A	782	VAL	C-N-CA	5.61	128.26	120.63
1	A	1452	GLY	CA-C-N	5.61	128.24	120.49
1	A	1452	GLY	C-N-CA	5.61	128.24	120.49
1	A	911	MET	N-CA-C	5.56	116.41	109.57
1	A	771	ASP	CA-C-N	5.52	132.09	121.54
1	A	771	ASP	C-N-CA	5.52	132.09	121.54
1	A	624	THR	N-CA-C	-5.46	101.68	110.14
1	A	749	TYR	CA-C-N	5.43	129.46	120.94
1	A	749	TYR	C-N-CA	5.43	129.46	120.94
1	A	625	LYS	CA-C-N	5.39	128.28	120.79
1	A	625	LYS	C-N-CA	5.39	128.28	120.79
1	A	618	PRO	CA-C-N	5.39	129.97	121.56
1	A	618	PRO	C-N-CA	5.39	129.97	121.56
1	A	1144	THR	CA-C-N	5.38	130.58	123.00
1	A	1144	THR	C-N-CA	5.38	130.58	123.00
1	A	562	PHE	CA-C-N	5.36	127.79	120.77
1	A	562	PHE	C-N-CA	5.36	127.79	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	VAL	N-CA-C	5.36	116.08	110.62
1	A	1077	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	659	CYS	N-CA-C	5.31	117.39	110.43
1	A	807	VAL	CA-C-N	5.24	127.56	120.38
1	A	807	VAL	C-N-CA	5.24	127.56	120.38
1	A	430	THR	CB-CA-C	5.23	120.42	110.27
1	A	846	TRP	N-CA-C	-5.23	105.66	111.36
1	A	1417	CYS	CA-C-N	5.21	128.11	120.71
1	A	1417	CYS	C-N-CA	5.21	128.11	120.71
1	A	368	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	1478	VAL	N-CA-CB	-5.20	106.14	112.33
1	A	464	LEU	CA-C-N	5.18	130.01	121.87
1	A	464	LEU	C-N-CA	5.18	130.01	121.87
1	A	1309	VAL	CB-CA-C	5.15	118.44	110.50
1	A	954	ILE	CA-C-N	5.14	130.54	122.21
1	A	954	ILE	C-N-CA	5.14	130.54	122.21
1	A	953	ASN	CA-C-N	5.14	131.22	121.97
1	A	953	ASN	C-N-CA	5.14	131.22	121.97
1	A	980	TYR	N-CA-C	5.13	118.39	107.67
1	A	1527	THR	CA-C-N	5.13	129.66	121.66
1	A	1527	THR	C-N-CA	5.13	129.66	121.66
1	A	905	GLU	CA-C-N	5.10	127.12	120.28
1	A	905	GLU	C-N-CA	5.10	127.12	120.28
1	A	871	LEU	CA-C-N	5.10	129.55	122.77
1	A	871	LEU	C-N-CA	5.10	129.55	122.77
1	A	967	PRO	N-CA-C	5.09	119.19	111.15
1	A	1007	LYS	N-CA-C	5.08	116.69	108.26
1	A	690	LEU	CA-C-N	5.06	131.21	121.54
1	A	690	LEU	C-N-CA	5.06	131.21	121.54
1	A	929	SER	N-CA-C	5.06	116.10	108.46
1	A	499	LYS	CA-C-N	5.04	127.30	120.44
1	A	499	LYS	C-N-CA	5.04	127.30	120.44
1	A	1540	ARG	N-CA-C	-5.04	102.45	109.96
1	A	1416	ILE	N-CA-CB	-5.04	104.16	111.52
1	A	544	SER	CA-C-N	5.03	127.72	120.38
1	A	544	SER	C-N-CA	5.03	127.72	120.38
1	A	709	ASP	N-CA-C	5.02	117.51	107.62
1	A	428	VAL	CA-C-N	5.01	128.61	120.60
1	A	428	VAL	C-N-CA	5.01	128.61	120.60
1	A	1554	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

There are no planarity outliers.

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	9110	0	8892	107	0
2	A	4	0	0	0	0
3	A	42	0	0	0	0
All	All	9156	0	8892	107	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 6.

All (107) 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:772:ASP:HB2	1:A:775:LYS:HG2	1.48	0.93
1:A:1428:MET:HE2	1:A:1542:LEU:HD22	1.64	0.79
1:A:595:GLY:HA3	1:A:1504:HIS:CE1	2.19	0.78
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.87	0.75
1:A:1330:PHE:H	1:A:1356:ASN:HD21	1.35	0.75
1:A:479:GLU:HA	1:A:516:LYS:HE2	1.70	0.72
1:A:1420:MET:HA	1:A:1420:MET:HE2	1.76	0.67
1:A:1030:THR:HG22	1:A:1032:ARG:H	1.60	0.67
1:A:567:VAL:HG13	1:A:581:ILE:HG22	1.77	0.67
1:A:1028:GLU:HG2	1:A:1037:SER:HB3	1.75	0.66
1:A:1543:HIS:HD2	1:A:1546:GLN:H	1.43	0.66
1:A:992:PRO:HG2	1:A:1336:VAL:HG22	1.79	0.64
1:A:1416:ILE:HG23	1:A:1571:ILE:HD12	1.80	0.64
1:A:1418:LYS:HB3	1:A:1420:MET:HE3	1.82	0.61
1:A:1027:PRO:HG2	1:A:1040:THR:HG21	1.82	0.61
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.83	0.61
1:A:1293:MET:HE2	1:A:1295:TYR:CE1	2.36	0.60
1:A:1543:HIS:CD2	1:A:1545:GLU:H	2.18	0.60
1:A:1543:HIS:CD2	1:A:1546:GLN:H	2.19	0.60
1:A:472:LEU:H	1:A:603:ALA:HB1	1.65	0.60
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:GLY:HA3	1:A:1504:HIS:HE1	1.69	0.57
1:A:1456:HIS:CG	1:A:1457:LYS:H	2.23	0.57
1:A:783:THR:HG21	1:A:897:CYS:HB2	1.87	0.57
1:A:1259:ASP:HA	1:A:1293:MET:HE3	1.85	0.56
1:A:1543:HIS:HD2	1:A:1545:GLU:H	1.53	0.56
1:A:446:LYS:HE2	1:A:452:ASN:O	2.04	0.56
1:A:379:ASP:HB3	1:A:460:ASN:HB2	1.88	0.56
1:A:1179:ALA:HA	1:A:1182:LEU:HD12	1.90	0.54
1:A:1306:GLN:HB3	1:A:1333:PRO:HB3	1.90	0.54
1:A:414:THR:HG23	1:A:496:GLU:H	1.73	0.54
1:A:535:ASN:O	1:A:539:THR:HB	2.09	0.53
1:A:1413:ARG:O	1:A:1553:ARG:HD3	2.08	0.53
1:A:1293:MET:HE2	1:A:1295:TYR:HE1	1.73	0.53
1:A:812:SER:HA	1:A:1288:ARG:HD3	1.91	0.53
1:A:414:THR:HG21	1:A:453:PRO:O	2.09	0.52
1:A:882:SER:H	1:A:1296:GLN:HE21	1.59	0.51
1:A:1332:GLU:HB3	1:A:1359:ARG:HD2	1.92	0.51
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.92	0.50
1:A:564:VAL:HG11	1:A:596:VAL:HG11	1.92	0.50
1:A:598:LEU:HB3	1:A:695:PRO:HB2	1.93	0.50
1:A:775:LYS:N	1:A:776:PRO:HD3	2.27	0.50
1:A:1143:ARG:NH1	1:A:1219:ASP:O	2.44	0.50
1:A:1096:THR:HB	1:A:1098:ASN:HD22	1.77	0.50
1:A:1236:ASN:O	1:A:1278:ARG:HA	2.12	0.50
1:A:836:LYS:HD2	1:A:866:THR:HG21	1.94	0.49
1:A:1231:GLY:HA3	1:A:1245:LYS:HG2	1.93	0.49
1:A:813:ASP:HB3	1:A:816:GLU:HB2	1.93	0.49
1:A:567:VAL:HG13	1:A:581:ILE:CG2	2.43	0.49
1:A:947:PRO:HA	1:A:996:ARG:HG2	1.94	0.49
1:A:553:GLU:O	1:A:557:LEU:HG	2.12	0.48
1:A:416:PHE:HA	1:A:442:SER:O	2.14	0.48
1:A:1333:PRO:HD2	1:A:1359:ARG:HB2	1.96	0.48
1:A:929:SER:HB3	1:A:938:ARG:HG2	1.96	0.48
1:A:558:ARG:HD3	1:A:559:HIS:CE1	2.49	0.47
1:A:412:ARG:HD2	1:A:495:MET:HE3	1.96	0.47
1:A:1040:THR:HG22	1:A:1366:ARG:HH22	1.78	0.47
1:A:655:ARG:HG3	1:A:662:CYS:SG	2.55	0.47
1:A:1005:CYS:SG	1:A:1006:GLY:N	2.83	0.47
1:A:979:LYS:HD3	1:A:1440:ARG:HB2	1.97	0.46
1:A:522:LEU:HB3	1:A:581:ILE:HG12	1.98	0.46
1:A:1416:ILE:HG23	1:A:1571:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:HIS:CG	1:A:1457:LYS:N	2.83	0.46
1:A:408:SER:HB3	1:A:491:GLU:HG2	1.98	0.46
1:A:1028:GLU:O	1:A:1033:SER:HA	2.15	0.46
1:A:1391:TYR:CE2	1:A:1412:LEU:HG	2.51	0.46
1:A:768:VAL:HG21	1:A:826:MET:HE1	1.98	0.45
1:A:769:ILE:HD11	1:A:832:HIS:CD2	2.51	0.45
1:A:357:PRO:HB2	1:A:366:LEU:HB2	1.98	0.45
1:A:360:PRO:HD2	1:A:422:ARG:HD2	1.98	0.45
1:A:1068:GLY:HA2	1:A:1071:LEU:HD12	1.99	0.45
1:A:630:ILE:HD11	1:A:1292:ARG:HB3	1.98	0.45
1:A:1600:SER:HA	1:A:1603:ARG:NE	2.31	0.45
1:A:690:LEU:HD23	1:A:693:ARG:HH21	1.82	0.45
1:A:871:LEU:HD13	1:A:880:PHE:HB3	1.98	0.44
1:A:414:THR:HG22	1:A:415:SER:H	1.83	0.44
1:A:478:GLY:C	1:A:480:LYS:H	2.25	0.44
1:A:1145:LEU:HA	1:A:1168:TRP:O	2.17	0.44
1:A:689:CYS:SG	1:A:690:LEU:N	2.91	0.44
1:A:770:PRO:HB3	1:A:778:TYR:CE1	2.52	0.44
1:A:513:TYR:HD2	1:A:551:PHE:HE1	1.66	0.44
1:A:1449:LEU:HD11	1:A:1455:ALA:HB2	2.00	0.44
1:A:483:ILE:HD12	1:A:483:ILE:H	1.83	0.44
1:A:1213:ARG:CD	1:A:1213:ARG:H	2.31	0.44
1:A:726:LYS:HA	1:A:770:PRO:HA	2.00	0.43
1:A:995:TYR:OH	1:A:1359:ARG:HG2	2.17	0.43
1:A:879:ARG:NH2	1:A:1328:PRO:O	2.52	0.43
1:A:1207:THR:HG23	1:A:1211:GLY:HA2	2.00	0.43
1:A:377:PRO:HD2	1:A:380:ALA:HB2	2.00	0.43
1:A:1173:TRP:CD1	1:A:1175:PRO:HD2	2.54	0.43
1:A:1311:GLN:HE21	1:A:1313:ARG:HB2	1.84	0.43
1:A:753:VAL:HG22	1:A:761:GLU:HG3	2.02	0.42
1:A:386:MET:HE3	1:A:386:MET:HB2	1.85	0.42
1:A:434:GLU:C	1:A:436:ASN:H	2.27	0.42
1:A:1386:ASN:C	1:A:1416:ILE:HD11	2.45	0.42
1:A:1478:VAL:HG13	1:A:1500:TRP:NE1	2.35	0.42
1:A:1293:MET:CE	1:A:1295:TYR:HE1	2.32	0.42
1:A:1570:ASN:O	1:A:1574:ARG:HG3	2.19	0.42
1:A:819:LEU:HB2	1:A:872:TRP:HA	2.01	0.42
1:A:744:GLU:O	1:A:747:ARG:N	2.52	0.42
1:A:630:ILE:HD13	1:A:1289:CYS:HA	2.02	0.41
1:A:1376:ASP:HB3	1:A:1400:GLN:OE1	2.21	0.41
1:A:1409:GLN:CD	1:A:1410:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:ARG:HG2	1:A:1279:ARG:HG3	2.03	0.41
1:A:1040:THR:CG2	1:A:1366:ARG:HH22	2.34	0.41
1:A:1374:MET:HE1	1:A:1525:PHE:CZ	2.55	0.41
1:A:1000:ILE:HG12	1:A:1019:LEU:HD23	2.03	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	1118/1330 (84%)	1007 (90%)	89 (8%)	22 (2%)	6	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ALA
1	A	456	GLU
1	A	465	GLY
1	A	573	ALA
1	A	603	ALA
1	A	637	GLU
1	A	639	ILE
1	A	690	LEU
1	A	772	ASP
1	A	954	ILE
1	A	1361	SER
1	A	477	GLY
1	A	896	PHE
1	A	1009	LYS
1	A	1203	ALA
1	A	1037	SER
1	A	1230	GLN

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Mol	Chain	Res	Type
1	A	995	TYR
1	A	1233	SER
1	A	1410	PRO
1	A	1450	GLY
1	A	762	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	1002/1162 (86%)	884 (88%)	118 (12%)	5 9

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	365	HIS
1	A	381	VAL
1	A	386	MET
1	A	387	LEU
1	A	408	SER
1	A	410	MET
1	A	414	THR
1	A	417	SER
1	A	421	SER
1	A	430	THR
1	A	433	ILE
1	A	448	ILE
1	A	451	GLU
1	A	459	ILE
1	A	469	GLN
1	A	483	ILE
1	A	493	ILE
1	A	507	LEU
1	A	529	VAL
1	A	533	LEU

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Mol	Chain	Res	Type
1	A	539	THR
1	A	545	THR
1	A	566	GLN
1	A	576	ASP
1	A	577	ASP
1	A	581	ILE
1	A	590	LEU
1	A	596	VAL
1	A	600	GLN
1	A	625	LYS
1	A	629	GLN
1	A	630	ILE
1	A	639	ILE
1	A	655	ARG
1	A	658	VAL
1	A	664	GLN
1	A	690	LEU
1	A	692	ARG
1	A	693	ARG
1	A	697	LEU
1	A	721	LEU
1	A	727	LYS
1	A	734	ILE
1	A	739	GLN
1	A	741	MET
1	A	743	ILE
1	A	749	TYR
1	A	755	ILE
1	A	759	MET
1	A	760	LEU
1	A	769	ILE
1	A	781	ARG
1	A	783	THR
1	A	787	GLU
1	A	804	THR
1	A	820	VAL
1	A	865	LYS
1	A	885	LYS
1	A	902	ARG
1	A	903	LEU
1	A	906	LEU
1	A	908	GLN

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Mol	Chain	Res	Type
1	A	911	MET
1	A	915	LEU
1	A	918	ILE
1	A	922	ASP
1	A	943	VAL
1	A	948	GLU
1	A	955	LYS
1	A	989	LEU
1	A	1004	HIS
1	A	1007	LYS
1	A	1009	LYS
1	A	1028	GLU
1	A	1042	ILE
1	A	1043	ASN
1	A	1054	VAL
1	A	1070	ASP
1	A	1071	LEU
1	A	1072	LEU
1	A	1094	SER
1	A	1163	ILE
1	A	1174	ASP
1	A	1178	GLN
1	A	1198	LEU
1	A	1206	VAL
1	A	1207	THR
1	A	1230	GLN
1	A	1270	ASN
1	A	1272	ARG
1	A	1275	VAL
1	A	1276	SER
1	A	1289	CYS
1	A	1309	VAL
1	A	1313	ARG
1	A	1336	VAL
1	A	1345	SER
1	A	1350	ASP
1	A	1354	VAL
1	A	1362	SER
1	A	1366	ARG
1	A	1394	GLU
1	A	1404	ARG
1	A	1411	ILE

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Mol	Chain	Res	Type
1	A	1412	LEU
1	A	1416	ILE
1	A	1451	ASP
1	A	1458	LEU
1	A	1478	VAL
1	A	1508	ARG
1	A	1526	SER
1	A	1528	THR
1	A	1530	THR
1	A	1537	LYS
1	A	1541	VAL
1	A	1549	VAL
1	A	1601	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	376	HIS
1	A	385	GLN
1	A	469	GLN
1	A	535	ASN
1	A	638	GLN
1	A	663	GLN
1	A	696	ASN
1	A	723	GLN
1	A	729	GLN
1	A	792	GLN
1	A	908	GLN
1	A	917	GLN
1	A	953	ASN
1	A	1039	HIS
1	A	1098	ASN
1	A	1105	HIS
1	A	1160	GLN
1	A	1296	GLN
1	A	1311	GLN
1	A	1356	ASN
1	A	1392	ASN
1	A	1407	HIS
1	A	1430	HIS
1	A	1509	HIS

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Mol	Chain	Res	Type
1	A	1543	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1140/1330 (85%)	0.74	151 (13%) 7 6	21, 59, 104, 128	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	851	GLY	5.2
1	A	688	ALA	5.0
1	A	749	TYR	4.9
1	A	956	VAL	4.8
1	A	1406	SER	4.7
1	A	639	ILE	4.6
1	A	1108	SER	4.6
1	A	690	LEU	4.5
1	A	722	HIS	4.3
1	A	489	PHE	4.2
1	A	721	LEU	4.2
1	A	689	CYS	4.2
1	A	1456	HIS	4.2
1	A	980	TYR	4.1
1	A	1612	ALA	4.1
1	A	641	LYS	4.0
1	A	409	PRO	3.9
1	A	405	TYR	3.9
1	A	376	HIS	3.8
1	A	1490	GLU	3.7
1	A	488	ALA	3.7
1	A	865	LYS	3.7
1	A	605	ARG	3.7
1	A	1609	ALA	3.6
1	A	1453	VAL	3.6
1	A	734	ILE	3.6
1	A	602	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	357	PRO	3.5
1	A	1610	VAL	3.5
1	A	748	THR	3.5
1	A	390	GLU	3.5
1	A	393	SER	3.4
1	A	776	PRO	3.4
1	A	408	SER	3.4
1	A	358	LYS	3.4
1	A	665	PRO	3.4
1	A	921	VAL	3.4
1	A	493	ILE	3.3
1	A	604	THR	3.3
1	A	1452	GLY	3.3
1	A	1004	HIS	3.3
1	A	378	GLU	3.2
1	A	1230	GLN	3.2
1	A	595	GLY	3.2
1	A	1048	SER	3.1
1	A	365	HIS	3.1
1	A	744	GLU	3.1
1	A	377	PRO	3.1
1	A	363	GLY	3.1
1	A	918	ILE	3.1
1	A	762	VAL	3.0
1	A	835	VAL	3.0
1	A	731	LYS	3.0
1	A	550	ARG	2.9
1	A	965	LYS	2.9
1	A	603	ALA	2.9
1	A	487	THR	2.8
1	A	633	THR	2.8
1	A	714	GLU	2.8
1	A	925	VAL	2.8
1	A	1408	TYR	2.8
1	A	836	LYS	2.7
1	A	1361	SER	2.7
1	A	1605	SER	2.7
1	A	989	LEU	2.7
1	A	933	ASN	2.7
1	A	379	ASP	2.7
1	A	577	ASP	2.7
1	A	743	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	769	ILE	2.7
1	A	885	LYS	2.7
1	A	693	ARG	2.7
1	A	1037	SER	2.7
1	A	747	ARG	2.6
1	A	1611	LYS	2.6
1	A	551	PHE	2.6
1	A	981	SER	2.5
1	A	915	LEU	2.5
1	A	1034	TYR	2.5
1	A	1002	GLU	2.5
1	A	547	ASN	2.5
1	A	964	LYS	2.5
1	A	1454	ILE	2.5
1	A	477	GLY	2.5
1	A	653	ARG	2.5
1	A	829	SER	2.5
1	A	1322	ALA	2.5
1	A	720	LYS	2.4
1	A	1043	ASN	2.4
1	A	448	ILE	2.4
1	A	872	TRP	2.4
1	A	1451	ASP	2.4
1	A	1015	ALA	2.4
1	A	716	PRO	2.4
1	A	834	LYS	2.4
1	A	917	GLN	2.4
1	A	777	LEU	2.4
1	A	954	ILE	2.4
1	A	479	GLU	2.4
1	A	919	GLU	2.4
1	A	1450	GLY	2.4
1	A	1025	TYR	2.3
1	A	866	THR	2.3
1	A	386	MET	2.3
1	A	435	LYS	2.3
1	A	625	LYS	2.3
1	A	789	LYS	2.3
1	A	895	LYS	2.3
1	A	729	GLN	2.3
1	A	1241	ARG	2.3
1	A	1005	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1012	VAL	2.3
1	A	1001	LYS	2.3
1	A	709	ASP	2.3
1	A	381	VAL	2.3
1	A	654	ARG	2.3
1	A	1006	GLY	2.3
1	A	391	LYS	2.2
1	A	715	MET	2.2
1	A	759	MET	2.2
1	A	366	LEU	2.2
1	A	548	VAL	2.2
1	A	635	PHE	2.2
1	A	909	LYS	2.2
1	A	955	LYS	2.2
1	A	1022	TYR	2.2
1	A	691	LYS	2.2
1	A	1003	ILE	2.2
1	A	1100	GLU	2.2
1	A	444	CYS	2.2
1	A	573	ALA	2.1
1	A	375	GLN	2.1
1	A	728	LYS	2.1
1	A	367	ASP	2.1
1	A	832	HIS	2.1
1	A	1170	ILE	2.1
1	A	1607	SER	2.1
1	A	1608	ALA	2.1
1	A	480	LYS	2.1
1	A	756	ASP	2.1
1	A	490	ALA	2.1
1	A	742	LYS	2.1
1	A	385	GLN	2.1
1	A	1606	ALA	2.1
1	A	514	ILE	2.1
1	A	914	VAL	2.1
1	A	412	ARG	2.0
1	A	572	GLU	2.0
1	A	939	LEU	2.0
1	A	1059	VAL	2.0
1	A	364	GLN	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
2	ZN	A	2001	1/1	0.98	0.07	35,35,35,35	0
2	ZN	A	2002	1/1	0.99	0.09	36,36,36,36	0
2	ZN	A	2004	1/1	1.00	0.07	32,32,32,32	0
2	ZN	A	2005	1/1	1.00	0.09	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.