



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:27 AM GMT

PDB ID : 3AV4
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

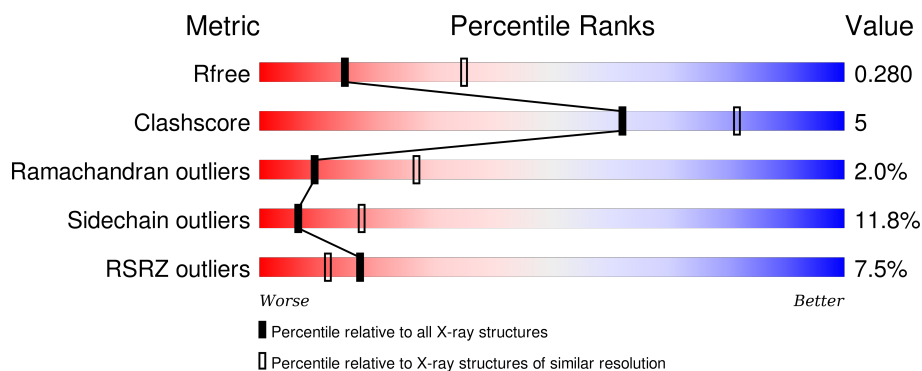
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1330	<div> <div>6%</div> <div>65%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>

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.

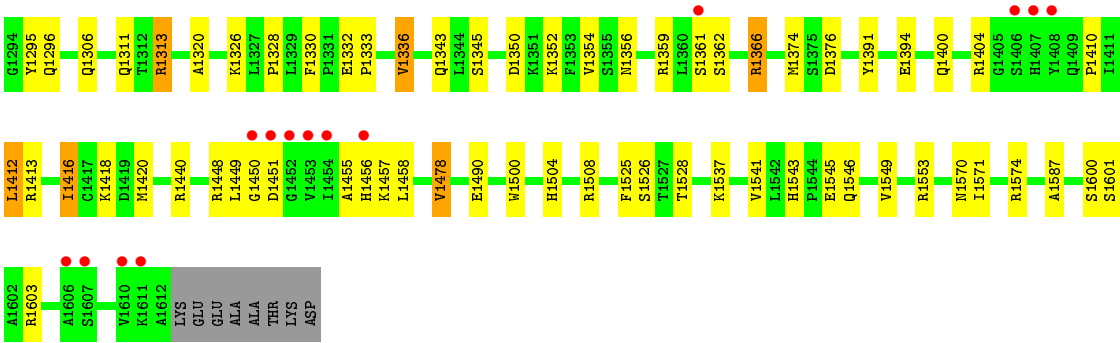
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0	0
			9110	5766	1586	1699	59			

- Molecule 2 is ZINC ION (three-letter code: 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		



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 2.8.0	Depositor
R, R_{free}	0.230 , 0.267 0.237 , 0.280	Depositor DCC
R_{free} test set	2315 reflections (5.33%)	DCC
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 , 57.7	EDS
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 45744 reflections (0.002%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/9330	0.79	3/12615 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1490	GLU	C-N-CA	5.61	135.73	121.70
1	A	1042	ILE	C-N-CA	5.20	134.69	121.70
1	A	689	CYS	C-N-CA	5.16	134.59	121.70

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	98	0
2	A	4	0	0	0	0
3	A	42	0	0	0	0
All	All	9156	0	8892	98	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 5.

All (98) 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: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: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: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: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
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:1543:HIS:HD2	1:A:1545:GLU:H	1.53	0.56
1:A:1293:MET:HE1	1:A:1295:TYR:CE1	2.40	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:1413:ARG:O	1:A:1553:ARG:HD3	2.08	0.53
1:A:535:ASN:O	1:A:539:THR:HB	2.09	0.53
1:A:1418:LYS:HE2	1:A:1420:MET:HE1	1.89	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:564:VAL:HG11	1:A:596:VAL:HG11	1.92	0.50
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.92	0.50
1:A:775:LYS:N	1:A:776:PRO:HD3	2.27	0.50
1:A:598:LEU:HB3	1:A:695:PRO:HB2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:ASN:O	1:A:1278:ARG:HA	2.12	0.50
1:A:1231:GLY:HA3	1:A:1245:LYS:HG2	1.93	0.49
1:A:836:LYS:HD2	1:A:866:THR:HG21	1.94	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: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
1:A:1456:HIS:CG	1:A:1457:LYS:N	2.83	0.46
1:A:1293:MET:HE1	1:A:1295:TYR:HE1	1.79	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:769:ILE:HD11	1:A:832:HIS:CD2	2.51	0.45
1:A:360:PRO:HD2	1:A:422:ARG:HD2	1.98	0.45
1:A:357:PRO:HB2	1:A:366:LEU:HB2	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: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:1213:ARG:H	1:A:1213:ARG:CD	2.31	0.44
1:A:483:ILE:H	1:A:483:ILE:HD12	1.83	0.44
1:A:995:TYR:OH	1:A:1359:ARG:HG2	2.17	0.43
1:A:726:LYS:HA	1:A:770:PRO:HA	2.00	0.43
1:A:879:ARG:NH2	1:A:1328:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1374:MET:HE1	1:A:1525:PHE:CZ	2.54	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: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: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:1293:MET:HE2	1:A:1293:MET:HB3	1.95	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

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	1118/1330 (84%)	1007 (90%)	89 (8%)	22 (2%)	9	27

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

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Mol	Chain	Res	Type
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
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%)	6	17

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	406	GLU
1	A	408	SER
1	A	410	MET

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Mol	Chain	Res	Type
1	A	414	THR
1	A	417	SER
1	A	421	SER
1	A	430	THR
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
1	A	539	THR
1	A	545	THR
1	A	577	ASP
1	A	581	ILE
1	A	590	LEU
1	A	600	GLN
1	A	625	LYS
1	A	629	GLN
1	A	639	ILE
1	A	653	ARG
1	A	655	ARG
1	A	658	VAL
1	A	664	GLN
1	A	692	ARG
1	A	693	ARG
1	A	697	LEU
1	A	707	GLU
1	A	721	LEU
1	A	727	LYS
1	A	728	LYS
1	A	734	ILE
1	A	739	GLN
1	A	741	MET
1	A	749	TYR
1	A	755	ILE
1	A	759	MET
1	A	760	LEU
1	A	781	ARG
1	A	792	GLN

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Mol	Chain	Res	Type
1	A	820	VAL
1	A	836	LYS
1	A	865	LYS
1	A	885	LYS
1	A	898	LEU
1	A	902	ARG
1	A	903	LEU
1	A	906	LEU
1	A	908	GLN
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	1009	LYS
1	A	1028	GLU
1	A	1042	ILE
1	A	1043	ASN
1	A	1054	VAL
1	A	1062	ARG
1	A	1070	ASP
1	A	1071	LEU
1	A	1072	LEU
1	A	1094	SER
1	A	1101	ASP
1	A	1107	ARG
1	A	1174	ASP
1	A	1178	GLN
1	A	1198	LEU
1	A	1206	VAL
1	A	1207	THR
1	A	1213	ARG
1	A	1230	GLN
1	A	1270	ASN
1	A	1272	ARG
1	A	1275	VAL
1	A	1276	SER
1	A	1279	ARG

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Mol	Chain	Res	Type
1	A	1289	CYS
1	A	1313	ARG
1	A	1326	LYS
1	A	1336	VAL
1	A	1343	GLN
1	A	1345	SER
1	A	1350	ASP
1	A	1352	LYS
1	A	1354	VAL
1	A	1362	SER
1	A	1366	ARG
1	A	1394	GLU
1	A	1404	ARG
1	A	1412	LEU
1	A	1416	ILE
1	A	1448	ARG
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	1537	LYS
1	A	1541	VAL
1	A	1549	VAL
1	A	1601	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	376	HIS
1	A	469	GLN
1	A	629	GLN
1	A	729	GLN
1	A	908	GLN
1	A	917	GLN
1	A	1098	ASN
1	A	1159	HIS
1	A	1160	GLN
1	A	1296	GLN
1	A	1311	GLN

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Mol	Chain	Res	Type
1	A	1356	ASN
1	A	1407	HIS
1	A	1430	HIS
1	A	1509	HIS
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 carbohydrates 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%)	0.45	86 (7%) 17 12	21, 59, 104, 128	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1072	LEU	6.5
1	A	1406	SER	6.4
1	A	390	GLU	5.6
1	A	489	PHE	5.2
1	A	1012	VAL	5.2
1	A	654	ARG	4.6
1	A	653	ARG	4.4
1	A	919	GLU	4.2
1	A	639	ILE	4.1
1	A	1611	LYS	4.0
1	A	1606	ALA	4.0
1	A	1408	TYR	3.9
1	A	715	MET	3.7
1	A	956	VAL	3.6
1	A	918	ILE	3.6
1	A	729	GLN	3.6
1	A	1008	LYS	3.6
1	A	1004	HIS	3.4
1	A	393	SER	3.4
1	A	436	ASN	3.3
1	A	379	ASP	3.2
1	A	573	ALA	3.2
1	A	915	LEU	3.1
1	A	749	TYR	3.1
1	A	921	VAL	3.1
1	A	1450	GLY	3.1
1	A	1610	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	409	PRO	3.1
1	A	1453	VAL	3.1
1	A	693	ARG	3.0
1	A	733	ARG	3.0
1	A	838	ILE	3.0
1	A	1009	LYS	3.0
1	A	722	HIS	2.9
1	A	1407	HIS	2.9
1	A	408	SER	2.9
1	A	453	PRO	2.9
1	A	965	LYS	2.8
1	A	954	ILE	2.8
1	A	920	GLU	2.8
1	A	924	ARG	2.8
1	A	716	PRO	2.8
1	A	923	GLY	2.8
1	A	1006	GLY	2.8
1	A	775	LYS	2.8
1	A	762	VAL	2.7
1	A	577	ASP	2.7
1	A	1451	ASP	2.7
1	A	832	HIS	2.7
1	A	1013	ASN	2.6
1	A	479	GLU	2.6
1	A	641	LYS	2.5
1	A	955	LYS	2.5
1	A	663	GLN	2.5
1	A	378	GLU	2.5
1	A	1456	HIS	2.5
1	A	1007	LYS	2.5
1	A	376	HIS	2.5
1	A	866	THR	2.5
1	A	730	ASN	2.5
1	A	769	ILE	2.5
1	A	1454	ILE	2.5
1	A	933	ASN	2.4
1	A	1002	GLU	2.4
1	A	1053	VAL	2.4
1	A	1095	LYS	2.3
1	A	1022	TYR	2.3
1	A	731	LYS	2.3
1	A	1241	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	547	ASN	2.2
1	A	691	LYS	2.2
1	A	1607	SER	2.2
1	A	387	LEU	2.2
1	A	835	VAL	2.2
1	A	1005	CYS	2.1
1	A	405	TYR	2.1
1	A	980	TYR	2.1
1	A	634	PHE	2.1
1	A	1452	GLY	2.1
1	A	890	GLU	2.1
1	A	1361	SER	2.1
1	A	493	ILE	2.0
1	A	365	HIS	2.0
1	A	719	LYS	2.0
1	A	815	LEU	2.0
1	A	637	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	2001	1/1	0.98	0.06	-2.28	35,35,35,35	0
2	ZN	A	2002	1/1	0.98	0.03	-3.26	36,36,36,36	0
2	ZN	A	2004	1/1	0.99	0.03	-	32,32,32,32	0
2	ZN	A	2005	1/1	0.99	0.05	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.