



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 02:28 PM EST

PDB ID : 3PT9
Title : Crystal structure of mouse DNMT1(731-1602) in the free state
Authors : Song, J.; Patel, D.J.
Deposited on : 2010-12-02
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
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

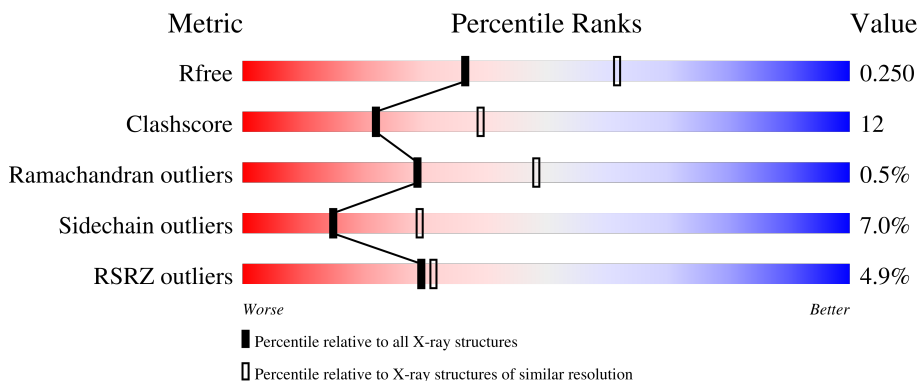
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	873	 5% 71% 21% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6827 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.

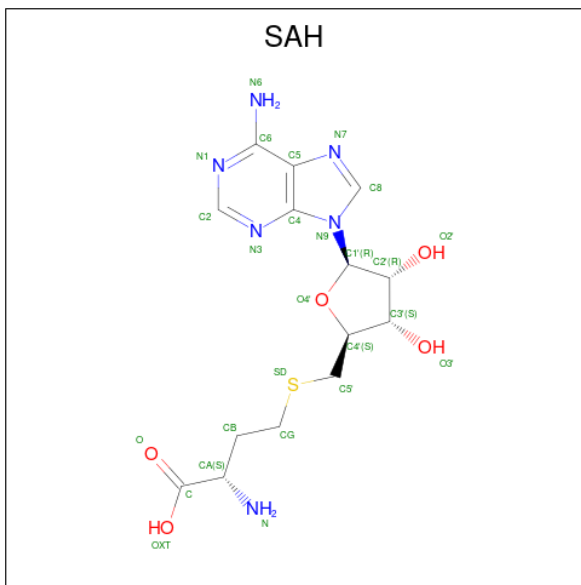
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	824	6472	4112	1130	1189	41	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	expression tag	UNP P13864

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

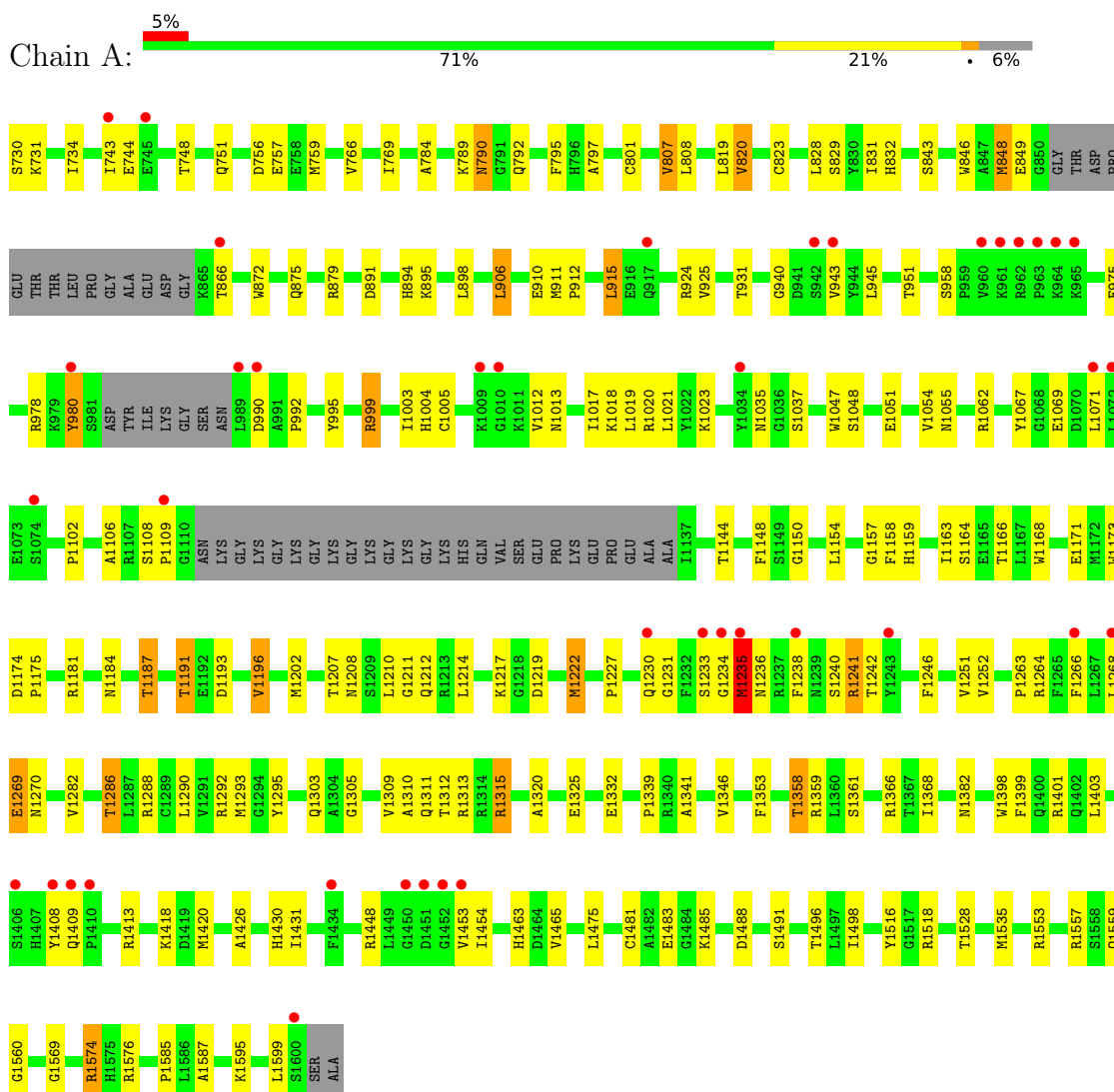
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	327	Total 327	O 327	0	0

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 21	Depositor
Cell constants a, b, c, α , β , γ	75.57Å 79.69Å 162.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.88-2.50) 99.2 (29.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.196 , 0.256 0.193 , 0.250	Depositor DCC
R_{free} test set	1737 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.555	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6827	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: SAH, 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	0.29	0/6644	0.47	0/9024

There are no bond length outliers.

There are no bond angle outliers.

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	6472	0	6159	149	0
2	A	26	0	19	1	0
3	A	2	0	0	0	0
4	A	327	0	0	19	0
All	All	6827	0	6178	149	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 12.

All (149) 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:1315:ARG:HH11	1:A:1315:ARG:HG2	1.17	1.03
1:A:1303:GLN:HE22	1:A:1313:ARG:H	1.11	0.93
1:A:1181:ARG:HH22	1:A:1191:THR:HG22	1.34	0.92
1:A:1303:GLN:HE21	1:A:1305:GLY:H	1.18	0.89
1:A:1315:ARG:HG2	1:A:1315:ARG:NH1	1.88	0.85
1:A:801:CYS:HB2	1:A:820:VAL:HG21	1.60	0.83
1:A:1207:THR:HG22	1:A:1208:ASN:O	1.77	0.83
1:A:1311:GLN:HE22	1:A:1313:ARG:HH11	1.26	0.83
1:A:924:ARG:HD2	1:A:1004:HIS:HD2	1.44	0.83
1:A:1184:ASN:HB3	1:A:1187:THR:HG23	1.62	0.81
1:A:1067:TYR:CE2	1:A:1102:PRO:HG2	2.15	0.81
1:A:866:THR:HA	4:A:46:HOH:O	1.79	0.80
1:A:1159:HIS:HD2	4:A:111:HOH:O	1.68	0.77
1:A:1290:LEU:HA	1:A:1293:MET:HE3	1.68	0.76
1:A:1181:ARG:HH22	1:A:1191:THR:CG2	1.99	0.75
1:A:1418:LYS:HE2	1:A:1420:MET:HE1	1.67	0.75
1:A:743:ILE:HG23	1:A:748:THR:HG22	1.69	0.74
1:A:1184:ASN:HB3	1:A:1187:THR:CG2	2.16	0.74
1:A:1303:GLN:NE2	1:A:1313:ARG:H	1.87	0.72
1:A:1418:LYS:HE2	1:A:1420:MET:CE	2.19	0.71
1:A:1576:ARG:HD2	4:A:286:HOH:O	1.89	0.71
1:A:1496:THR:HG22	4:A:28:HOH:O	1.90	0.71
1:A:801:CYS:HB2	1:A:820:VAL:CG2	2.21	0.71
1:A:1019:LEU:HB2	4:A:313:HOH:O	1.91	0.70
1:A:924:ARG:HD2	1:A:1004:HIS:CD2	2.26	0.70
1:A:945:LEU:HD21	1:A:1054:VAL:HG11	1.74	0.69
1:A:1496:THR:HG23	1:A:1498:ILE:O	1.93	0.68
1:A:915:LEU:HD21	1:A:931:THR:HB	1.76	0.67
1:A:1108:SER:HB3	1:A:1109:PRO:HD2	1.77	0.67
1:A:1181:ARG:NH2	1:A:1191:THR:HG22	2.09	0.66
1:A:1560:GLY:HA3	1:A:1585:PRO:CD	2.26	0.66
1:A:766:VAL:HG13	1:A:831:ILE:HG23	1.78	0.65
1:A:1191:THR:HG21	4:A:61:HOH:O	1.96	0.65
1:A:1312:THR:HG23	1:A:1341:ALA:HB1	1.77	0.65
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.80	0.64
1:A:1159:HIS:HE1	1:A:1166:THR:H	1.45	0.63
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.97	0.63
1:A:1311:GLN:NE2	1:A:1313:ARG:HH11	1.96	0.63
1:A:1054:VAL:HB	4:A:313:HOH:O	1.98	0.63
1:A:1037:SER:HB2	4:A:202:HOH:O	1.98	0.63
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.79	0.63
1:A:1023:LYS:O	1:A:1048:SER:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:ARG:HA	1:A:1454:ILE:HD13	1.81	0.63
1:A:1516:TYR:CE2	1:A:1535:MET:HG3	2.34	0.62
1:A:1005:CYS:HB3	1:A:1017:ILE:HA	1.81	0.62
1:A:1516:TYR:HE2	1:A:1535:MET:HG3	1.64	0.61
1:A:1413:ARG:O	1:A:1553:ARG:HD2	2.01	0.61
1:A:1332:GLU:HG3	1:A:1359:ARG:HD2	1.84	0.60
1:A:1150:GLY:HA3	2:A:1603:SAH:HB1	1.83	0.60
1:A:790:ASN:HD21	1:A:792:GLN:HB2	1.67	0.59
1:A:1303:GLN:HE22	1:A:1313:ARG:N	1.93	0.59
1:A:1315:ARG:HD2	4:A:20:HOH:O	2.03	0.58
1:A:1382:ASN:HD21	1:A:1420:MET:H	1.51	0.58
1:A:1311:GLN:NE2	1:A:1528:THR:H	2.01	0.58
1:A:1207:THR:CG2	1:A:1208:ASN:O	2.50	0.57
1:A:1303:GLN:NE2	1:A:1305:GLY:H	1.97	0.57
1:A:1418:LYS:HB2	1:A:1420:MET:CE	2.33	0.57
1:A:848:MET:HA	1:A:1217:LYS:HE2	1.87	0.57
1:A:1067:TYR:CE1	1:A:1069:GLU:HB2	2.40	0.56
1:A:846:TRP:HH2	1:A:1295:TYR:CZ	2.24	0.56
1:A:1488:ASP:HB3	1:A:1491:SER:OG	2.07	0.55
1:A:1560:GLY:HA3	1:A:1585:PRO:HD3	1.90	0.54
1:A:1003:ILE:HG12	1:A:1019:LEU:HD22	1.90	0.54
1:A:795:PHE:CD2	1:A:828:LEU:HD23	2.43	0.54
1:A:731:LYS:HB3	1:A:734:ILE:HD11	1.89	0.53
1:A:769:ILE:HD11	1:A:832:HIS:CE1	2.43	0.53
1:A:790:ASN:ND2	1:A:792:GLN:H	2.07	0.53
1:A:1184:ASN:CB	1:A:1187:THR:HG23	2.35	0.52
1:A:730:SER:O	1:A:731:LYS:HD2	2.09	0.52
1:A:1311:GLN:HE22	1:A:1313:ARG:NH1	2.02	0.52
1:A:1282:VAL:O	1:A:1286:THR:HG23	2.09	0.52
1:A:1332:GLU:OE2	1:A:1358:THR:N	2.30	0.52
1:A:1403:LEU:HD23	1:A:1557:ARG:HD3	1.93	0.51
1:A:980:TYR:HA	4:A:269:HOH:O	2.10	0.51
1:A:1269:GLU:OE2	1:A:1315:ARG:HD3	2.11	0.51
1:A:819:LEU:HA	4:A:6:HOH:O	2.11	0.51
1:A:1021:LEU:O	1:A:1051:GLU:HA	2.12	0.50
1:A:1207:THR:HG21	1:A:1211:GLY:HA2	1.93	0.50
1:A:1315:ARG:HH11	1:A:1315:ARG:CG	2.01	0.50
1:A:795:PHE:HB3	1:A:828:LEU:HD21	1.95	0.49
1:A:1268:LEU:C	1:A:1268:LEU:HD23	2.32	0.49
1:A:731:LYS:HB2	1:A:829:SER:HA	1.95	0.49
1:A:1018:LYS:HE2	1:A:1055:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:PRO:HD3	1:A:1339:PRO:HD3	1.95	0.49
1:A:1067:TYR:HE2	1:A:1102:PRO:HG2	1.75	0.49
1:A:1148:PHE:CE2	1:A:1227:PRO:HB3	2.48	0.49
1:A:1158:PHE:HB3	1:A:1164:SER:OG	2.13	0.49
1:A:1163:ILE:CG2	1:A:1595:LYS:HB2	2.43	0.48
1:A:945:LEU:CD2	1:A:1054:VAL:HG11	2.41	0.48
1:A:1366:ARG:NE	4:A:270:HOH:O	2.39	0.48
1:A:1418:LYS:CB	1:A:1420:MET:CE	2.92	0.48
1:A:843:SER:HB3	1:A:849:GLU:OE1	2.13	0.48
1:A:1241:ARG:HG2	1:A:1242:THR:N	2.28	0.47
1:A:1263:PRO:HD2	1:A:1295:TYR:OH	2.14	0.47
1:A:1288:ARG:HE	1:A:1292:ARG:HH21	1.60	0.47
1:A:766:VAL:HG11	1:A:831:ILE:HG12	1.96	0.47
1:A:915:LEU:CD2	1:A:931:THR:HB	2.44	0.47
1:A:1174:ASP:HB3	1:A:1175:PRO:HD3	1.97	0.46
1:A:759:MET:HE3	4:A:259:HOH:O	2.14	0.46
1:A:1398:TRP:HA	1:A:1401:ARG:NH1	2.29	0.46
1:A:1399:PHE:CE2	1:A:1403:LEU:HD22	2.51	0.46
1:A:1413:ARG:O	1:A:1553:ARG:CD	2.64	0.46
1:A:797:ALA:O	1:A:823:CYS:HA	2.15	0.45
1:A:1465:VAL:HG23	1:A:1483:GLU:HA	1.98	0.45
1:A:1047:TRP:CG	1:A:1048:SER:N	2.84	0.45
1:A:906:LEU:HA	1:A:906:LEU:HD13	1.73	0.45
1:A:790:ASN:C	1:A:790:ASN:HD22	2.20	0.45
1:A:879:ARG:HD2	4:A:19:HOH:O	2.17	0.45
1:A:1418:LYS:HE2	1:A:1420:MET:HE3	1.97	0.45
1:A:1426:ALA:O	1:A:1430:HIS:HD2	2.00	0.45
1:A:1171:GLU:O	1:A:1191:THR:HA	2.17	0.44
1:A:1233:SER:O	1:A:1235:MET:HG2	2.17	0.44
1:A:1264:ARG:HD2	1:A:1325:GLU:OE1	2.16	0.44
1:A:1018:LYS:HE2	1:A:1055:ASN:ND2	2.32	0.44
1:A:1246:PHE:O	1:A:1252:VAL:HG21	2.18	0.43
1:A:807:VAL:HG13	1:A:1353:PHE:CE2	2.53	0.43
1:A:1108:SER:HB3	1:A:1109:PRO:CD	2.43	0.43
1:A:1154:LEU:HB3	4:A:24:HOH:O	2.18	0.43
1:A:819:LEU:HB2	1:A:872:TRP:HA	2.01	0.43
1:A:925:VAL:O	1:A:1004:HIS:HA	2.19	0.43
1:A:1071:LEU:HD23	1:A:1071:LEU:HA	1.81	0.43
1:A:1208:ASN:OD1	1:A:1212:GLN:HB2	2.18	0.43
1:A:790:ASN:ND2	1:A:790:ASN:C	2.72	0.43
1:A:1310:ALA:HB2	1:A:1368:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:ARG:NE	1:A:1292:ARG:HH21	2.17	0.42
1:A:1481:CYS:HA	1:A:1485:LYS:O	2.20	0.42
1:A:784:ALA:HB2	1:A:895:LYS:HA	1.99	0.42
1:A:1282:VAL:O	1:A:1286:THR:CG2	2.67	0.42
1:A:1418:LYS:HB2	1:A:1420:MET:HE2	2.01	0.42
1:A:911:MET:HA	1:A:912:PRO:HD3	1.87	0.42
1:A:995:TYR:OH	1:A:1359:ARG:HG2	2.19	0.42
1:A:1431:ILE:HG22	1:A:1518:ARG:HE	1.85	0.41
1:A:1569:GLY:O	1:A:1574:ARG:NH1	2.51	0.41
1:A:1144:THR:HG23	1:A:1222:MET:HG2	2.03	0.41
1:A:756:ASP:O	1:A:757:GLU:HB2	2.20	0.41
1:A:789:LYS:HG2	4:A:167:HOH:O	2.19	0.41
1:A:1144:THR:HB	1:A:1166:THR:HA	2.03	0.41
1:A:1193:ASP:HB3	1:A:1196:VAL:HG13	2.01	0.41
1:A:1217:LYS:HE3	4:A:302:HOH:O	2.20	0.41
1:A:891:ASP:O	1:A:894:HIS:HE1	2.04	0.41
1:A:940:GLY:O	1:A:999:ARG:HD2	2.20	0.41
1:A:1168:TRP:CH2	1:A:1219:ASP:HB3	2.56	0.41
1:A:1217:LYS:CE	4:A:302:HOH:O	2.69	0.41
1:A:1557:ARG:O	1:A:1559:GLN:O	2.38	0.41
1:A:1173:TRP:CD1	1:A:1175:PRO:HD2	2.56	0.40
1:A:1463:HIS:HD2	4:A:256:HOH:O	2.04	0.40
1:A:999:ARG:NH2	1:A:1106:ALA:O	2.54	0.40
1:A:891:ASP:O	1:A:894:HIS:CE1	2.75	0.40
1:A:1234:GLY:O	1:A:1236:ASN:N	2.47	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	816/873 (94%)	772 (95%)	40 (5%)	4 (0%)	29 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	980	TYR
1	A	1235	MET
1	A	1231	GLY
1	A	1453	VAL

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	682/759 (90%)	634 (93%)	48 (7%)	15 29

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	GLU
1	A	751	GLN
1	A	790	ASN
1	A	807	VAL
1	A	808	LEU
1	A	820	VAL
1	A	848	MET
1	A	875	GLN
1	A	898	LEU
1	A	906	LEU
1	A	910	GLU
1	A	915	LEU
1	A	943	VAL
1	A	951	THR
1	A	958	SER
1	A	990	ASP
1	A	999	ARG
1	A	1012	VAL
1	A	1013	ASN
1	A	1020	ARG
1	A	1035	ASN

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Mol	Chain	Res	Type
1	A	1062	ARG
1	A	1187	THR
1	A	1191	THR
1	A	1196	VAL
1	A	1202	MET
1	A	1210	LEU
1	A	1214	LEU
1	A	1222	MET
1	A	1230	GLN
1	A	1235	MET
1	A	1238	PHE
1	A	1240	SER
1	A	1241	ARG
1	A	1251	VAL
1	A	1269	GLU
1	A	1270	ASN
1	A	1286	THR
1	A	1309	VAL
1	A	1315	ARG
1	A	1346	VAL
1	A	1358	THR
1	A	1361	SER
1	A	1408	TYR
1	A	1409	GLN
1	A	1475	LEU
1	A	1574	ARG
1	A	1599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	790	ASN
1	A	870	GLN
1	A	875	GLN
1	A	894	HIS
1	A	1004	HIS
1	A	1013	ASN
1	A	1055	ASN
1	A	1159	HIS
1	A	1184	ASN
1	A	1216	GLN
1	A	1303	GLN

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Mol	Chain	Res	Type
1	A	1311	GLN
1	A	1343	GLN
1	A	1382	ASN
1	A	1430	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	A	1603	-	24,28,28	1.18	3 (12%)	25,40,40	1.54	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	1603	-	-	3/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1603	SAH	C2-N3	3.59	1.37	1.32
2	A	1603	SAH	C2-N1	2.56	1.38	1.33
2	A	1603	SAH	OXT-C	-2.02	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1603	SAH	N3-C2-N1	-5.12	120.68	128.68
2	A	1603	SAH	OXT-C-O	-2.48	118.46	124.09
2	A	1603	SAH	C5'-SD-CG	-2.10	95.95	102.27
2	A	1603	SAH	OXT-C-CA	2.04	120.34	113.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

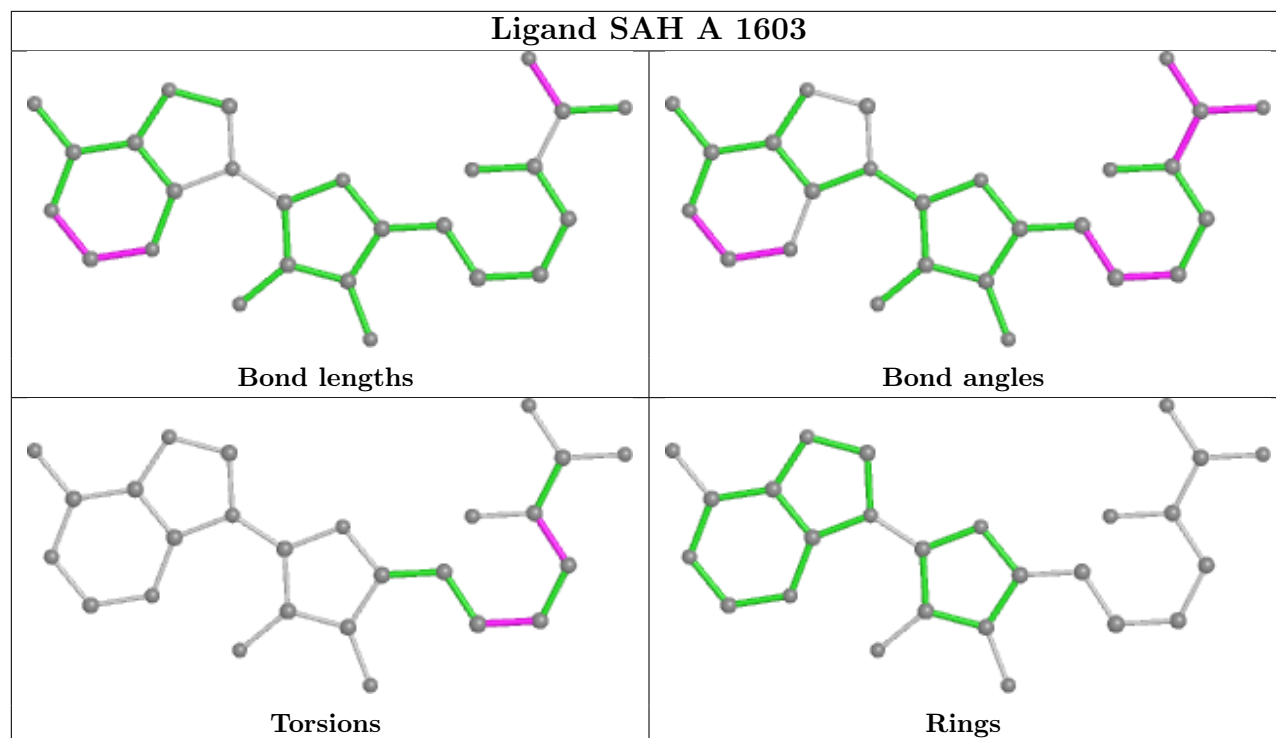
Mol	Chain	Res	Type	Atoms
2	A	1603	SAH	N-CA-CB-CG
2	A	1603	SAH	CB-CG-SD-C5'
2	A	1603	SAH	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1603	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	824/873 (94%)	0.09	40 (4%) 29 31	21, 34, 57, 104	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	964	LYS	5.5
1	A	963	PRO	5.4
1	A	989	LEU	5.4
1	A	1238	PHE	5.1
1	A	1451	ASP	5.0
1	A	1109	PRO	4.6
1	A	1450	GLY	4.2
1	A	866	THR	4.1
1	A	980	TYR	4.1
1	A	990	ASP	3.9
1	A	1408	TYR	3.5
1	A	962	ARG	3.5
1	A	1600	SER	3.5
1	A	961	LYS	3.4
1	A	965	LYS	3.2
1	A	1233	SER	3.1
1	A	1072	LEU	3.1
1	A	1452	GLY	3.0
1	A	1034	TYR	2.9
1	A	1410	PRO	2.9
1	A	1243	TYR	2.9
1	A	1453	VAL	2.9
1	A	1409	GLN	2.8
1	A	1434	PHE	2.7
1	A	1266	PHE	2.6
1	A	1010	GLY	2.5
1	A	1406	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1235	MET	2.5
1	A	745	GLU	2.5
1	A	1268	LEU	2.4
1	A	1071	LEU	2.4
1	A	1009	LYS	2.3
1	A	1074	SER	2.3
1	A	942	SER	2.2
1	A	1230	GLN	2.2
1	A	1234	GLY	2.2
1	A	960	VAL	2.2
1	A	743	ILE	2.1
1	A	917	GLN	2.1
1	A	943	VAL	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](#)

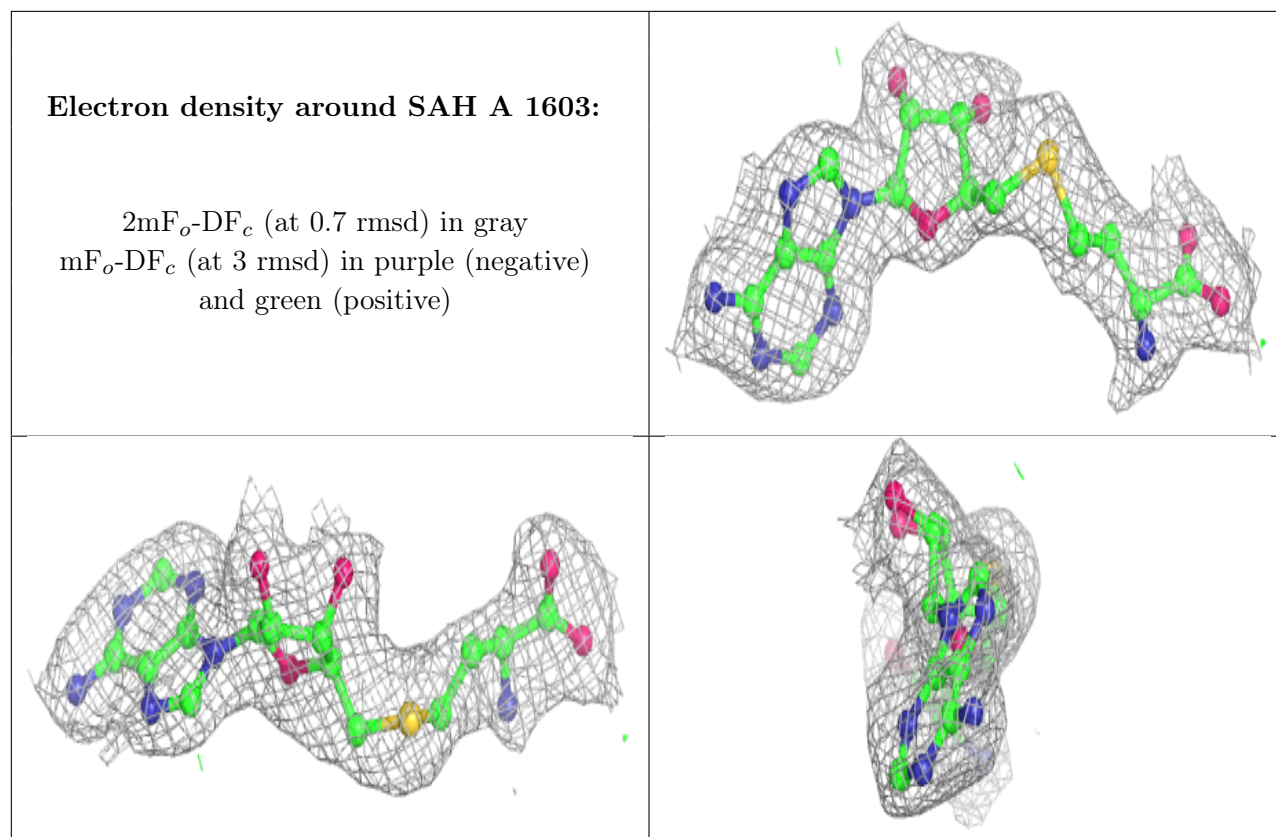
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
2	SAH	A	1603	26/26	0.96	0.15	20,24,25,28	0
3	ZN	A	1	1/1	0.98	0.04	48,48,48,48	0
3	ZN	A	2	1/1	0.99	0.04	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.