



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:16 pm BST

PDB ID : 4U7P  
Title : Crystal structure of DNMT3A-DNMT3L complex  
Authors : Wang, L.; Guo, X.; Li, J.; Xiao, J.; Yin, X.; He, S.; Wang, J.; Xu, Y.  
Deposited on : 2014-07-31  
Resolution : 3.82 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](mailto: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.

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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 : 2.11  
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) : 2.11

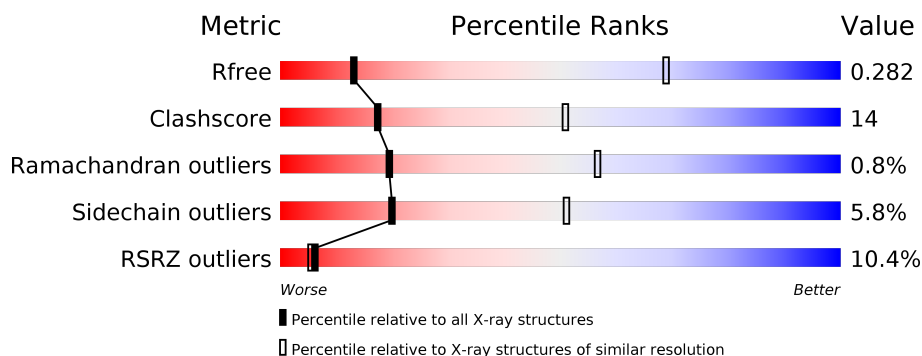
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.82 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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  $\geq 3$ , 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	466	
2	B	209	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5072 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 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3422	2166	609	612	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y6K1
A	448	PRO	-	expression tag	UNP Q9Y6K1
A	449	LEU	-	expression tag	UNP Q9Y6K1
A	450	GLY	-	expression tag	UNP Q9Y6K1
A	451	SER	-	expression tag	UNP Q9Y6K1
A	452	PRO	-	expression tag	UNP Q9Y6K1
A	453	GLU	-	expression tag	UNP Q9Y6K1
A	454	PHE	-	expression tag	UNP Q9Y6K1

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1621	1055	277	285	4			

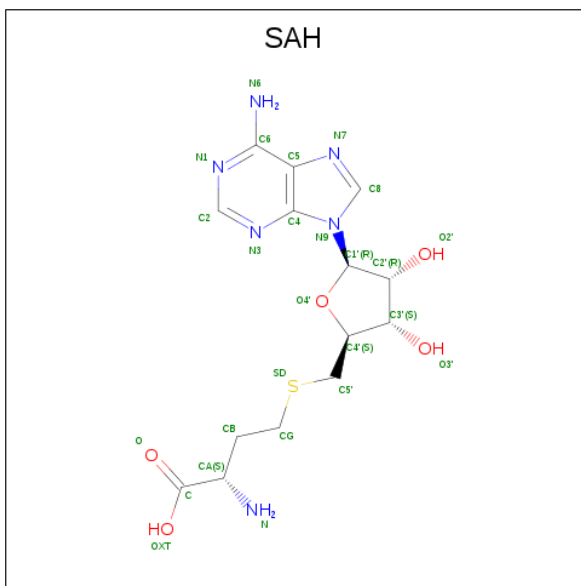
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP Q9UJW3
B	172	PRO	-	expression tag	UNP Q9UJW3
B	173	LEU	-	expression tag	UNP Q9UJW3
B	174	GLY	-	expression tag	UNP Q9UJW3
B	175	SER	-	expression tag	UNP Q9UJW3
B	176	GLU	-	expression tag	UNP Q9UJW3
B	177	PHE	-	expression tag	UNP Q9UJW3

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

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

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).

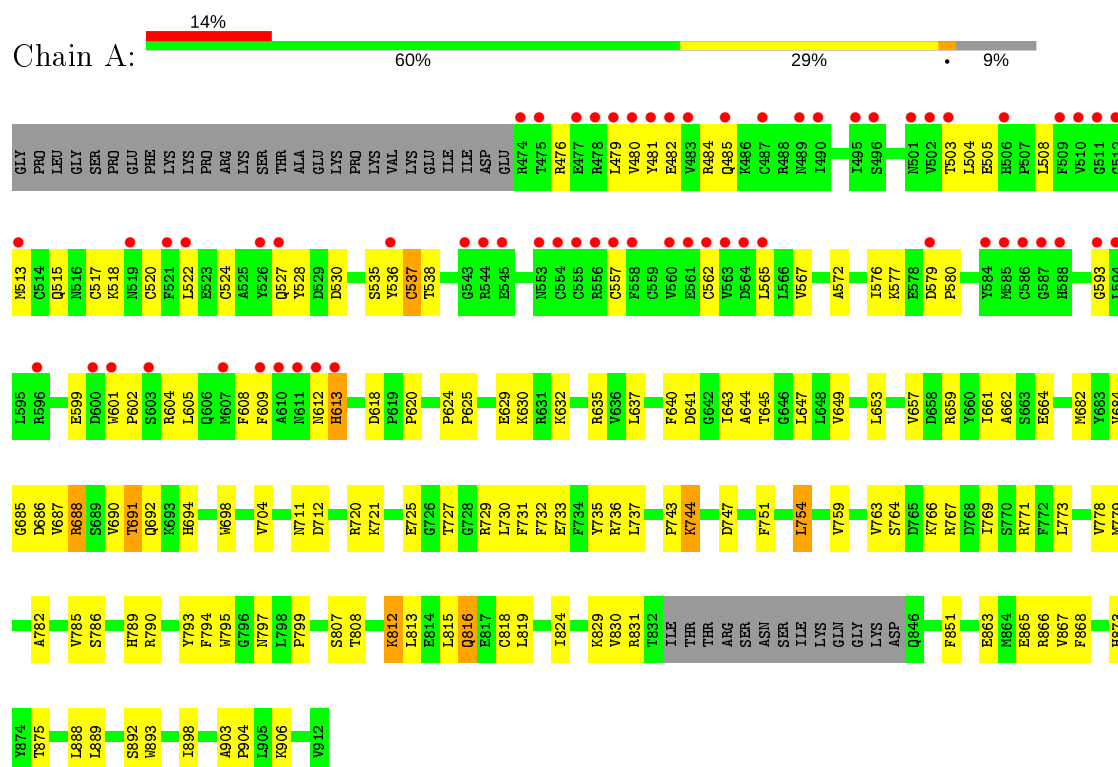


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

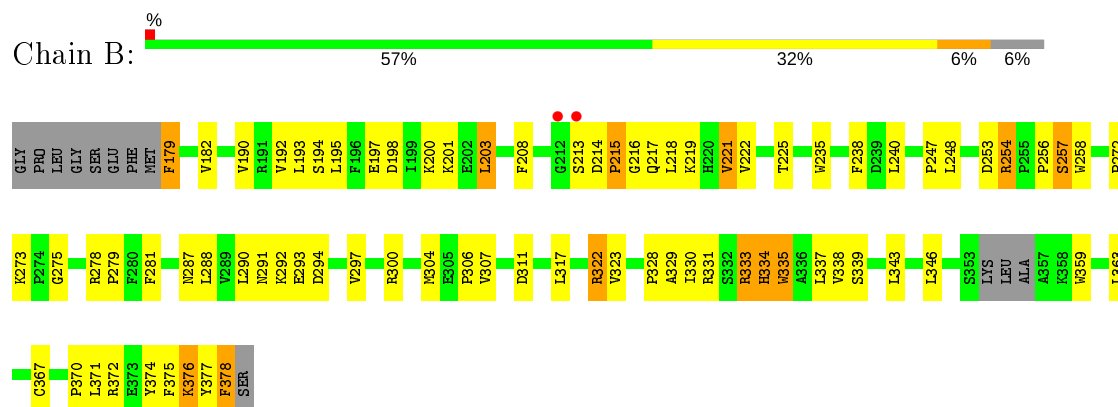
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 3A



#### • Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	252.03 Å   252.03 Å   75.34 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	42.01 – 3.82 42.01 – 3.82	Depositor EDS
% Data completeness (in resolution range)	79.2 (42.01-3.82) 98.7 (42.01-3.82)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 3.88 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.224   ,   0.269 0.246   ,   0.282	Depositor DCC
$R_{free}$ test set	1392 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SAH

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	0.31	0/3505	0.49	0/4736
2	B	0.31	0/1673	0.51	0/2278
All	All	0.31	0/5178	0.50	0/7014

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

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	3422	0	3337	86	0
2	B	1621	0	1599	54	0
3	A	3	0	0	0	0
4	A	26	0	19	1	0
All	All	5072	0	4955	138	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 14.

All (138) 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)
2:B:376:LYS:NZ	2:B:378:PHE:O	2.13	0.81
1:A:733:GLU:OE2	1:A:736:ARG:NH1	2.19	0.76
1:A:524:CYS:HA	1:A:527:GLN:HB2	1.66	0.76
1:A:528:TYR:O	1:A:535:SER:OG	2.04	0.75
1:A:637:LEU:HB3	1:A:704:VAL:HG22	1.69	0.75
1:A:643:ILE:HD11	1:A:888:LEU:HB3	1.70	0.74
1:A:790:ARG:NH2	1:A:892:SER:O	2.21	0.74
2:B:198:ASP:O	2:B:201:LYS:NZ	2.21	0.73
1:A:690:VAL:O	1:A:736:ARG:NH2	2.25	0.69
1:A:711:ASN:HB3	1:A:727:THR:HG21	1.77	0.67
1:A:744:LYS:H	1:A:744:LYS:HD3	1.62	0.65
1:A:712:ASP:HB3	1:A:721:LYS:H	1.63	0.63
2:B:333:ARG:O	2:B:335:TRP:N	2.33	0.62
1:A:505:GLU:OE1	1:A:604:ARG:NH2	2.32	0.62
1:A:484:ARG:NH2	1:A:565:LEU:O	2.31	0.61
2:B:213:SER:H	2:B:214:ASP:HA	1.66	0.59
1:A:476:ARG:NH2	1:A:562:CYS:SG	2.70	0.59
1:A:721:LYS:HB3	1:A:725:GLU:HB2	1.85	0.58
2:B:287:ASN:HB2	2:B:359:TRP:CZ3	2.39	0.58
1:A:536:TYR:HB3	1:A:537:CYS:CA	2.34	0.58
1:A:527:GLN:HG2	1:A:763:VAL:HB	1.85	0.58
1:A:813:LEU:O	1:A:829:LYS:NZ	2.36	0.58
1:A:875:THR:HG21	1:A:889:LEU:HD11	1.85	0.58
1:A:865:GLU:OE2	1:A:873:HIS:N	2.34	0.57
2:B:273:LYS:HG2	2:B:275:GLY:H	1.69	0.57
1:A:732:PHE:HA	1:A:735:TYR:HB3	1.87	0.57
1:A:686:ASP:HB3	1:A:688:ARG:HD3	1.86	0.57
1:A:645:THR:HG21	1:A:893:TRP:HB2	1.87	0.56
1:A:536:TYR:HB3	1:A:537:CYS:C	2.26	0.56
1:A:576:ILE:HG22	1:A:577:LYS:H	1.68	0.56
2:B:307:VAL:HG21	2:B:330:ILE:HG13	1.87	0.56
2:B:328:PRO:HG2	2:B:370:PRO:HB2	1.87	0.56
2:B:219:LYS:HE2	2:B:235:TRP:CE2	2.42	0.55
2:B:213:SER:HB3	2:B:214:ASP:C	2.27	0.55
1:A:649:VAL:HG21	1:A:898:ILE:HB	1.89	0.54
1:A:789:HIS:O	1:A:789:HIS:ND1	2.39	0.54
1:A:618:ASP:O	1:A:620:PRO:HD3	2.08	0.54
1:A:612:ASN:O	1:A:613:HIS:ND1	2.41	0.54
1:A:733:GLU:OE1	2:B:300:ARG:NH1	2.41	0.53
1:A:522:LEU:HD22	1:A:612:ASN:HB2	1.91	0.53
1:A:643:ILE:O	1:A:645:THR:N	2.41	0.52
2:B:272:PRO:HB3	2:B:278:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:GLU:HG2	1:A:889:LEU:HD21	1.92	0.52
2:B:293:GLU:O	2:B:297:VAL:HG23	2.10	0.52
2:B:182:VAL:HB	2:B:374:TYR:HA	1.92	0.51
1:A:812:LYS:HD2	1:A:812:LYS:O	2.11	0.51
1:A:503:THR:HG21	1:A:515:GLN:HG2	1.93	0.51
1:A:729:ARG:HH12	2:B:257:SER:HB3	1.76	0.50
1:A:480:VAL:HG11	1:A:565:LEU:HG	1.92	0.50
1:A:536:TYR:HB3	1:A:537:CYS:HA	1.93	0.50
1:A:684:VAL:HG21	1:A:698:TRP:CH2	2.46	0.50
1:A:782:ALA:HB1	1:A:786:SER:HB3	1.93	0.50
2:B:339:SER:O	2:B:343:LEU:N	2.37	0.50
1:A:785:VAL:HG23	1:A:807:SER:HA	1.93	0.49
1:A:572:ALA:O	1:A:576:ILE:HG13	2.12	0.49
1:A:816:GLN:OE1	1:A:824:ILE:HA	2.11	0.49
1:A:764:SER:HB3	1:A:767:ARG:HH21	1.78	0.49
2:B:304:MET:HE3	2:B:331:ARG:HE	1.78	0.49
2:B:208:PHE:CZ	2:B:372:ARG:HG2	2.48	0.49
1:A:508:LEU:HD21	1:A:605:LEU:HD11	1.95	0.48
2:B:213:SER:HB3	2:B:215:PRO:N	2.27	0.48
2:B:193:LEU:HB2	2:B:238:PHE:CD1	2.48	0.48
1:A:831:ARG:O	1:A:831:ARG:NH2	2.46	0.48
2:B:192:VAL:HG13	2:B:240:LEU:HB3	1.96	0.47
2:B:311:ASP:HB2	2:B:363:LEU:HD21	1.96	0.47
2:B:337:LEU:HD12	2:B:337:LEU:H	1.80	0.47
1:A:818:CYS:O	1:A:866:ARG:HD2	2.14	0.47
2:B:200:LYS:HB2	2:B:218:LEU:HD22	1.96	0.47
2:B:214:ASP:OD2	2:B:217:GLN:N	2.45	0.47
1:A:751:PHE:O	1:A:797:ASN:ND2	2.39	0.47
2:B:214:ASP:C	2:B:216:GLY:HA2	2.35	0.47
1:A:530:ASP:HB2	1:A:535:SER:HB3	1.96	0.46
1:A:731:PHE:HE1	1:A:773:LEU:HD11	1.80	0.46
1:A:536:TYR:HB3	1:A:538:THR:N	2.30	0.46
1:A:567:VAL:HG13	1:A:593:GLY:HA3	1.98	0.46
1:A:605:LEU:HD22	1:A:609:PHE:HE1	1.81	0.46
2:B:253:ASP:HB3	2:B:254:ARG:HD2	1.96	0.46
1:A:522:LEU:HB3	1:A:612:ASN:ND2	2.31	0.46
1:A:481:TYR:O	1:A:485:GLN:HG2	2.16	0.45
2:B:330:ILE:HD12	2:B:330:ILE:HA	1.79	0.45
2:B:367:CYS:O	2:B:370:PRO:HD2	2.16	0.45
1:A:640:PHE:CZ	1:A:730:LEU:HB3	2.52	0.45
2:B:247:PRO:HG3	2:B:359:TRP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HB2	2:B:322:ARG:HB2	1.97	0.45
1:A:664:GLU:OE2	4:A:1004:SAH:O2'	2.22	0.45
2:B:219:LYS:HE3	2:B:221:VAL:HG13	1.98	0.45
2:B:333:ARG:C	2:B:335:TRP:H	2.19	0.45
1:A:624:PRO:HA	1:A:625:PRO:HD3	1.78	0.45
2:B:254:ARG:HG3	2:B:258:TRP:CE3	2.52	0.44
2:B:329:ALA:HB3	2:B:370:PRO:HG3	1.99	0.44
1:A:731:PHE:CE1	1:A:769:ILE:HG23	2.52	0.44
1:A:517:CYS:HA	1:A:520:CYS:HB2	2.00	0.44
1:A:579:ASP:HB3	1:A:580:PRO:HD3	2.00	0.44
2:B:317:LEU:HD21	2:B:343:LEU:HD12	1.99	0.44
1:A:799:PRO:HB2	1:A:904:PRO:HG2	2.00	0.44
2:B:195:LEU:C	2:B:197:GLU:H	2.20	0.44
2:B:214:ASP:O	2:B:216:GLY:HA2	2.17	0.44
2:B:291:ASN:N	2:B:294:ASP:HB2	2.32	0.44
1:A:635:ARG:HD2	1:A:659:ARG:NH2	2.33	0.44
2:B:240:LEU:HA	2:B:281:PHE:O	2.18	0.44
2:B:333:ARG:HB2	2:B:334:HIS:H	1.72	0.44
2:B:214:ASP:HA	2:B:215:PRO:HD3	1.68	0.43
1:A:661:ILE:HG12	1:A:682:MET:HB3	2.00	0.43
1:A:686:ASP:HB3	1:A:688:ARG:H	1.83	0.43
1:A:518:LYS:HA	1:A:608:PHE:HZ	1.83	0.43
1:A:790:ARG:CZ	1:A:868:PHE:HE2	2.32	0.43
1:A:712:ASP:HA	1:A:720:ARG:HA	2.00	0.43
1:A:778:VAL:HG23	1:A:794:PHE:HB2	2.01	0.43
2:B:307:VAL:HG23	2:B:323:VAL:HB	2.00	0.43
1:A:754:LEU:HD23	1:A:795:TRP:O	2.19	0.43
1:A:630:LYS:HD2	1:A:632:LYS:HZ1	1.84	0.42
1:A:641:ASP:HB2	1:A:662:ALA:HB1	2.01	0.42
1:A:691:THR:HG23	1:A:694:HIS:ND1	2.34	0.42
1:A:711:ASN:HB3	1:A:727:THR:CG2	2.48	0.42
1:A:759:VAL:HA	1:A:793:TYR:CD2	2.54	0.42
1:A:601:TRP:CG	1:A:602:PRO:HD3	2.54	0.42
1:A:647:LEU:HD11	1:A:657:VAL:HG11	2.01	0.42
1:A:903:ALA:HB3	1:A:904:PRO:HD3	2.02	0.42
2:B:307:VAL:HG11	2:B:331:ARG:HA	2.02	0.42
1:A:759:VAL:HG11	1:A:779:MET:HG3	2.02	0.42
2:B:190:VAL:HB	2:B:375:PHE:CG	2.55	0.42
2:B:248:LEU:HD13	2:B:288:LEU:HB2	2.02	0.41
2:B:256:PRO:HB3	2:B:290:LEU:HD23	2.01	0.41
1:A:743:PRO:HB2	1:A:747:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:SER:OG	2:B:198:ASP:HA	2.20	0.41
1:A:903:ALA:O	1:A:906:LYS:HG2	2.20	0.41
2:B:200:LYS:HA	2:B:218:LEU:HD13	2.02	0.41
1:A:766:LYS:HE2	1:A:766:LYS:HB3	1.75	0.41
1:A:504:LEU:O	1:A:513:MET:N	2.52	0.41
1:A:736:ARG:HH21	1:A:737:LEU:HD21	1.86	0.41
2:B:371:LEU:HA	2:B:371:LEU:HD23	1.81	0.41
2:B:179:PHE:CE2	2:B:279:PRO:HA	2.56	0.41
1:A:479:LEU:O	1:A:482:GLU:HG2	2.21	0.40
2:B:304:MET:CE	2:B:331:ARG:HE	2.34	0.40
2:B:192:VAL:HG21	2:B:203:LEU:HD23	2.03	0.40
2:B:377:TYR:O	2:B:378:PHE:HB2	2.21	0.40
1:A:815:LEU:O	1:A:819:LEU:HD22	2.20	0.40
1:A:863:GLU:O	1:A:867:VAL:HG23	2.21	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	422/466 (91%)	388 (92%)	32 (8%)	2 (0%)	29	66
2	B	193/209 (92%)	167 (86%)	23 (12%)	3 (2%)	9	44
All	All	615/675 (91%)	555 (90%)	55 (9%)	5 (1%)	19	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	ALA
2	B	334	HIS
2	B	335	TRP
1	A	685	GLY

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Mol	Chain	Res	Type
2	B	215	PRO

### 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	374/410 (91%)	356 (95%)	18 (5%)	25	55
2	B	180/189 (95%)	166 (92%)	14 (8%)	12	42
All	All	554/599 (92%)	522 (94%)	32 (6%)	20	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	CYS
1	A	557	CYS
1	A	599	GLU
1	A	613	HIS
1	A	629	GLU
1	A	653	LEU
1	A	687	VAL
1	A	688	ARG
1	A	691	THR
1	A	692	GLN
1	A	744	LYS
1	A	754	LEU
1	A	771	ARG
1	A	808	THR
1	A	812	LYS
1	A	816	GLN
1	A	830	VAL
1	A	851	PHE
2	B	179	PHE
2	B	203	LEU
2	B	221	VAL
2	B	222	VAL

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Mol	Chain	Res	Type
2	B	225	THR
2	B	254	ARG
2	B	257	SER
2	B	292	LYS
2	B	322	ARG
2	B	333	ARG
2	B	338	VAL
2	B	346	LEU
2	B	376	LYS
2	B	378	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	757	ASN

### 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, 3 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
4	SAH	A	1004	-	21,28,28	1.24	2 (9%)	20,40,40	1.59	3 (15%)

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
4	SAH	A	1004	-	-	2/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1004	SAH	C2-N3	4.08	1.38	1.32
4	A	1004	SAH	C2-N1	2.59	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	SAH	N3-C2-N1	-5.43	120.19	128.68
4	A	1004	SAH	C5'-SD-CG	-2.75	94.02	102.27
4	A	1004	SAH	C3'-C2'-C1'	2.20	104.28	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	SAH	N-CA-CB-CG
4	A	1004	SAH	C-CA-CB-CG

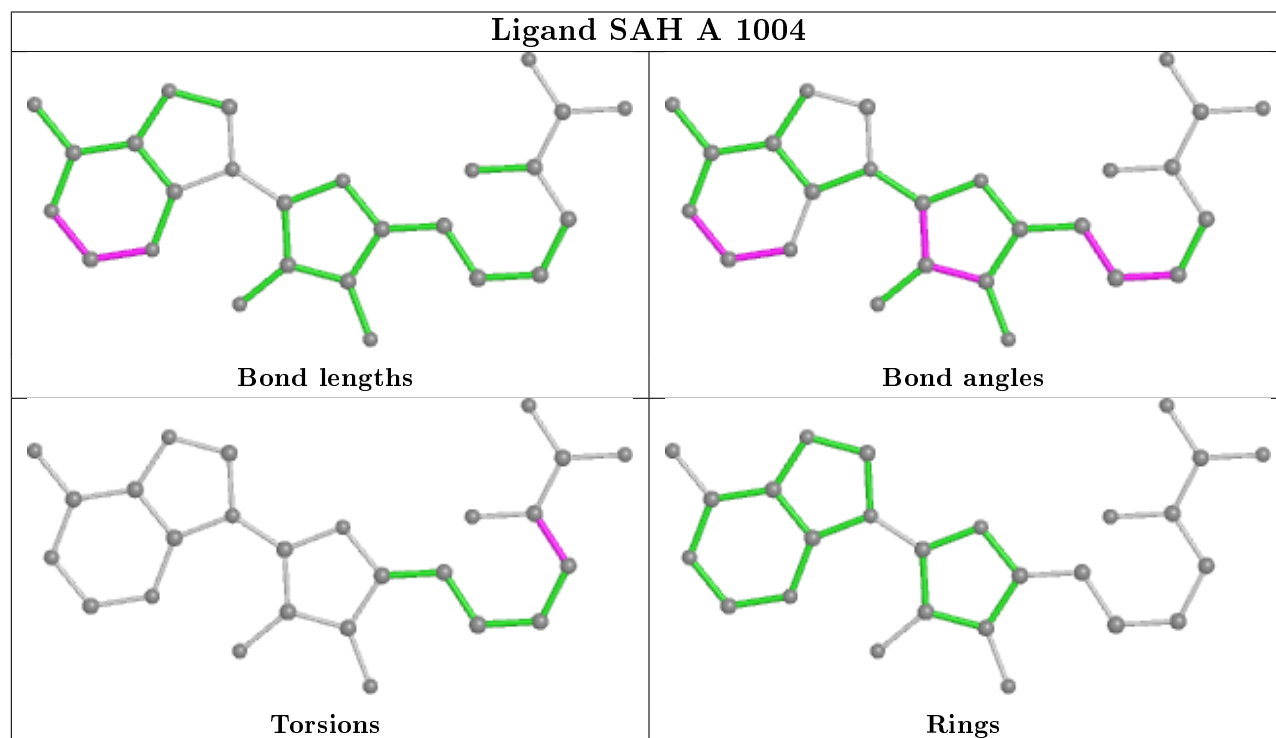
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	426/466 (91%)	0.46	63 (14%) 2 2	20, 67, 208, 251	0
2	B	197/209 (94%)	-0.31	2 (1%) 82 76	13, 34, 99, 128	0
All	All	623/675 (92%)	0.22	65 (10%) 6 5	13, 54, 198, 251	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	GLY	7.7
1	A	543	GLY	6.1
1	A	495	ILE	5.9
1	A	556	ARG	5.4
1	A	501	ASN	5.1
1	A	564	ASP	5.1
1	A	555	CYS	4.6
1	A	554	CYS	4.5
1	A	536	TYR	4.4
1	A	587	GLY	4.3
1	A	481	TYR	4.1
1	A	557	CYS	3.9
1	A	612	ASN	3.8
1	A	506	HIS	3.8
1	A	502	VAL	3.7
1	A	593	GLY	3.7
1	A	512	GLY	3.6
1	A	560	VAL	3.6
1	A	611	ASN	3.4
1	A	601	TRP	3.3
1	A	561	GLU	3.0
1	A	483	VAL	2.9
1	A	588	HIS	2.9
1	A	480	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	586	CYS	2.8
1	A	496	SER	2.8
1	A	585	MET	2.8
1	A	503	THR	2.8
1	A	490	ILE	2.8
1	A	487	CYS	2.8
1	A	600	ASP	2.7
1	A	609	PHE	2.7
1	A	610	ALA	2.7
1	A	482	GLU	2.7
1	A	522	LEU	2.7
1	A	521	PHE	2.7
1	A	558	PHE	2.6
2	B	212	GLY	2.6
1	A	519	ASN	2.6
1	A	562	CYS	2.6
1	A	485	GLN	2.5
1	A	563	VAL	2.5
1	A	513	MET	2.5
1	A	596	ARG	2.5
1	A	579	ASP	2.5
1	A	565	LEU	2.5
1	A	474	ARG	2.5
1	A	527	GLN	2.4
1	A	489	ASN	2.4
1	A	545	GLU	2.4
2	B	213	SER	2.4
1	A	607	MET	2.4
1	A	475	THR	2.4
1	A	509	PHE	2.4
1	A	478	ARG	2.3
1	A	479	LEU	2.3
1	A	526	TYR	2.3
1	A	477	GLU	2.3
1	A	594	LEU	2.3
1	A	553	ASN	2.2
1	A	510	VAL	2.2
1	A	544	ARG	2.2
1	A	603	SER	2.2
1	A	613	HIS	2.0
1	A	584	TYR	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](#)

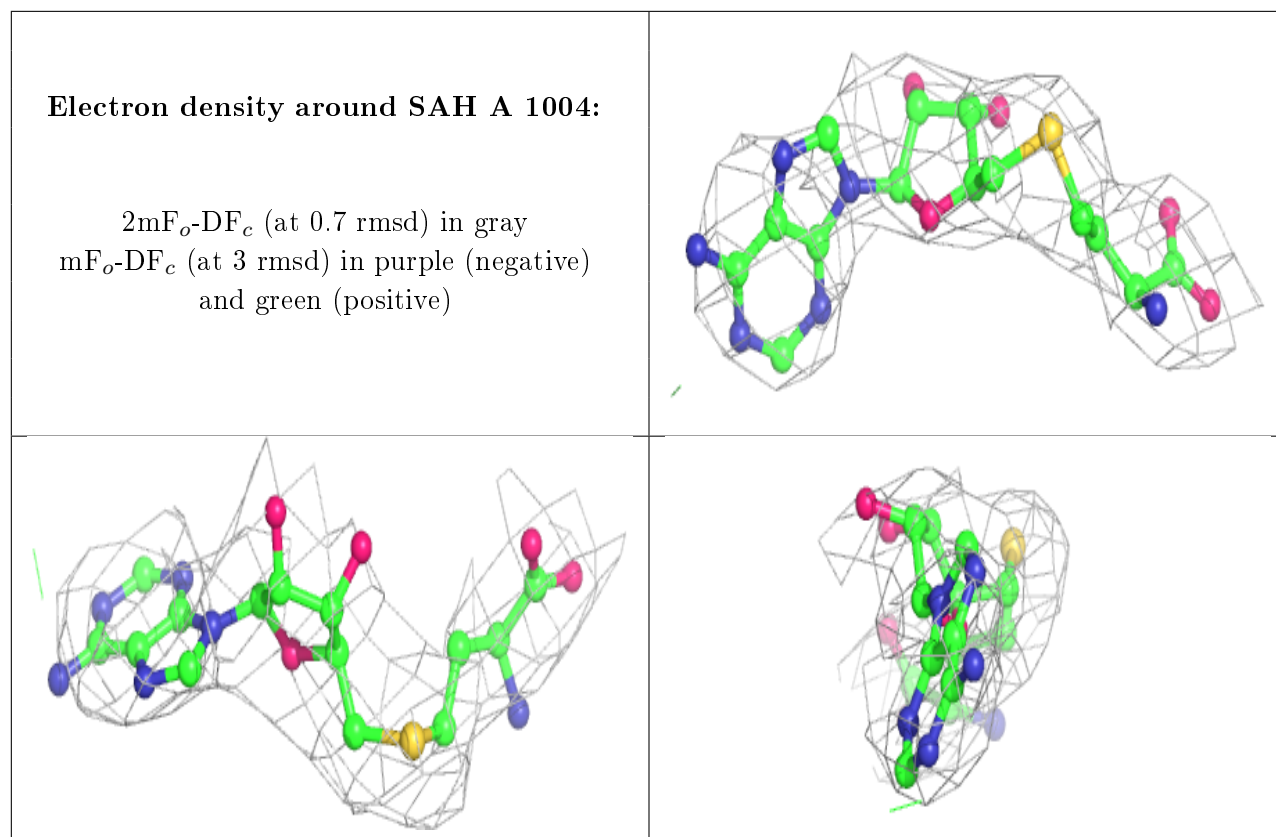
There are no carbohydrates in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	1003	1/1	0.58	0.28	431,431,431,431	0
3	ZN	A	1001	1/1	0.62	0.15	187,187,187,187	0
3	ZN	A	1002	1/1	0.93	0.38	188,188,188,188	0
4	SAH	A	1004	26/26	0.95	0.19	25,34,40,52	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.