Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 03:58 PM EST

PDB ID	:	2ADM
Title	:	ADENINE-N6-DNA-METHYLTRANSFERASE TAQI
Authors	:	Schluckebier, G.; Saenger, W.
Deposited on	:	1996-07-15
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

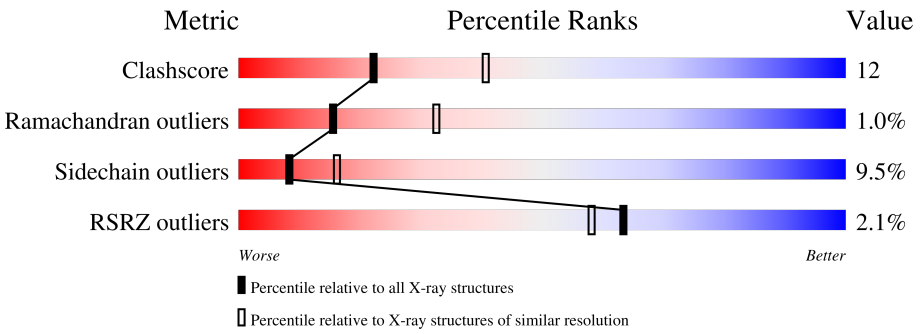
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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 <=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	421	2% 63% 25% • 9%
1	B	421	% 65% 23% • • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6394 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.

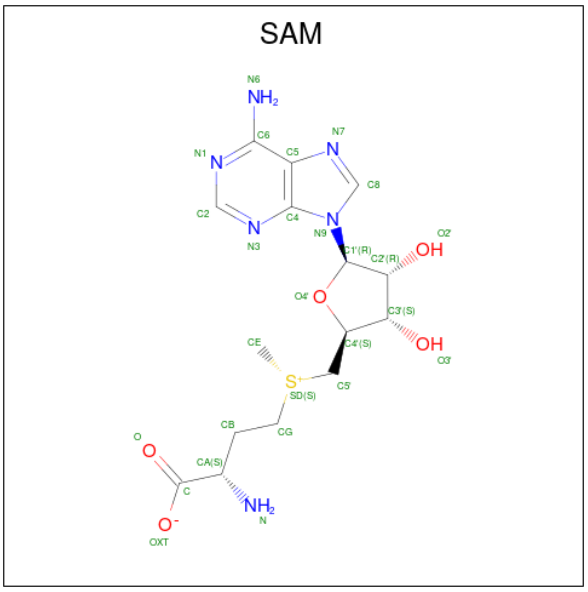
- Molecule 1 is a protein called ADENINE-N6-DNA-METHYLTRANSFERASE TAQI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3123	2044	537	536	6	0	0	0
1	B	385	3123	2044	537	536	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	THR	SER	conflict	UNP P14385
B	370	THR	SER	conflict	UNP P14385

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	27	15	6	5	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	27	15	6	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	47	47	47	0	0
			Total	O		
3	B	47	47	47	0	0

3 Residue-property plots (i)

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: ADENINE-N6-DNA-METHYLTRANSFERASE TAQI

Chain A: 2% 63% 25% • 9%

MET GLY LEU PRO PRO LEU LEU SER LEU PRO SER ASN SER ALA PRO ARG SER LEU GLY ARG V21 E26 V27 V28 M31 V32 R39 R42 V43 L44 E45 P46 A47 H50 G51 P52 F53 L54 H61 R66 E71 L77 D78 L87 W93 E94 P95 G96 E97

L101 I102 L103 G104 N105 P106 P107 I110 V111 G112 GLU ALA SER LYS TYR PRO ILE HIS V121 F122 K123 A124 V125 K126 D127 K130 K131 K139 L154 V159 V163 L171 E172 A175 R178 E179 F180 L181 A182 R183 E184 G185 K186 V204 V205 I206 Q209 K210

S211 G212 K213 G214 L215 S216 L217 E241 R244 T247 E248 E249 T250 R251 E254 I255 S256 G257 M258 P259 L260 F264 R271 S272 P273 H278 P279 A280 V281 R282 K283 L289 V290 L298 Y305 E306 H309 M314 P315 R318 A319 K320 R323 D324 F325

T328 P329 H330 L331 A334 H335 G338 T339 R340 R348 E355 F356 H357 L358 L359 V364 R365 L366 L371 V372 Q373 S377 Q381 P393 H394 R398 R402 R406 H412 T413 SER PRO GLU SER ALA ARG ASN PHE

• Molecule 1: ADENINE-N6-DNA-METHYLTRANSFERASE TAQI

Chain B: % 65% 23% • • 9%

MET GLY LEU PRO PRO LEU LEU SER LEU PRO SER ASN SER ALA PRO ARG SER LEU GLY ARG V21 E26 F30 M31 R39 R42 V43 L44 E45 P46 A47 H50 G51 P52 F53 L54 R66 E71 D78 L87 F90 W93 E94 P95 G96 E97 A98 F99

N105 P106 P107 Y108 G109 I110 V111 G112 GLU ALA SER LYS TYR PRO ILE HIS V121 F122 K123 A124 V125 K126 D127 K130 K131 K139 Y140 M141 L142 E148 K149 R152 L153 L154 L160 V163 V164 P165 L171 R178 L181 G185 K186 T187 K199 V204 V205 I206

R207 F208 Q209 K210 S211 G212 K213 G214 L215 S216 L217 P229 T247 E248 E249 T250 R251 E254 I255 S256 G257 M258 P259 L260 F264 A269 A270 R271 S272 P273 H278 P279 A280 V281 R282 K283 L289 V290 L298 Y305 E306 P315 R318 A319 K320 D324 F325

T328 P329 H330 L331 A334 H335 G338 T339 R340 W345 R348 F356 H357 L358 L359 V364 R365 L366 L371 V372 Q373 E378 P393 L397 R398 E401 R402 R406 H412 T413 SER PRO GLU SER ALA ARG ASN PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	130.66Å 141.83Å 53.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 9.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 92.8 (9.99-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.91 (at 2.41Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.214 , 0.273 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 75.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6394	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7752e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SAM

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	0.42	0/3223	0.71	2/4378 (0.0%)
1	B	0.41	0/3223	0.69	4/4378 (0.1%)
All	All	0.42	0/6446	0.70	6/8756 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	LEU	CA-CB-CG	6.46	130.15	115.30
1	B	215	LEU	CA-CB-CG	6.12	129.38	115.30
1	B	44	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	160	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	44	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	199	LYS	N-CA-C	5.08	124.71	111.00

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	3123	0	3120	81	0
1	B	3123	0	3120	67	0
2	A	27	0	22	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	22	2	0
3	A	47	0	0	2	0
3	B	47	0	0	1	0
All	All	6394	0	6284	147	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 (147) 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:47:ALA:HB1	2:A:500:SAM:H5'2	1.52	0.92
1:B:31:MET:SD	1:B:163:VAL:HG22	2.11	0.91
1:A:31:MET:SD	1:A:163:VAL:HG22	2.12	0.90
1:A:330:HIS:HE1	1:A:357:HIS:HD2	1.22	0.87
1:A:330:HIS:HE1	1:A:357:HIS:CD2	1.95	0.84
1:A:394:HIS:HB2	3:A:1676:HOH:O	1.80	0.81
1:A:364:VAL:HG22	1:A:412:HIS:HB2	1.68	0.76
1:A:247:THR:OG1	1:A:249:GLU:HG3	1.91	0.70
1:A:186:LYS:HB2	1:A:213:LYS:HB3	1.74	0.69
1:A:398:ARG:HH12	1:A:402:ARG:HD2	1.57	0.69
1:A:305:TYR:CE2	1:A:348:ARG:HD3	2.28	0.68
1:A:338:GLY:HA2	1:A:393:PRO:O	1.95	0.67
1:A:93:TRP:CH2	1:A:95:PRO:HB3	2.29	0.66
1:B:330:HIS:HE1	1:B:357:HIS:CD2	2.13	0.66
1:A:71:GLU:OE2	2:A:500:SAM:H1'	1.95	0.66
1:A:47:ALA:HB1	2:A:500:SAM:C5'	2.25	0.65
1:A:107:PRO:HG3	2:A:500:SAM:H5'1	1.78	0.64
1:B:185:GLY:HA2	1:B:212:GLY:HA2	1.79	0.64
1:A:330:HIS:CE1	1:A:357:HIS:HD2	2.11	0.64
1:B:47:ALA:HB1	2:B:500:SAM:O4'	1.97	0.63
1:B:127:ASP:O	1:B:131:LYS:HG2	1.99	0.62
1:B:330:HIS:HE1	1:B:357:HIS:HD2	1.47	0.62
1:A:328:THR:O	1:A:330:HIS:HD2	1.82	0.61
1:B:186:LYS:HB2	1:B:213:LYS:HB3	1.80	0.61
1:B:315:PRO:HG2	1:B:318:ARG:HB2	1.81	0.61
1:A:110:ILE:HD13	1:A:139:LYS:O	2.01	0.61
1:B:186:LYS:HD3	1:B:213:LYS:HD2	1.82	0.61
1:A:309:HIS:HE1	3:A:1622:HOH:O	1.83	0.60
1:B:338:GLY:HA2	1:B:393:PRO:O	2.01	0.60
1:A:335:HIS:O	1:A:394:HIS:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:NE	1:A:271:ARG:H	2.00	0.60
1:B:110:ILE:HD13	1:B:139:LYS:O	2.02	0.60
1:B:111:VAL:HA	3:B:1656:HOH:O	2.02	0.59
1:A:31:MET:SD	1:A:163:VAL:CG2	2.89	0.58
1:A:331:LEU:HD23	1:A:358:LEU:HD22	1.84	0.58
1:A:185:GLY:HA2	1:A:212:GLY:HA2	1.84	0.58
1:A:47:ALA:HB1	2:A:500:SAM:O4'	2.04	0.58
1:B:364:VAL:HG22	1:B:412:HIS:HB2	1.85	0.58
1:B:139:LYS:HD3	1:B:139:LYS:H	1.68	0.57
1:B:298:LEU:HD23	1:B:334:ALA:HB2	1.87	0.57
1:A:320:LYS:HD2	1:A:324:ASP:HA	1.86	0.57
1:B:328:THR:O	1:B:330:HIS:HD2	1.88	0.57
1:B:247:THR:OG1	1:B:249:GLU:HG3	2.05	0.57
1:B:305:TYR:CE2	1:B:348:ARG:HD3	2.39	0.56
1:B:260:LEU:HD21	1:B:358:LEU:HD21	1.87	0.56
1:A:278:HIS:CD2	1:A:279:PRO:O	2.58	0.56
1:A:260:LEU:HD21	1:A:358:LEU:HD21	1.87	0.55
1:A:186:LYS:HD3	1:A:213:LYS:HD2	1.88	0.55
1:A:127:ASP:O	1:A:131:LYS:HG2	2.07	0.54
1:B:213:LYS:HG2	1:B:214:GLY:H	1.72	0.54
1:A:139:LYS:HD3	1:A:139:LYS:H	1.73	0.54
1:B:269:ALA:HB2	1:B:357:HIS:HE1	1.74	0.53
1:A:121:VAL:O	1:A:125:VAL:HG23	2.09	0.53
1:A:315:PRO:HG2	1:A:318:ARG:HB2	1.92	0.52
1:A:110:ILE:HD12	1:A:111:VAL:H	1.74	0.52
1:B:26:GLU:H	1:B:26:GLU:CD	2.13	0.52
1:B:45:GLU:HB2	1:B:54:LEU:HD13	1.92	0.52
1:A:186:LYS:CB	1:A:213:LYS:HB3	2.39	0.52
1:B:335:HIS:HB3	1:B:356:PHE:CE2	2.45	0.51
1:A:71:GLU:O	1:A:87:LEU:HA	2.11	0.51
1:A:377:SER:O	1:A:381:GLN:HG2	2.10	0.51
1:A:305:TYR:CZ	1:A:348:ARG:HD3	2.45	0.51
1:B:31:MET:SD	1:B:163:VAL:CG2	2.93	0.51
1:B:160:LEU:HG	1:B:208:PHE:HB3	1.93	0.51
1:A:298:LEU:HD23	1:A:334:ALA:HB2	1.93	0.50
1:B:71:GLU:O	1:B:87:LEU:HA	2.11	0.50
1:B:44:LEU:HD22	1:B:45:GLU:N	2.26	0.50
1:B:42:ARG:HG2	1:B:66:ARG:HD3	1.93	0.50
1:A:102:ILE:CD1	1:A:154:LEU:HD13	2.42	0.50
1:A:325:PHE:HB3	1:A:359:LEU:HD11	1.93	0.49
1:B:315:PRO:HG2	1:B:318:ARG:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:HA	1:B:406:ARG:HH11	1.76	0.49
1:B:279:PRO:O	1:B:280:ALA:HB3	2.11	0.49
1:A:130:LYS:HB3	1:A:130:LYS:NZ	2.28	0.49
1:B:186:LYS:CB	1:B:213:LYS:HB3	2.43	0.48
1:B:107:PRO:HG3	2:B:500:SAM:H5'1	1.94	0.48
1:A:213:LYS:HG2	1:A:214:GLY:H	1.78	0.48
1:A:28:VAL:HG22	1:A:53:PHE:CE1	2.49	0.47
1:B:278:HIS:CD2	1:B:279:PRO:O	2.68	0.47
1:A:279:PRO:O	1:A:280:ALA:HB3	2.14	0.47
1:A:42:ARG:HG2	1:A:66:ARG:HD3	1.97	0.47
1:B:121:VAL:O	1:B:125:VAL:HG23	2.15	0.47
1:A:93:TRP:CZ3	1:A:95:PRO:HB3	2.50	0.46
1:A:101:LEU:HA	1:A:159:VAL:O	2.15	0.46
1:B:110:ILE:HD12	1:B:111:VAL:H	1.80	0.46
1:A:26:GLU:CD	1:A:26:GLU:H	2.19	0.46
1:B:130:LYS:NZ	1:B:130:LYS:HB3	2.31	0.46
1:B:51:GLY:N	1:B:52:PRO:HD3	2.31	0.45
1:A:71:GLU:HB3	1:A:77:LEU:HD13	1.97	0.45
1:A:256:SER:CB	1:A:406:ARG:HH22	2.29	0.45
1:A:264:PHE:CZ	1:A:366:LEU:HD22	2.51	0.45
1:B:171:LEU:O	1:B:178:ARG:NH2	2.49	0.45
1:B:250:THR:O	1:B:254:GLU:HG3	2.16	0.45
1:A:271:ARG:NH2	1:A:323:ARG:HH21	2.15	0.45
1:A:171:LEU:O	1:A:178:ARG:NH2	2.49	0.45
1:A:175:ALA:O	1:A:179:GLU:HG3	2.16	0.45
1:B:90:PHE:O	1:B:149:LYS:HE2	2.17	0.45
1:A:264:PHE:HZ	1:A:366:LEU:HD22	1.82	0.45
1:A:51:GLY:N	1:A:52:PRO:HD3	2.31	0.45
1:B:154:LEU:HB3	1:B:210:LYS:HD2	1.98	0.44
1:A:355:GLU:HA	1:A:355:GLU:OE1	2.17	0.44
1:B:30:PHE:HE1	1:B:229:PRO:HG3	1.83	0.44
1:B:271:ARG:HB2	1:B:273:PRO:HD2	1.99	0.44
1:B:398:ARG:HH12	1:B:402:ARG:HD2	1.82	0.44
1:B:325:PHE:HB3	1:B:359:LEU:HD11	2.00	0.44
1:A:102:ILE:HD12	1:A:154:LEU:HD13	1.99	0.44
1:A:271:ARG:N	1:A:271:ARG:HE	2.16	0.44
1:B:30:PHE:CE1	1:B:229:PRO:HG3	2.52	0.43
1:B:269:ALA:HB2	1:B:357:HIS:CE1	2.53	0.43
1:A:39:ARG:HH22	1:B:378:GLU:CD	2.20	0.43
1:B:320:LYS:HD2	1:B:324:ASP:HA	2.00	0.43
1:B:50:HIS:NE2	1:B:52:PRO:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:CG	1:B:213:LYS:HB3	2.49	0.43
1:A:282:ARG:HG3	1:A:289:LEU:HD11	2.00	0.43
1:A:44:LEU:HD22	1:A:45:GLU:N	2.33	0.43
1:A:47:ALA:HB1	2:A:500:SAM:C4'	2.48	0.43
1:B:50:HIS:HA	1:B:78:ASP:O	2.18	0.43
1:B:305:TYR:CZ	1:B:348:ARG:HD3	2.54	0.42
1:A:50:HIS:HA	1:A:78:ASP:O	2.19	0.42
1:A:121:VAL:O	1:A:124:ALA:HB3	2.20	0.42
1:B:148:GLU:O	1:B:152:ARG:HG3	2.19	0.42
1:B:106:PRO:HA	1:B:107:PRO:HD3	1.88	0.42
1:B:282:ARG:HG3	1:B:289:LEU:HD11	2.02	0.42
1:B:331:LEU:HB2	1:B:345:TRP:CZ3	2.55	0.42
1:A:314:MET:HE2	1:A:318:ARG:HB3	2.01	0.41
1:A:272:SER:HB3	1:A:273:PRO:HD3	2.03	0.41
1:B:397:LEU:O	1:B:401:GLU:HG3	2.20	0.41
1:A:213:LYS:CG	1:A:214:GLY:H	2.33	0.41
1:B:264:PHE:CZ	1:B:366:LEU:HD22	2.55	0.41
1:A:50:HIS:CE1	1:A:52:PRO:HG3	2.55	0.41
1:A:331:LEU:HD23	1:A:358:LEU:CD2	2.50	0.41
1:A:255:ILE:HD12	1:A:256:SER:N	2.35	0.41
1:B:93:TRP:CH2	1:B:95:PRO:HB3	2.55	0.41
1:A:244:ARG:NH2	1:A:254:GLU:OE2	2.53	0.41
1:A:335:HIS:HB3	1:A:356:PHE:CE2	2.56	0.41
1:A:339:THR:O	1:A:339:THR:HG22	2.20	0.41
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.93	0.40
1:A:406:ARG:HA	1:A:406:ARG:HH11	1.86	0.40
1:A:46:PRO:HD2	1:A:103:LEU:O	2.21	0.40
1:B:44:LEU:HB2	1:B:99:PHE:CD2	2.56	0.40
1:A:32:VAL:O	1:A:61:HIS:HE1	2.03	0.40
1:A:209:GLN:O	1:A:211:SER:N	2.48	0.40
1:B:108:TYR:CE1	1:B:165:PRO:HD3	2.56	0.40
1:B:187:THR:O	1:B:215:LEU:HA	2.21	0.40
1:B:199:LYS:HA	1:B:199:LYS:HD2	1.89	0.40
1:A:278:HIS:HD2	1:A:281:VAL:HG23	1.85	0.40
1:B:256:SER:CB	1:B:406:ARG:HH22	2.35	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	381/421 (90%)	356 (93%)	21 (6%)	4 (1%)	15 32
1	B	381/421 (90%)	357 (94%)	20 (5%)	4 (1%)	15 32
All	All	762/842 (90%)	713 (94%)	41 (5%)	8 (1%)	15 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	PHE
1	A	212	GLY
1	B	122	PHE
1	A	213	LYS
1	B	212	GLY
1	B	213	LYS
1	B	111	VAL
1	A	111	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	325/356 (91%)	293 (90%)	32 (10%)	8 15
1	B	325/356 (91%)	295 (91%)	30 (9%)	9 17
All	All	650/712 (91%)	588 (90%)	62 (10%)	8 16

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	44	LEU
1	A	54	LEU
1	A	93	TRP
1	A	94	GLU
1	A	97	GLU
1	A	105	ASN
1	A	123	LYS
1	A	139	LYS
1	A	154	LEU
1	A	172	GLU
1	A	181	LEU
1	A	183	ARG
1	A	204	VAL
1	A	206	ILE
1	A	217	LEU
1	A	241	GLU
1	A	249	GLU
1	A	251	ARG
1	A	258	MET
1	A	271	ARG
1	A	272	SER
1	A	283	LYS
1	A	290	VAL
1	A	306	GLU
1	A	318	ARG
1	A	340	ARG
1	A	366	LEU
1	A	371	LEU
1	A	373	GLN
1	A	398	ARG
1	A	406	ARG
1	B	39	ARG
1	B	44	LEU
1	B	54	LEU
1	B	93	TRP
1	B	94	GLU
1	B	97	GLU
1	B	105	ASN
1	B	139	LYS
1	B	140	TYR
1	B	142	LEU
1	B	154	LEU

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Mol	Chain	Res	Type
1	B	160	LEU
1	B	181	LEU
1	B	204	VAL
1	B	206	ILE
1	B	215	LEU
1	B	217	LEU
1	B	249	GLU
1	B	251	ARG
1	B	258	MET
1	B	271	ARG
1	B	283	LYS
1	B	290	VAL
1	B	306	GLU
1	B	318	ARG
1	B	324	ASP
1	B	340	ARG
1	B	371	LEU
1	B	373	GLN
1	B	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	105	ASN
1	A	278	HIS
1	A	309	HIS
1	A	330	HIS
1	A	335	HIS
1	A	357	HIS
1	A	394	HIS
1	B	61	HIS
1	B	105	ASN
1	B	278	HIS
1	B	330	HIS
1	B	335	HIS
1	B	357	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)

2 ligands are modelled in this entry.

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	SAM	B	500	-	24,29,29	0.96	2 (8%)	23,42,42	1.16	1 (4%)
2	SAM	A	500	-	24,29,29	0.93	1 (4%)	23,42,42	1.18	1 (4%)

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	SAM	B	500	-	-	6/12/33/33	0/3/3/3
2	SAM	A	500	-	-	2/12/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	SAM	C8-N7	-3.08	1.29	1.34
2	A	500	SAM	C8-N7	-2.76	1.29	1.34
2	B	500	SAM	O4'-C1'	2.09	1.44	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	SAM	C3'-C2'-C1'	3.29	105.93	100.98
2	B	500	SAM	C3'-C2'-C1'	3.29	105.93	100.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

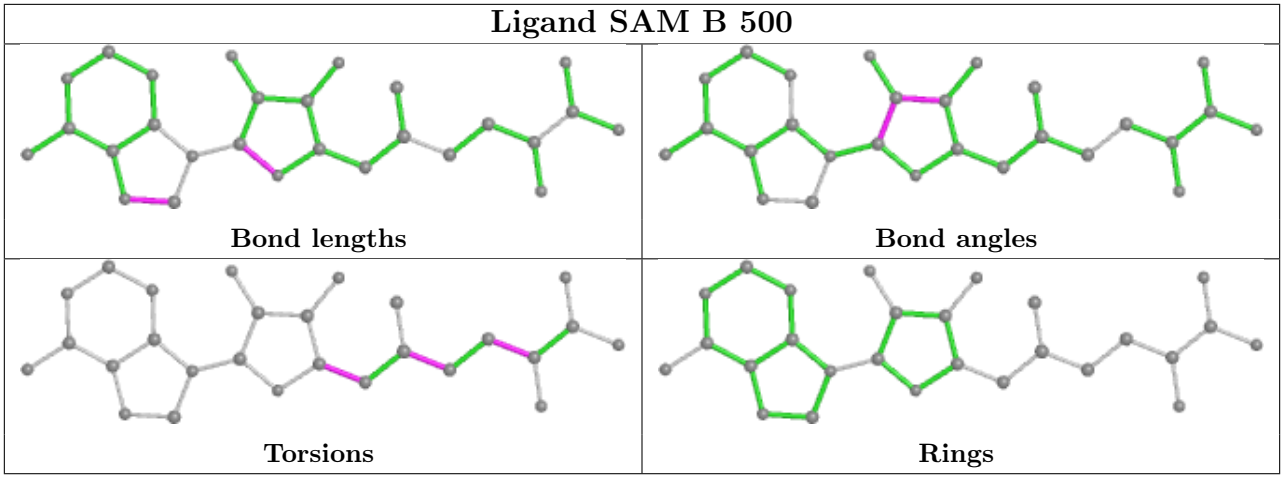
Mol	Chain	Res	Type	Atoms
2	B	500	SAM	CB-CG-SD-C5'
2	B	500	SAM	CB-CG-SD-CE
2	B	500	SAM	C-CA-CB-CG
2	A	500	SAM	CB-CG-SD-CE
2	A	500	SAM	CB-CG-SD-C5'
2	B	500	SAM	O4'-C4'-C5'-SD
2	B	500	SAM	C3'-C4'-C5'-SD
2	B	500	SAM	N-CA-CB-CG

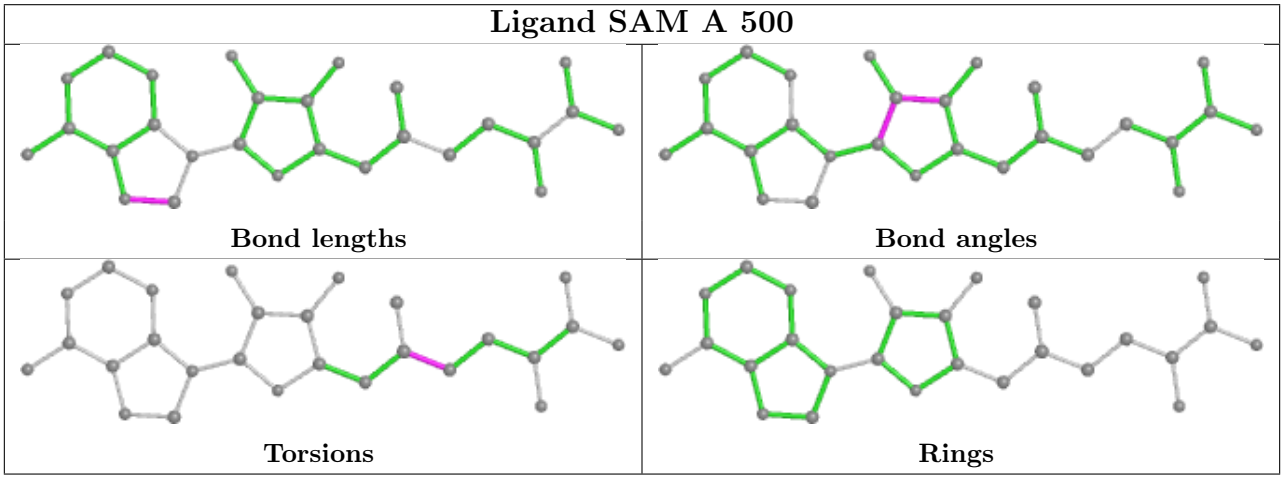
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	SAM	2	0
2	A	500	SAM	6	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 then 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	385/421 (91%)	-0.75	10 (2%)	56	50	4, 20, 61, 125	0
1	B	385/421 (91%)	-0.75	6 (1%)	72	68	4, 22, 63, 119	0
All	All	770/842 (91%)	-0.75	16 (2%)	63	58	4, 22, 63, 125	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	14.9
1	B	413	THR	10.8
1	A	413	THR	7.1
1	B	122	PHE	7.1
1	A	122	PHE	4.9
1	A	111	VAL	4.6
1	A	124	ALA	4.5
1	B	412	HIS	4.4
1	A	123	LYS	4.3
1	A	412	HIS	3.7
1	A	121	VAL	3.5
1	A	21	VAL	2.8
1	B	21	VAL	2.7
1	B	123	LYS	2.6
1	B	112	GLY	2.3
1	A	125	VAL	2.3

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)

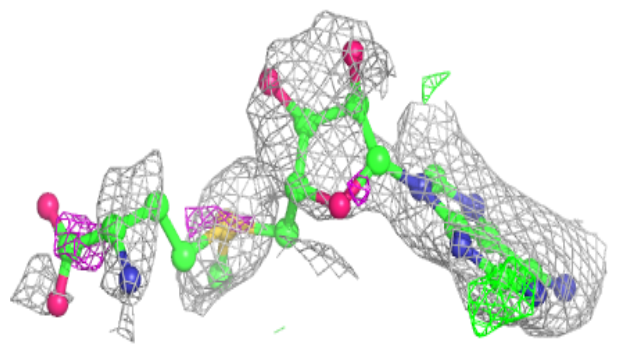
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

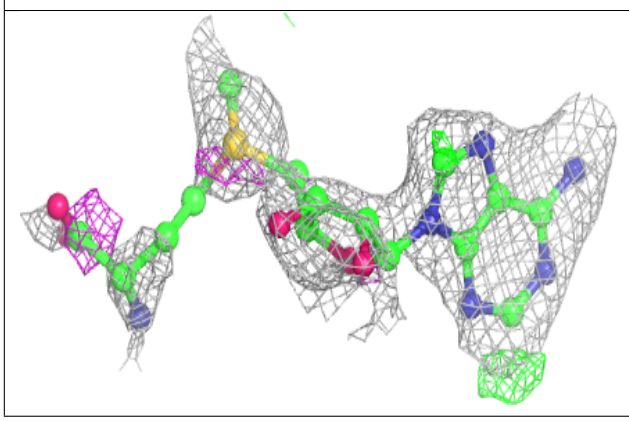
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAM	A	500	27/27	0.78	0.30	43,65,79,82	0
2	SAM	B	500	27/27	0.89	0.21	29,64,75,78	0

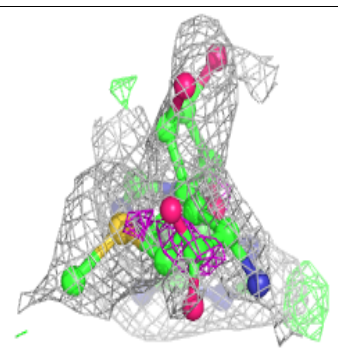
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM A 500:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

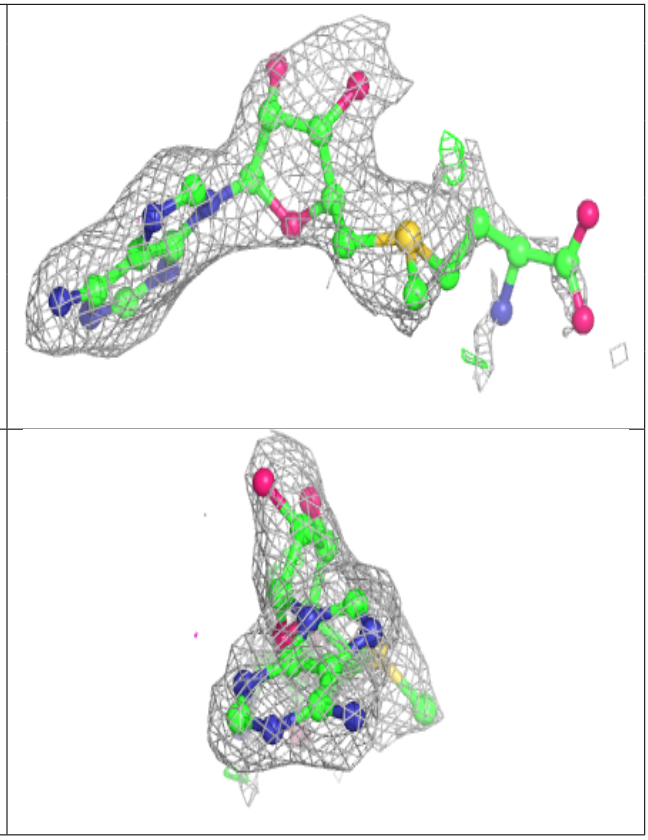






Electron density around SAM B 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.