Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 03:59 AM EST

PDB ID	:	1XVA
Title	:	METHYLTRANSFERASE
Authors	:	Fu, Z.; Hu, Y.; Konishi, K.; Takata, Y.; Ogawa, H.; Gomi, T.; Fujioka, M.; Takusagawa, F.
Deposited on	:	1996-07-20
Resolution	:	2.20 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 (1)) were used in the production of this report:

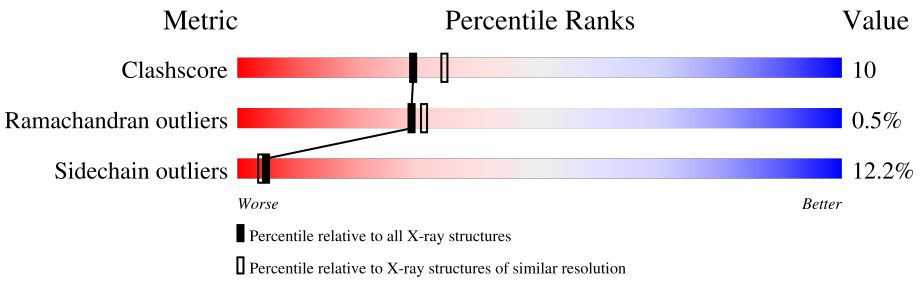
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	292	66% 24% 9% •
1	B	292	69% 23% 8% •

2 Entry composition (i)

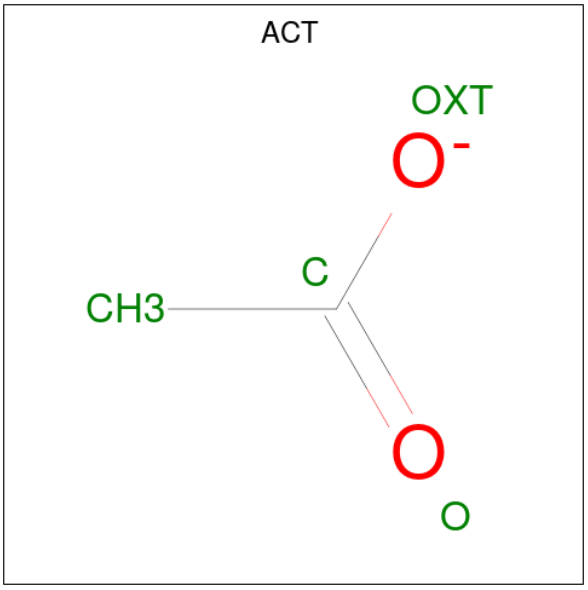
There are 4 unique types of molecules in this entry. The entry contains 4724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCINE N-METHYLTRANSFERASE.

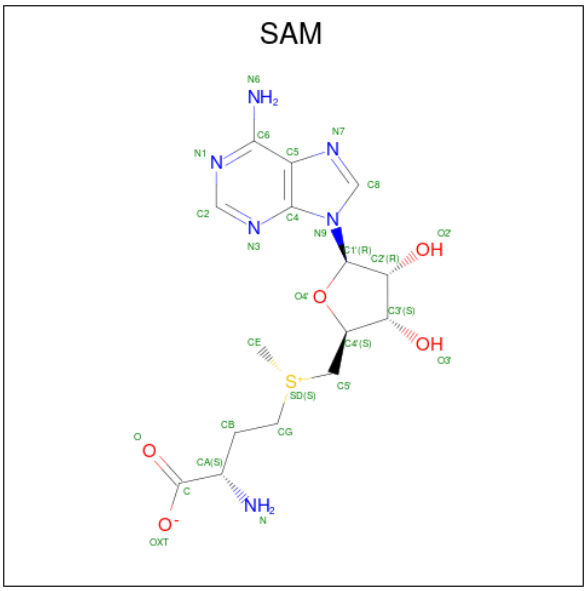
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2284	1450	399	424	11	0	0	0
1	B	292	2284	1450	399	424	11	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0

- Molecule 3 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		
3	A	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
3	B	1	27	15	6	5	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	59	59	59	0	0
			Total	O		
4	B	35	35	35	0	0

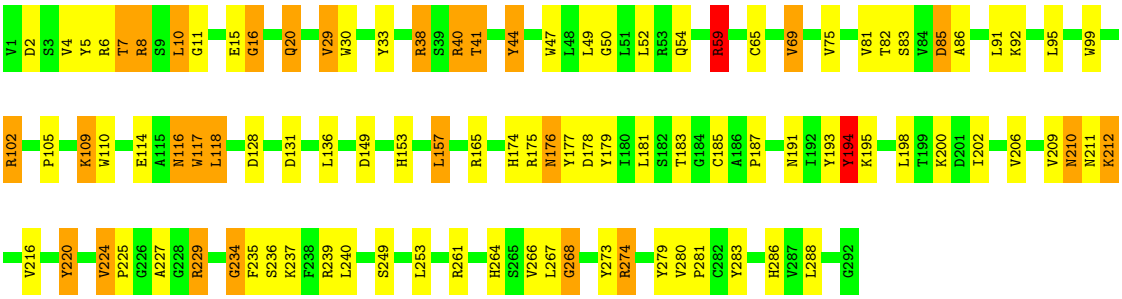
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

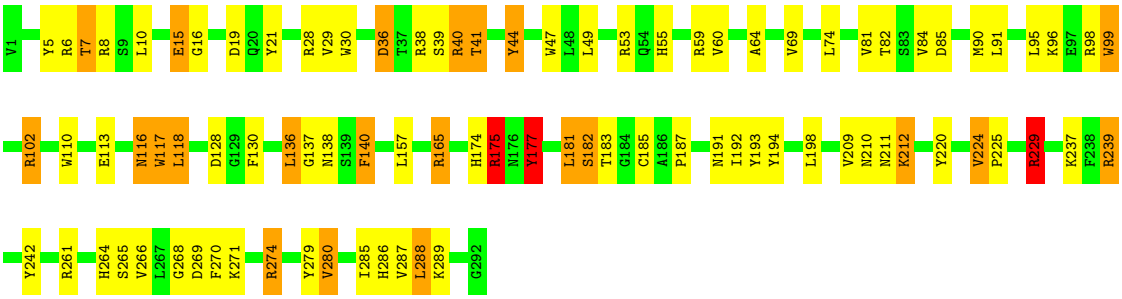
• Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain A: 66% 24% 9% •



• Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain B: 69% 23% 8% •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.40Å 175.70Å 45.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.5 (10.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4724	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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: ACT, 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	0.93	0/2340	1.68	47/3174 (1.5%)
1	B	1.02	2/2340 (0.1%)	1.72	48/3174 (1.5%)
All	All	0.98	2/4680 (0.0%)	1.70	95/6348 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	SER	C-N	20.12	1.80	1.34
1	B	140	PHE	N-CA	-5.63	1.35	1.46

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	SER	O-C-N	-16.53	96.25	122.70
1	B	182	SER	C-N-CA	11.62	150.76	121.70
1	B	182	SER	CA-C-N	11.06	141.53	117.20
1	A	7	THR	CA-CB-CG2	9.04	125.05	112.40
1	B	177	TYR	CB-CG-CD1	-8.94	115.64	121.00
1	B	136	LEU	CB-CA-C	-8.57	93.92	110.20
1	A	102	ARG	NE-CZ-NH1	8.53	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	B	30	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	A	30	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	A	102	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	229	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	210	ASN	CB-CA-C	7.91	126.22	110.40
1	B	47	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	A	210	ASN	O-C-N	7.75	135.10	122.70
1	B	117	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	B	99	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	A	235	PHE	CB-CA-C	-7.64	95.12	110.40
1	B	7	THR	CA-CB-CG2	7.48	122.87	112.40
1	A	110	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	B	175	ARG	CB-CG-CD	-7.43	92.29	111.60
1	A	99	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	B	90	MET	CA-CB-CG	-7.33	100.83	113.30
1	A	20	GLN	CA-C-N	7.29	133.25	117.20
1	B	279	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	A	47	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	B	117	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B	99	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	117	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	B	47	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	B	110	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	B	30	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	38	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	99	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	A	110	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	B	239	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	283	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	B	175	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	30	TRP	CG-CD1-NE1	-6.52	103.58	110.10
1	B	288	LEU	CA-CB-CG	6.49	130.24	115.30
1	A	179	TYR	CB-CG-CD2	-6.49	117.11	121.00
1	B	110	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	A	75	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	B	53	ARG	CA-CB-CG	-6.41	99.29	113.40
1	A	117	TRP	CE2-CD2-CG	-6.39	102.18	107.30
1	A	47	TRP	CB-CG-CD1	-6.37	118.71	127.00
1	B	165	ARG	CA-CB-CG	6.35	127.38	113.40
1	A	30	TRP	CE2-CD2-CG	-6.32	102.25	107.30
1	B	98	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	8	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	21	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	B	102	ARG	CA-CB-CG	6.20	127.03	113.40
1	A	268	GLY	CA-C-N	6.07	130.54	117.20
1	B	269	ASP	N-CA-CB	6.02	121.43	110.60
1	A	59	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	165	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	47	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	B	269	ASP	CA-C-N	5.96	130.31	117.20
1	A	20	GLN	CA-CB-CG	-5.94	100.33	113.40
1	B	210	ASN	CB-CA-C	5.94	122.27	110.40
1	A	47	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	A	210	ASN	CA-C-N	-5.91	104.21	117.20
1	A	273	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	B	261	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	280	VAL	CA-CB-CG2	5.83	119.65	110.90
1	A	59	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	149	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	15	GLU	O-C-N	-5.73	113.46	123.20
1	A	40	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	191	ASN	CA-C-N	-5.62	104.85	117.20
1	B	191	ASN	CA-C-N	-5.62	104.84	117.20
1	A	229	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	234	GLY	N-CA-C	-5.57	99.17	113.10
1	A	194	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	85	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	110	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	B	30	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	117	TRP	CG-CD2-CE3	5.46	138.81	133.90
1	B	274	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	274	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	40	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	B	175	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	20	GLN	O-C-N	-5.37	114.11	122.70
1	B	6	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	19	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	53	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	240	LEU	N-CA-CB	-5.29	99.83	110.40
1	B	268	GLY	CA-C-N	5.25	128.74	117.20
1	B	38	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	A	279	TYR	CB-CG-CD1	-5.21	117.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	69	VAL	CA-CB-CG1	-5.02	103.37	110.90
1	B	41	THR	N-CA-CB	-5.00	100.79	110.30
1	B	44	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	GLY	Peptide
1	A	165	ARG	Sidechain
1	A	193	TYR	Sidechain
1	A	194	TYR	Sidechain
1	A	239	ARG	Sidechain
1	A	44	TYR	Sidechain
1	A	5	TYR	Sidechain
1	A	59	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	177	TYR	Sidechain
1	B	28	ARG	Sidechain
1	B	5	TYR	Sidechain

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	2284	0	2243	43	0
1	B	2284	0	2242	48	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
3	A	27	0	22	1	0
3	B	27	0	22	4	0
4	A	59	0	0	0	0
4	B	35	0	0	1	0
All	All	4724	0	4535	88	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 10.

All (88) 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:B:182:SER:C	1:B:183:THR:N	1.80	1.31
1:A:227:ALA:HB3	1:A:234:GLY:HA3	1.58	0.86
1:B:175:ARG:HG3	3:B:293:SAM:H8	1.68	0.75
2:A:294:ACT:H2	3:A:293:SAM:H3'	1.69	0.75
1:B:116:ASN:HD22	1:B:118:LEU:H	1.35	0.73
1:A:38:ARG:HB2	1:A:69:VAL:HG11	1.71	0.73
1:B:41:THR:HG22	1:B:44:TYR:H	1.55	0.70
1:A:10:LEU:HA	1:A:20:GLN:HE22	1.60	0.67
1:B:40:ARG:HB3	1:B:194:TYR:CE1	2.31	0.65
1:B:182:SER:O	1:B:183:THR:N	2.28	0.65
1:A:185:CYS:O	1:A:187:PRO:HD3	1.97	0.65
1:A:15:GLU:OE1	3:B:293:SAM:HB1	1.97	0.65
1:B:185:CYS:O	1:B:187:PRO:HD3	1.97	0.64
1:A:174:HIS:HD2	1:A:175:ARG:O	1.80	0.64
1:A:85:ASP:OD1	1:B:15:GLU:O	2.16	0.63
1:A:209:VAL:CG2	1:A:212:LYS:HE2	2.29	0.62
1:A:105:PRO:O	1:A:109:LYS:HD2	2.00	0.61
1:B:193:TYR:CD1	1:B:270:PHE:HZ	2.19	0.61
1:A:117:TRP:CH2	1:B:16:GLY:HA3	2.36	0.61
1:B:137:GLY:O	1:B:138:ASN:HB3	1.99	0.60
1:A:209:VAL:HG23	1:A:212:LYS:HE2	1.83	0.59
1:A:50:GLY:O	1:A:54:GLN:HB2	2.03	0.59
1:A:175:ARG:HB3	1:A:177:TYR:CE2	2.39	0.58
1:A:264:HIS:HE1	1:A:286:HIS:ND1	2.01	0.58
1:A:33:TYR:HE1	1:A:200:LYS:HE2	1.69	0.57
1:B:130:PHE:O	1:B:165:ARG:HB2	2.04	0.57
1:B:140:PHE:CZ	1:B:157:LEU:HD13	2.40	0.57
1:A:33:TYR:CE1	1:A:200:LYS:HE2	2.42	0.55
1:A:11:GLY:H	1:A:20:GLN:HE22	1.55	0.55
1:B:39:SER:O	1:B:194:TYR:HA	2.07	0.55
1:B:116:ASN:ND2	1:B:118:LEU:H	2.03	0.54
1:B:174:HIS:HD2	1:B:175:ARG:O	1.91	0.54
1:B:137:GLY:O	3:B:293:SAM:H4'	2.08	0.54
1:A:41:THR:HG22	1:A:44:TYR:H	1.74	0.53
1:A:116:ASN:HD22	1:A:117:TRP:N	2.07	0.53
1:A:176:ASN:HD21	1:A:178:ASP:HB2	1.74	0.51
1:B:264:HIS:HE1	1:B:286:HIS:ND1	2.08	0.51
1:B:7:THR:HG22	1:B:8:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:CG1	1:A:236:SER:HB2	2.41	0.50
1:A:11:GLY:H	1:A:20:GLN:NE2	2.10	0.49
1:A:206:VAL:HG22	1:A:216:VAL:HG22	1.94	0.49
1:A:220:TYR:O	1:A:237:LYS:HA	2.12	0.49
1:A:209:VAL:HG23	1:A:209:VAL:O	2.11	0.48
1:B:193:TYR:CE1	1:B:270:PHE:CZ	3.01	0.48
1:B:41:THR:HG21	1:B:192:ILE:O	2.13	0.48
1:A:116:ASN:HD22	1:A:118:LEU:H	1.61	0.48
1:B:116:ASN:HD21	1:B:118:LEU:HD22	1.80	0.47
1:B:99:TRP:O	1:B:102:ARG:HB2	2.14	0.47
1:A:16:GLY:HA2	1:B:117:TRP:CH2	2.50	0.46
1:B:85:ASP:HB3	1:B:91:LEU:HD13	1.98	0.46
1:A:224:VAL:HG13	1:A:234:GLY:O	2.16	0.46
1:A:6:ARG:O	1:B:239:ARG:HD3	2.16	0.46
1:A:40:ARG:HB3	1:A:194:TYR:CE1	2.51	0.45
1:B:55:HIS:HD2	1:B:289:LYS:NZ	2.14	0.45
1:B:174:HIS:CE1	1:B:286:HIS:HE2	2.33	0.45
1:B:40:ARG:HH21	1:B:69:VAL:CG1	2.30	0.45
1:B:96:LYS:HZ2	1:B:96:LYS:HB2	1.82	0.45
1:B:137:GLY:O	1:B:138:ASN:CB	2.65	0.45
1:B:60:VAL:HG21	1:B:74:LEU:HD13	2.00	0.44
1:B:177:TYR:O	1:B:181:LEU:HB2	2.18	0.44
1:A:176:ASN:ND2	1:A:178:ASP:HB2	2.33	0.43
1:B:242:TYR:CD1	1:B:242:TYR:N	2.85	0.43
1:A:59:ARG:O	1:A:131:ASP:HB2	2.17	0.43
1:A:153:HIS:O	1:A:157:LEU:HB2	2.18	0.43
1:A:224:VAL:HA	1:A:225:PRO:HD3	1.72	0.43
1:B:36:ASP:OD2	1:B:198:LEU:HB2	2.18	0.43
1:A:280:VAL:HA	1:A:281:PRO:HD3	1.84	0.43
1:A:7:THR:HG22	1:A:8:ARG:HG2	2.01	0.42
1:A:65:CYS:SG	1:A:83:SER:HB3	2.58	0.42
1:B:84:VAL:HA	1:B:113:GLU:O	2.19	0.42
1:B:175:ARG:HG3	3:B:293:SAM:C8	2.45	0.42
1:A:85:ASP:OD1	1:A:86:ALA:N	2.52	0.42
1:A:116:ASN:ND2	1:A:118:LEU:H	2.17	0.42
1:B:209:VAL:HB	1:B:212:LYS:NZ	2.35	0.42
1:B:193:TYR:HE1	1:B:270:PHE:CE1	2.38	0.41
1:A:202:ILE:HD13	1:A:202:ILE:HG21	1.90	0.41
1:B:64:ALA:HB3	4:B:311:HOH:O	2.20	0.41
1:B:117:TRP:CH2	1:B:140:PHE:HA	2.55	0.41
1:A:267:LEU:HD22	1:A:267:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG11	1:A:236:SER:HB2	2.01	0.41
1:A:183:THR:HG22	1:A:185:CYS:HB2	2.03	0.41
1:B:183:THR:HG22	1:B:185:CYS:HB2	2.03	0.41
1:B:220:TYR:O	1:B:237:LYS:HA	2.21	0.41
1:B:40:ARG:HH21	1:B:69:VAL:HG12	1.86	0.41
1:B:44:TYR:CD1	1:B:193:TYR:HD1	2.40	0.40
1:B:224:VAL:HA	1:B:225:PRO:HD3	1.77	0.40
1:B:209:VAL:HB	1:B:212:LYS:HZ3	1.86	0.40
1:B:44:TYR:CD1	1:B:193:TYR:CD1	3.09	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	290/292 (99%)	270 (93%)	18 (6%)	2 (1%)	22	22
1	B	290/292 (99%)	271 (93%)	18 (6%)	1 (0%)	41	46
All	All	580/584 (99%)	541 (93%)	36 (6%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ARG
1	A	268	GLY
1	B	229	ARG

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	242/242 (100%)	208 (86%)	34 (14%)	3 3
1	B	242/242 (100%)	217 (90%)	25 (10%)	7 6
All	All	484/484 (100%)	425 (88%)	59 (12%)	5 4

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	4	VAL
1	A	10	LEU
1	A	29	VAL
1	A	41	THR
1	A	49	LEU
1	A	52	LEU
1	A	81	VAL
1	A	82	THR
1	A	91	LEU
1	A	92	LYS
1	A	95	LEU
1	A	102	ARG
1	A	109	LYS
1	A	114	GLU
1	A	116	ASN
1	A	118	LEU
1	A	128	ASP
1	A	136	LEU
1	A	157	LEU
1	A	176	ASN
1	A	181	LEU
1	A	195	LYS
1	A	198	LEU
1	A	210	ASN
1	A	211	ASN
1	A	212	LYS
1	A	224	VAL
1	A	249	SER
1	A	253	LEU
1	A	261	ARG
1	A	266	VAL
1	A	274	ARG

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Mol	Chain	Res	Type
1	A	288	LEU
1	B	10	LEU
1	B	29	VAL
1	B	36	ASP
1	B	49	LEU
1	B	81	VAL
1	B	82	THR
1	B	95	LEU
1	B	116	ASN
1	B	118	LEU
1	B	128	ASP
1	B	136	LEU
1	B	175	ARG
1	B	181	LEU
1	B	211	ASN
1	B	212	LYS
1	B	224	VAL
1	B	229	ARG
1	B	265	SER
1	B	266	VAL
1	B	271	LYS
1	B	274	ARG
1	B	280	VAL
1	B	285	ILE
1	B	287	VAL
1	B	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	116	ASN
1	A	150	GLN
1	A	153	HIS
1	A	159	ASN
1	A	174	HIS
1	A	176	ASN
1	A	211	ASN
1	A	223	GLN
1	A	245	HIS
1	A	264	HIS
1	B	55	HIS

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Mol	Chain	Res	Type
1	B	100	ASN
1	B	116	ASN
1	B	150	GLN
1	B	153	HIS
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN
1	B	211	ASN
1	B	264	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)

4 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	ACT	A	294	-	3,3,3	0.77	0	3,3,3	0.92	0
3	SAM	B	293	-	24,29,29	1.36	4 (16%)	23,42,42	1.97	4 (17%)
3	SAM	A	293	-	24,29,29	1.48	5 (20%)	23,42,42	1.25	3 (13%)
2	ACT	B	294	-	3,3,3	0.77	0	3,3,3	0.91	0

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
3	SAM	B	293	-	-	5/12/33/33	0/3/3/3
3	SAM	A	293	-	-	6/12/33/33	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	SAM	O4'-C1'	3.75	1.46	1.41
3	B	293	SAM	O4'-C1'	3.49	1.45	1.41
3	A	293	SAM	C5'-C4'	-3.13	1.44	1.53
3	A	293	SAM	C3'-C4'	2.63	1.59	1.53
3	B	293	SAM	C3'-C4'	2.37	1.59	1.53
3	A	293	SAM	C8-N7	-2.32	1.30	1.34
3	B	293	SAM	C5'-C4'	-2.31	1.46	1.53
3	A	293	SAM	OXT-C	-2.23	1.23	1.30
3	B	293	SAM	OXT-C	-2.17	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	293	SAM	C1'-N9-C4	-6.84	114.62	126.64
3	B	293	SAM	CG-SD-C5'	3.64	112.70	103.40
3	A	293	SAM	C1'-N9-C4	2.92	131.78	126.64
3	B	293	SAM	C5-C6-N6	2.91	124.78	120.35
3	B	293	SAM	OXT-C-O	-2.82	117.69	124.09
3	A	293	SAM	OXT-C-O	-2.71	117.93	124.09
3	A	293	SAM	OXT-C-CA	2.42	121.61	113.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	293	SAM	O-C-CA-N
3	A	293	SAM	N-CA-CB-CG
3	A	293	SAM	C-CA-CB-CG
3	A	293	SAM	OXT-C-CA-N
3	A	293	SAM	OXT-C-CA-CB
3	B	293	SAM	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	A	293	SAM	O-C-CA-CB
3	B	293	SAM	O4'-C4'-C5'-SD
3	B	293	SAM	C3'-C4'-C5'-SD
3	B	293	SAM	OXT-C-CA-CB
3	B	293	SAM	C-CA-CB-CG

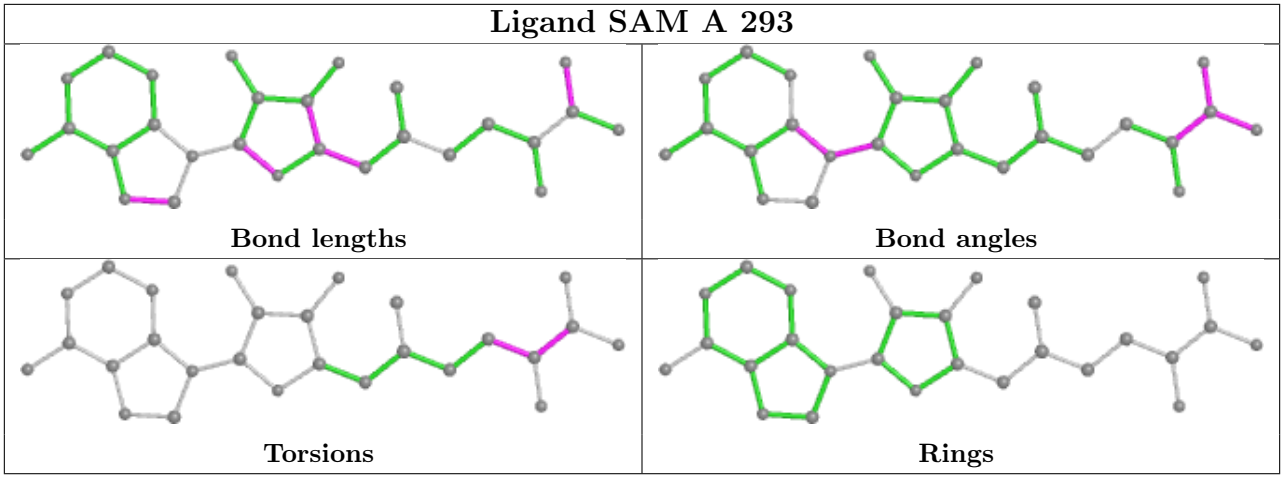
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	294	ACT	1	0
3	B	293	SAM	4	0
3	A	293	SAM	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 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.

Ligand SAM B 293



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	182:SER	C	183:THR	N	1.80

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.