



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:04 PM UTC

PDB ID : 1XVA / pdb_00001xva
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

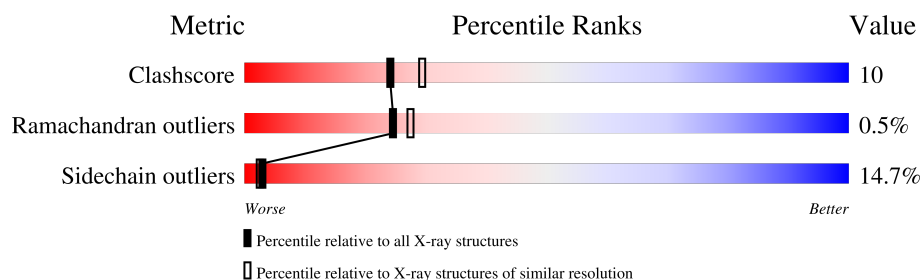
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	294	-	-	X	-

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
1	A	292	Total	C	N	O	S	0	0	0
			2284	1450	399	424	11			
1	B	292	Total	C	N	O	S	0	0	0
			2284	1450	399	424	11			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



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

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

- Molecule 4 is water.

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

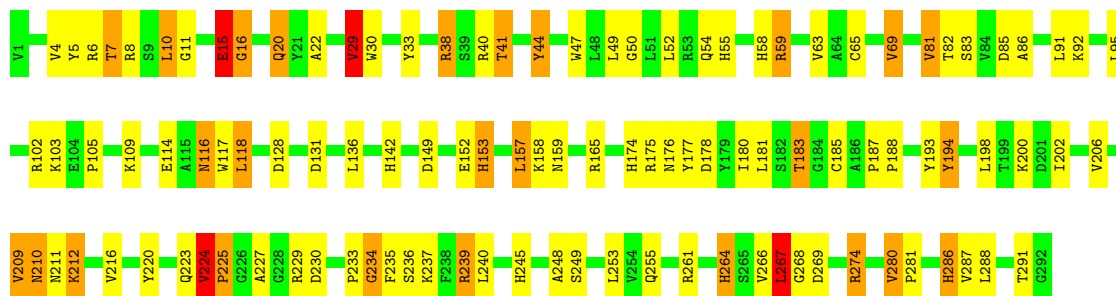
3 Residue-property plots

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. 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.

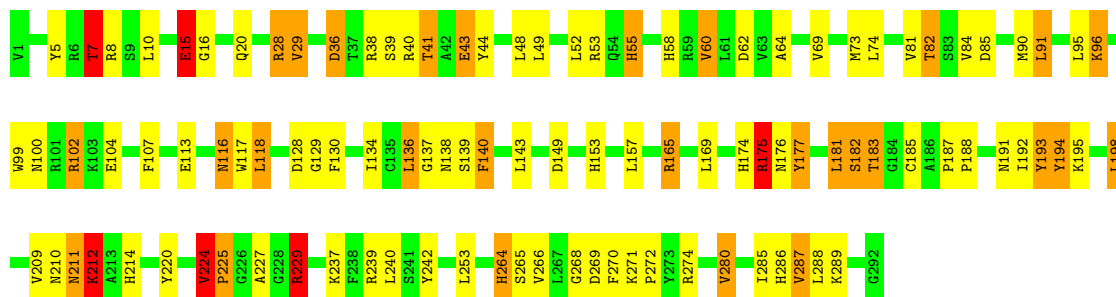
• Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain A: 



• Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain B: 



4 Data and refinement statistics

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	86.40 Å 175.70 Å 45.50 Å 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAM, ACT

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	1.22	9/2340 (0.4%)	1.93	67/3174 (2.1%)
1	B	1.36	12/2340 (0.5%)	1.98	67/3174 (2.1%)
All	All	1.29	21/4680 (0.4%)	1.96	134/6348 (2.1%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	SER	C-N	31.19	1.80	1.33
1	B	140	PHE	N-CA	-8.77	1.35	1.46
1	B	194	TYR	N-CA	7.81	1.55	1.45
1	A	142	HIS	CD2-NE2	-7.62	1.29	1.37
1	A	264	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	214	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	20	GLN	C-N	-6.26	1.24	1.33
1	B	280	VAL	CA-CB	6.15	1.59	1.53
1	A	55	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	55	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	193	TYR	CA-C	6.05	1.59	1.52
1	A	286	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	264	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	153	HIS	CD2-NE2	-5.95	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	LEU	CA-C	-5.88	1.45	1.52
1	B	153	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	245	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	58	HIS	CD2-NE2	-5.22	1.32	1.37
1	B	58	HIS	CD2-NE2	-5.22	1.32	1.37
1	B	139	SER	C-N	-5.13	1.26	1.34
1	A	264	HIS	CG-ND1	-5.04	1.32	1.38

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	SER	O-C-N	-22.72	96.25	122.15
1	B	182	SER	CA-C-N	16.93	150.76	121.14
1	B	182	SER	C-N-CA	16.93	150.76	121.14
1	B	191	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	A	210	ASN	O-C-N	9.41	135.10	122.59
1	A	210	ASN	CA-CB-CG	9.34	121.94	112.60
1	B	176	ASN	OD1-CG-ND2	-9.27	113.33	122.60
1	A	224	VAL	N-CA-C	8.81	116.27	107.55
1	A	7	THR	CA-CB-CG2	8.56	125.05	110.50
1	B	175	ARG	CB-CG-CD	-8.27	92.29	111.30
1	B	136	LEU	CB-CA-C	-8.09	93.92	109.37
1	A	210	ASN	CB-CA-C	7.94	126.22	110.42
1	A	20	GLN	CA-C-O	-7.76	112.53	121.07
1	A	230	ASP	CA-CB-CG	7.67	120.27	112.60
1	A	149	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	20	GLN	O-C-N	-7.45	114.11	122.08
1	B	53	ARG	CA-CB-CG	-7.40	99.29	114.10
1	A	224	VAL	CB-CA-C	7.38	119.75	111.04
1	B	7	THR	CA-CB-CG2	7.28	122.87	110.50
1	B	15	GLU	O-C-N	-7.22	113.46	122.20
1	B	191	ASN	CB-CG-ND2	7.22	127.22	116.40
1	B	29	VAL	CB-CA-C	-7.19	102.30	112.22
1	A	235	PHE	CB-CA-C	-7.19	95.12	109.35
1	A	20	GLN	CA-CB-CG	-6.88	100.33	114.10
1	A	149	ASP	O-C-N	-6.81	115.31	122.94
1	A	29	VAL	CB-CA-C	-6.81	102.82	112.22
1	A	63	VAL	N-CA-C	-6.68	106.01	112.29
1	A	233	PRO	CA-C-N	6.65	129.17	122.66
1	A	233	PRO	C-N-CA	6.65	129.17	122.66
1	B	165	ARG	CA-CB-CG	6.64	127.38	114.10
1	B	29	VAL	N-CA-CB	6.64	120.54	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	MET	CA-CB-CG	-6.63	100.83	114.10
1	A	209	VAL	O-C-N	6.58	130.18	123.20
1	A	81	VAL	N-CA-C	6.56	117.29	108.11
1	A	224	VAL	CA-C-N	6.55	128.03	119.84
1	A	224	VAL	C-N-CA	6.55	128.03	119.84
1	A	20	GLN	N-CA-C	6.53	118.99	111.02
1	B	269	ASP	N-CA-CB	6.48	121.43	110.49
1	B	102	ARG	CA-CB-CG	6.47	127.03	114.10
1	A	69	VAL	N-CA-CB	6.46	119.33	110.54
1	A	15	GLU	CA-C-N	-6.40	112.07	120.13
1	A	15	GLU	C-N-CA	-6.40	112.07	120.13
1	B	7	THR	CA-CB-OG1	-6.39	100.02	109.60
1	A	153	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	B	52	LEU	N-CA-CB	-6.32	100.85	110.33
1	A	234	GLY	N-CA-C	-6.32	99.17	111.12
1	B	100	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	B	7	THR	N-CA-CB	-6.31	100.84	110.12
1	A	269	ASP	CA-C-N	-6.31	112.13	122.54
1	A	269	ASP	C-N-CA	-6.31	112.13	122.54
1	A	240	LEU	N-CA-CB	-6.30	99.83	110.99
1	B	41	THR	N-CA-CB	-6.24	100.79	109.97
1	B	20	GLN	N-CA-C	6.24	121.66	111.37
1	B	225	PRO	N-CA-C	6.17	122.10	113.53
1	A	223	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	191	ASN	CA-CB-CG	5.99	118.59	112.60
1	B	107	PHE	CA-CB-CG	-5.93	107.87	113.80
1	B	136	LEU	O-C-N	5.90	130.90	123.23
1	A	267	LEU	O-C-N	5.86	129.96	123.16
1	B	104	GLU	CA-C-N	5.82	125.68	119.28
1	B	104	GLU	C-N-CA	5.82	125.68	119.28
1	A	20	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	B	136	LEU	N-CA-C	5.80	118.86	109.40
1	A	183	THR	N-CA-CB	-5.79	101.40	110.44
1	A	29	VAL	N-CA-CB	5.76	119.22	110.58
1	B	211	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	B	28	ARG	CA-C-O	-5.74	114.79	120.82
1	B	38	ARG	O-C-N	5.74	130.22	122.59
1	B	269	ASP	CA-C-O	-5.74	112.30	120.51
1	B	58	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	255	GLN	CA-CB-CG	-5.71	102.69	114.10
1	B	224	VAL	CA-C-N	5.70	125.37	119.05
1	B	224	VAL	C-N-CA	5.70	125.37	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	55	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	212	LYS	N-CA-C	5.68	117.98	108.73
1	B	229	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	B	82	THR	CB-CA-C	5.67	119.53	109.72
1	A	58	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	B	176	ASN	CB-CG-ND2	5.63	124.85	116.40
1	A	225	PRO	N-CA-C	5.63	124.06	112.47
1	B	129	GLY	N-CA-C	-5.62	106.00	112.29
1	A	158	LYS	N-CA-CB	-5.62	101.93	110.07
1	B	149	ASP	O-C-N	-5.57	116.50	122.85
1	A	291	THR	CA-C-O	-5.56	114.07	120.24
1	B	183	THR	N-CA-CB	-5.54	101.37	110.40
1	A	235	PHE	N-CA-C	5.51	118.44	109.24
1	A	47	TRP	CB-CG-CD1	-5.46	118.71	126.90
1	B	272	PRO	N-CA-C	5.45	119.79	111.34
1	B	210	ASN	CB-CA-C	5.45	122.27	115.79
1	B	274	ARG	N-CA-C	-5.45	100.06	109.15
1	B	280	VAL	CA-CB-CG2	5.44	119.65	110.40
1	A	153	HIS	CB-CG-ND1	5.43	130.84	122.70
1	B	227	ALA	N-CA-C	5.42	119.20	112.59
1	A	264	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	274	ARG	CA-C-N	5.39	125.39	119.89
1	A	274	ARG	C-N-CA	5.39	125.39	119.89
1	B	269	ASP	CA-C-N	-5.39	113.28	122.56
1	B	269	ASP	C-N-CA	-5.39	113.28	122.56
1	A	47	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	A	159	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	22	ALA	N-CA-C	5.37	119.00	112.23
1	A	55	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	B	264	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	152	GLU	N-CA-C	5.33	117.09	111.28
1	A	142	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	210	ASN	CA-C-N	5.27	131.60	121.54
1	A	210	ASN	C-N-CA	5.27	131.60	121.54
1	B	214	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	159	ASN	CB-CG-ND2	5.25	124.27	116.40
1	B	268	GLY	N-CA-C	-5.23	100.78	113.18
1	A	245	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	43	GLU	CB-CA-C	-5.21	102.69	110.88
1	A	245	HIS	CA-C-O	5.21	126.53	120.49
1	A	188	PRO	O-C-N	5.20	129.46	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ASP	N-CA-C	-5.20	100.25	108.73
1	A	20	GLN	CG-CD-NE2	5.19	124.19	116.40
1	A	20	GLN	CA-C-N	-5.18	114.93	122.86
1	A	20	GLN	C-N-CA	-5.18	114.93	122.86
1	B	287	VAL	CB-CA-C	5.18	118.12	110.77
1	B	188	PRO	O-C-N	5.16	129.41	123.06
1	B	55	HIS	CA-CB-CG	-5.16	108.64	113.80
1	B	20	GLN	CA-C-N	-5.16	114.54	123.25
1	B	20	GLN	C-N-CA	-5.16	114.54	123.25
1	A	239	ARG	N-CA-CB	-5.12	102.00	111.53
1	A	248	ALA	CB-CA-C	-5.12	102.84	110.88
1	B	210	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	30	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	B	224	VAL	CB-CA-C	5.08	116.62	110.78
1	B	15	GLU	N-CA-C	5.07	119.69	111.37
1	A	38	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	149	ASP	N-CA-C	-5.06	103.72	110.55
1	A	180	ILE	CB-CG1-CD1	5.02	124.34	113.80
1	A	20	GLN	N-CA-CB	5.01	117.43	109.82

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

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	50	0
2	A	4	0	3	1	0
2	B	4	0	3	2	0
3	A	27	0	22	1	0
3	B	27	0	22	6	0
4	A	59	0	0	0	0
4	B	35	0	0	1	0
All	All	4724	0	4535	92	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 (92) 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	1.36
1:A:227:ALA:HB3	1:A:234:GLY:HA3	1.58	0.86
2:B:294:ACT:CH3	3:B:293:SAM:HE1	2.10	0.81
2:B:294:ACT:H3	3:B:293:SAM:HE1	1.63	0.81
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:LYS:HZ2	1:B:96:LYS:HB2	1.71	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:B:209:VAL:HB	1:B:212:LYS:HZ3	1.73	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
1:A:29:VAL:CG1	1:A:236:SER:HB2	2.41	0.50
1:B:48:LEU:HD23	1:B:73:MET:HE1	1.94	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:55:HIS:HD2	1:B:289:LYS:HZ1	1.65	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: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
1:B:209:VAL:HB	1:B:212:LYS:NZ	2.35	0.41
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: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%)	18	19
1	B	290/292 (99%)	271 (93%)	18 (6%)	1 (0%)	36	42
All	All	580/584 (99%)	541 (93%)	36 (6%)	3 (0%)	24	27

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 ⓘ

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%)	207 (86%)	35 (14%)	3	2
1	B	242/242 (100%)	206 (85%)	36 (15%)	3	2
All	All	484/484 (100%)	413 (85%)	71 (15%)	3	2

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	10	LEU
1	A	15	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	103	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	181	LEU
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	267	LEU
1	A	274	ARG
1	A	280	VAL
1	A	287	VAL
1	A	288	LEU
1	B	7	THR
1	B	10	LEU
1	B	15	GLU
1	B	29	VAL
1	B	36	ASP
1	B	43	GLU
1	B	49	LEU
1	B	60	VAL
1	B	81	VAL
1	B	82	THR
1	B	91	LEU
1	B	95	LEU
1	B	96	LYS
1	B	116	ASN
1	B	118	LEU
1	B	128	ASP
1	B	134	ILE
1	B	136	LEU
1	B	169	LEU
1	B	175	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	181	LEU
1	B	195	LYS
1	B	198	LEU
1	B	211	ASN
1	B	212	LYS
1	B	224	VAL
1	B	229	ARG
1	B	240	LEU
1	B	253	LEU
1	B	265	SER
1	B	266	VAL
1	B	271	LYS
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	116	ASN
1	A	142	HIS
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	54	GLN
1	B	55	HIS
1	B	100	ASN
1	B	116	ASN
1	B	138	ASN
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN
1	B	210	ASN
1	B	211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	214	HIS
1	B	245	HIS
1	B	255	GLN
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 oligosaccharides 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	$\# Z > 2$
3	SAM	A	293	-	27,29,29	1.35	4 (14%)	34,42,42	1.38	3 (8%)
3	SAM	B	293	-	27,29,29	1.69	4 (14%)	34,42,42	2.20	6 (17%)
2	ACT	B	294	-	3,3,3	0.82	0	3,3,3	0.92	0
2	ACT	A	294	-	3,3,3	0.82	0	3,3,3	0.92	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	-	-	6/17/33/33	0/3/3/3
3	SAM	A	293	-	-	8/17/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	293	SAM	C1'-N9	6.81	1.65	1.46
3	A	293	SAM	C5'-C4'	-3.13	1.44	1.53
3	A	293	SAM	C3'-C4'	2.65	1.59	1.53
3	B	293	SAM	C3'-C4'	2.39	1.59	1.53
3	A	293	SAM	C1'-N9	2.36	1.52	1.46
3	A	293	SAM	OXT-C	-2.33	1.23	1.30
3	B	293	SAM	C5'-C4'	-2.31	1.46	1.53
3	B	293	SAM	OXT-C	-2.26	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	SAM	C2'-C1'-N9	6.33	129.04	113.30
3	A	293	SAM	O4'-C1'-N9	5.93	119.48	108.09
3	B	293	SAM	O4'-C1'-N9	5.61	118.86	108.09
3	B	293	SAM	C1'-N9-C8	5.58	139.47	127.09
3	B	293	SAM	C4-N9-C1'	-5.14	114.62	126.63
3	B	293	SAM	CG-SD-C5'	3.79	112.70	103.43
3	B	293	SAM	OXT-C-O	-2.82	117.69	124.08
3	A	293	SAM	OXT-C-O	-2.71	117.93	124.08
3	A	293	SAM	C4-N9-C1'	2.20	131.78	126.63

There are no chirality outliers.

All (14) 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	B	293	SAM	C4'-C5'-SD-CE
3	A	293	SAM	OXT-C-CA-N
3	A	293	SAM	OXT-C-CA-CB
3	B	293	SAM	O-C-CA-CB
3	A	293	SAM	O-C-CA-CB
3	B	293	SAM	O4'-C4'-C5'-SD
3	B	293	SAM	C3'-C4'-C5'-SD

Continued on next page...

Continued from previous page...

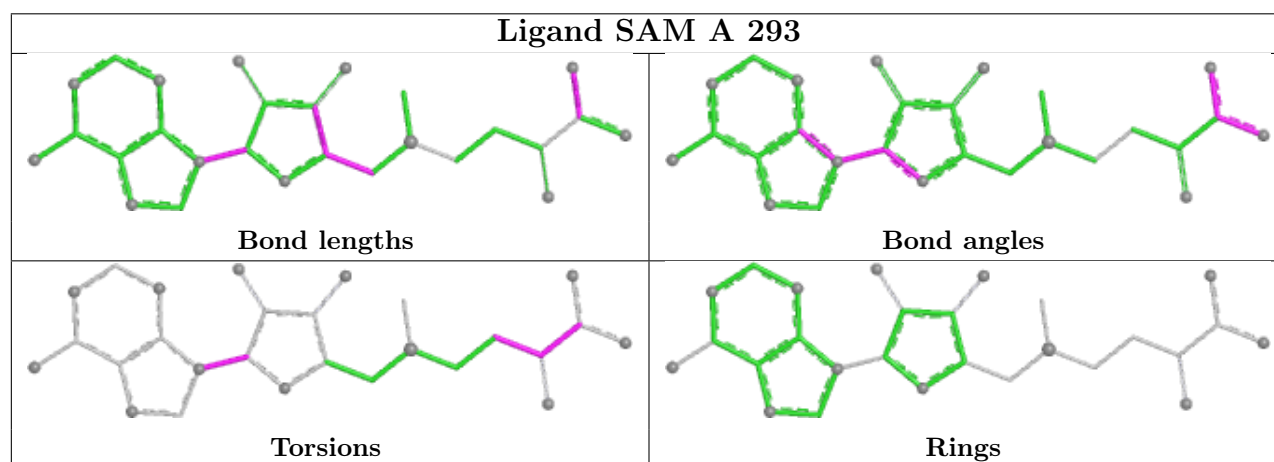
Mol	Chain	Res	Type	Atoms
3	B	293	SAM	OXT-C-CA-CB
3	B	293	SAM	C-CA-CB-CG
3	A	293	SAM	O4'-C1'-N9-C8
3	A	293	SAM	O4'-C1'-N9-C4

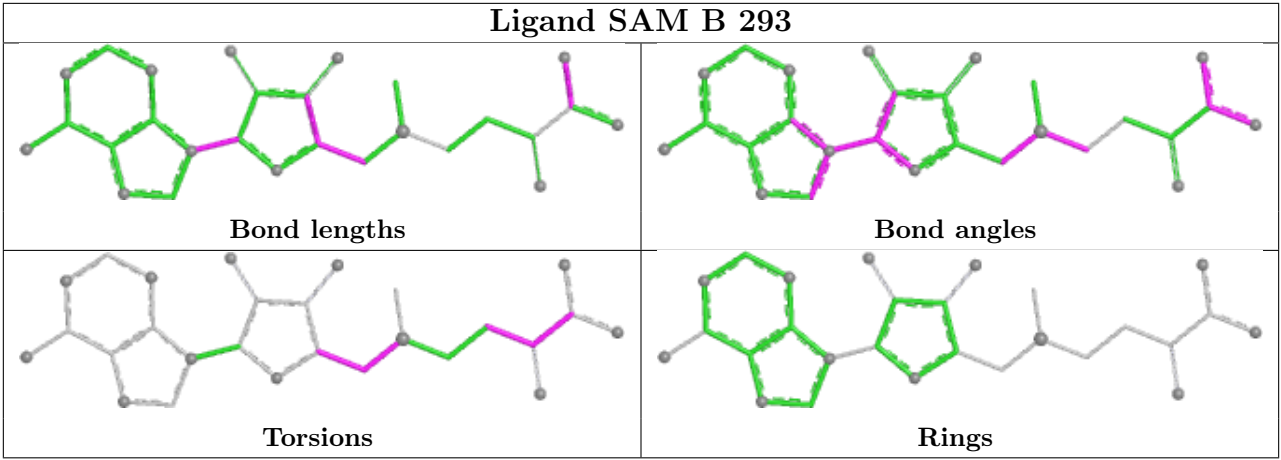
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	293	SAM	1	0
3	B	293	SAM	6	0
2	B	294	ACT	2	0
2	A	294	ACT	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.