



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:16 AM UTC

PDB ID : 1D2H / pdb\_00001d2h  
Title : CRYSTAL STRUCTURE OF R175K MUTANT GLYCINE N-METHYLTRANSFERASE COMPLEXED WITH S-ADENOSYLHOMOCYSTEINE  
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Deposited on : 1999-10-11  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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<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>.

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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)  
Xtrriage (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

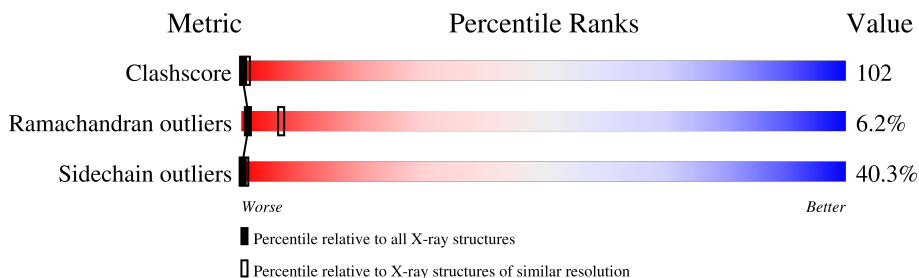
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	292	13% 44% 27% • 14%
1	B	292	11% 47% 26% • 14%
1	C	292	20% 38% 27% • 14%
1	D	292	13% 46% 25% • 14%

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	SAH	A	1301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8492 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	252	1970	1257	339	363	11	0	0	0
1	B	252	1970	1257	339	363	11	0	0	0
1	C	252	1970	1257	339	363	11	0	0	0
1	D	252	1970	1257	339	363	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LYS	ARG	engineered mutation	UNP P13255
B	89	LYS	ARG	engineered mutation	UNP P13255
C	89	LYS	ARG	engineered mutation	UNP P13255
D	89	LYS	ARG	engineered mutation	UNP P13255

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



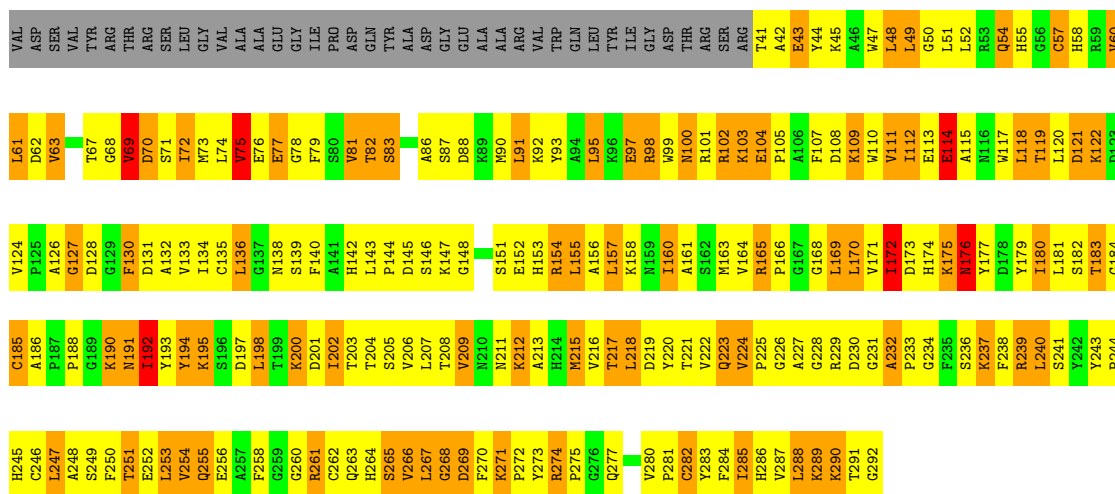
### 3 Residue-property plots

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.

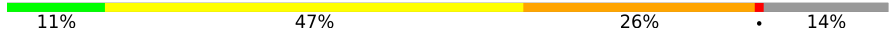
Note EDS was not executed.

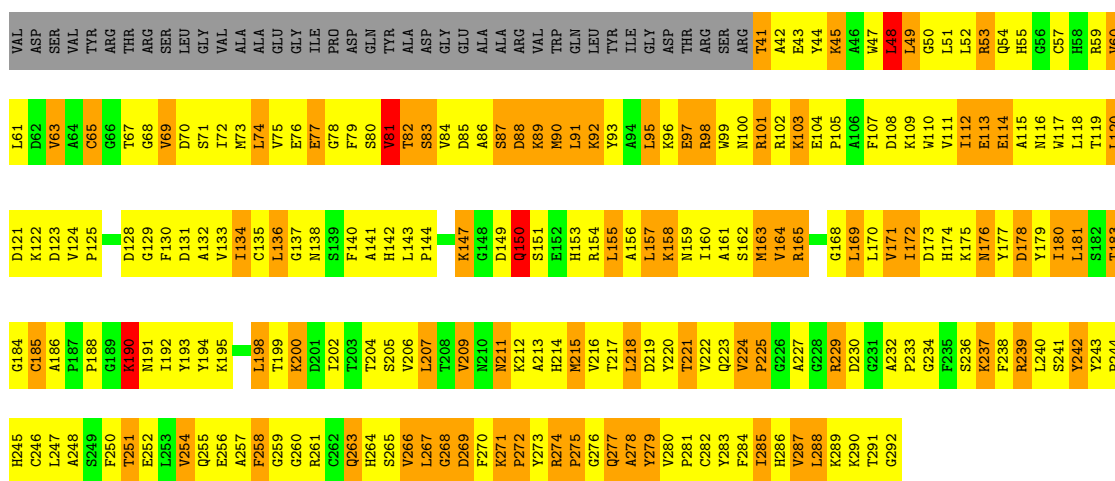
#### • Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain A: 

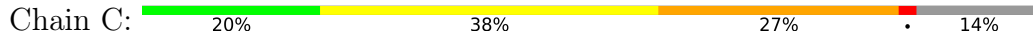


#### • Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain B: 



#### • Molecule 1: GLYCINE N-METHYLTRANSFERASE



VAL	ASP	SER	VAL	TYR	ARG	THR	THR	ARG	SER	SER	LEU	GLY	LEU	VAL	ALA	ALA	GLU	GLY	ILE	PRO	ASP	GLN	GLY	GLY	ALA	ALA	ARG	VAL	TRP	GLN	LEU	TYR	ILE	GLY	ASP	THR	ARG	SER	ARG	T41	A42	E43	Y44	K45	A46	W47	L48	L49	G50	L51	L52	R53	Q54	Q54	V60	L61	A64	C65			
G66	T67	G68	V69	D70	S71	L72	M73	L74	W75	E76	F79	S80	W81	T82	S83	V84	D85	A86	S87	D88	R89	M90	L91	K92	Y93	A94	A94	L95	E97	G97	L98	M99	M100	R101	R102	R103	E104	P105	A106	G106	F107	D108	K109	W110	V111	I112	W113	E114	W117	W117	L118	L118	T119	L120	D121	K122	L123	V124	P125	A126	G127
D128	G129	F130	D131	A132	Y133	L134	C135	L136	G137	S138	F139	L143	P144	H145	S146	K147	G148	D149	Q150	S151	E152	H153	R154	L155	A156	L157	K158	N159	I160	A161	V164	G165	P166	G167	G168	L169	L170	L171	V172	D173	H174	K175	M176	Y177	D178	Y179	I180	L181	S182	T183	G184	C185	P188	A126	G189						
K190	N191	I192	Y193	K194	K195	L196	T199	K200	D201	L202	T203	T204	S205	D206	L207	T208	W209	N210	R211	K212	A213	H214	M215	V216	T217	Y220	T221	W222	Q223	V224	P225	G226	A227	G228	R229	D230	G231	A232	P233	G234	F235	S236	K237	L240	S241	Y242	Y243	H244	H245	C246	L247	A248	S249	F250	T251						
V254	Q255	E256	A257	G260	K261	Q262	Q263	H264	S265	V266	L267	G268	D269	F270	Y273	R274	Q277	A278	V279	P281	C282	L285	L288	K289	R290	T291	G292																																		

● Molecule 1: GLYCINE N-METHYLTRANSFERASE



VAL	ASP	SER	VAL	TYR	ARG	THR	THR	ARG	SER	SER	LEU	GLY	LEU	VAL	ALA	ALA	GLU	GLY	ILE	PRO	ASP	GLN	GLY	GLY	ALA	ALA	ARG	VAL	TRP	GLN	LEU	TYR	ILE	GLY	ASP	THR	ARG	SER	ARG	T41	A42	E43	Y44	K45	A46	W47	L48	L49	G50	L51	L52	R53	Q54	Q54	H55	H55	G56	C57	H58	R59	L120	F189	V60
L61	D62	V63	A64	C65	G66	T67	G68	S71	I72	M73	L74	V75	E77	G78	F79	S80	W81	T82	S83	V84	D85	A86	S87	D88	R89	L91	K92	Y93	A94	L95	E97	G97	R98	W99	M100	R101	R102	K103	V104	E104	P105	A106	F107	G108	L109	W110	V111	I112	W113	E114	A115	N116	W117	L118	T119	L120	D121						
K122	D123	V124	A125	G126	D128	G129	F130	S131	A132	V133	L134	C135	L136	S139	F140	A141	H142	L143	P144	D145	S146	K147	G148	D149	Q150	S151	E152	H153	R154	L155	A156	L157	K158	N159	I160	A161	M163	V164	R165	P166	G167	G168	L169	L170	W171	I172	D173	H174	K175	P244	N176	Y177	D178	Y179	I180	L181	S182						
T183	G184	A186	P187	P188	G189	K190	H191	I192	Y193	G194	K195	S196	D197	L198	L199	K200	D201	L202	T203	T204	S205	V206	L207	T208	V209	N210	N211	V216	T217	L218	D219	Y220	T221	V222	Q223	V224	P225	G226	A227	G228	D230	G231	A232	P233	G234	K237	F238	R239	L240	S241	Y242	Y243	P244	H245	C246								
L247	F250	E252	L253	V254	Q255	E256	A257	F258	G259	G260	R261	C262	Q263	H264	S265	V266	L267	G268	Y273	R274	P275	G276	Q277	A278	Y279	V280	P281	C282	Y283	F284	I285	H286	V287	L288	K289	K290	T291	G292																									

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.90Å 77.90Å 227.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	92.5 (10.00-3.00)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: 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	0.37	0/2020	0.93	7/2737 (0.3%)
1	B	0.35	0/2020	0.90	6/2737 (0.2%)
1	C	0.36	0/2020	0.84	6/2737 (0.2%)
1	D	0.36	0/2020	0.86	4/2737 (0.1%)
All	All	0.36	0/8080	0.88	23/10948 (0.2%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	GLY	N-CA-C	-10.28	95.03	112.30
1	A	268	GLY	N-CA-C	-8.98	97.22	112.30
1	D	81	VAL	N-CA-C	7.65	119.59	108.58
1	B	81	VAL	N-CA-C	6.99	118.19	107.99
1	C	81	VAL	N-CA-C	6.68	117.74	108.12

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	1970	0	1941	423	0
1	B	1970	0	1941	394	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1970	0	1941	398	0
1	D	1970	0	1941	423	0
2	A	26	0	19	10	0
2	B	26	0	19	5	0
2	C	26	0	19	5	0
2	D	26	0	19	6	0
3	A	157	0	0	6	0
3	B	119	0	0	4	0
3	C	114	0	0	3	0
3	D	118	0	0	3	0
All	All	8492	0	7840	1610	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 102.

The worst 5 of 1610 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:247:LEU:HD12	1:A:247:LEU:O	1.23	1.36
1:C:193:TYR:HB3	1:C:194:TYR:CE1	1.62	1.34
1:A:247:LEU:HD12	1:A:247:LEU:C	1.46	1.32
1:C:223:GLN:HB2	1:C:235:PHE:CE2	1.65	1.31
1:A:122:LYS:HA	1:A:122:LYS:NZ	1.49	1.26

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	250/292 (86%)	185 (74%)	49 (20%)	16 (6%)	<b>1</b> <b>6</b>
1	B	250/292 (86%)	186 (74%)	49 (20%)	15 (6%)	<b>1</b> <b>7</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	250/292 (86%)	187 (75%)	50 (20%)	13 (5%)	1	9
1	D	250/292 (86%)	184 (74%)	48 (19%)	18 (7%)	1	4
All	All	1000/1168 (86%)	742 (74%)	196 (20%)	62 (6%)	1	6

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	269	ASP
1	B	269	ASP
1	C	261	ARG
1	D	48	LEU

### 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	211/242 (87%)	121 (57%)	90 (43%)	0	0
1	B	211/242 (87%)	124 (59%)	87 (41%)	0	0
1	C	211/242 (87%)	127 (60%)	84 (40%)	0	1
1	D	211/242 (87%)	132 (63%)	79 (37%)	0	1
All	All	844/968 (87%)	504 (60%)	340 (40%)	0	0

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	202	ILE
1	D	122	LYS
1	C	229	ARG
1	C	290	LYS
1	D	173	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	176	ASN
1	D	116	ASN
1	C	210	ASN
1	C	263	GLN
1	D	159	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 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
2	SAH	D	4301	-	27,28,28	1.11	2 (7%)	36,40,40	2.30	9 (25%)
2	SAH	C	3301	-	27,28,28	1.02	1 (3%)	36,40,40	2.46	13 (36%)
2	SAH	A	1301	-	27,28,28	1.09	2 (7%)	36,40,40	2.63	12 (33%)
2	SAH	B	2301	-	27,28,28	1.09	1 (3%)	36,40,40	2.25	6 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	D	4301	-	-	6/15/31/31	0/3/3/3
2	SAH	C	3301	-	-	7/15/31/31	0/3/3/3
2	SAH	A	1301	-	-	3/15/31/31	0/3/3/3
2	SAH	B	2301	-	-	4/15/31/31	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	SAH	C5-N7	-3.66	1.32	1.39
2	D	4301	SAH	C5-N7	-3.63	1.32	1.39
2	A	1301	SAH	C5-N7	-3.58	1.32	1.39
2	C	3301	SAH	C5-N7	-3.23	1.33	1.39
2	D	4301	SAH	C4-N9	-2.12	1.33	1.37

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	SAH	C5-C4-N3	-7.25	116.74	126.72
2	B	2301	SAH	C5-C4-N3	-7.08	116.97	126.72
2	D	4301	SAH	C5-C4-N3	-6.93	117.18	126.72
2	C	3301	SAH	C5-C4-N3	-6.75	117.42	126.72
2	A	1301	SAH	N3-C4-N9	6.45	138.13	127.17

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

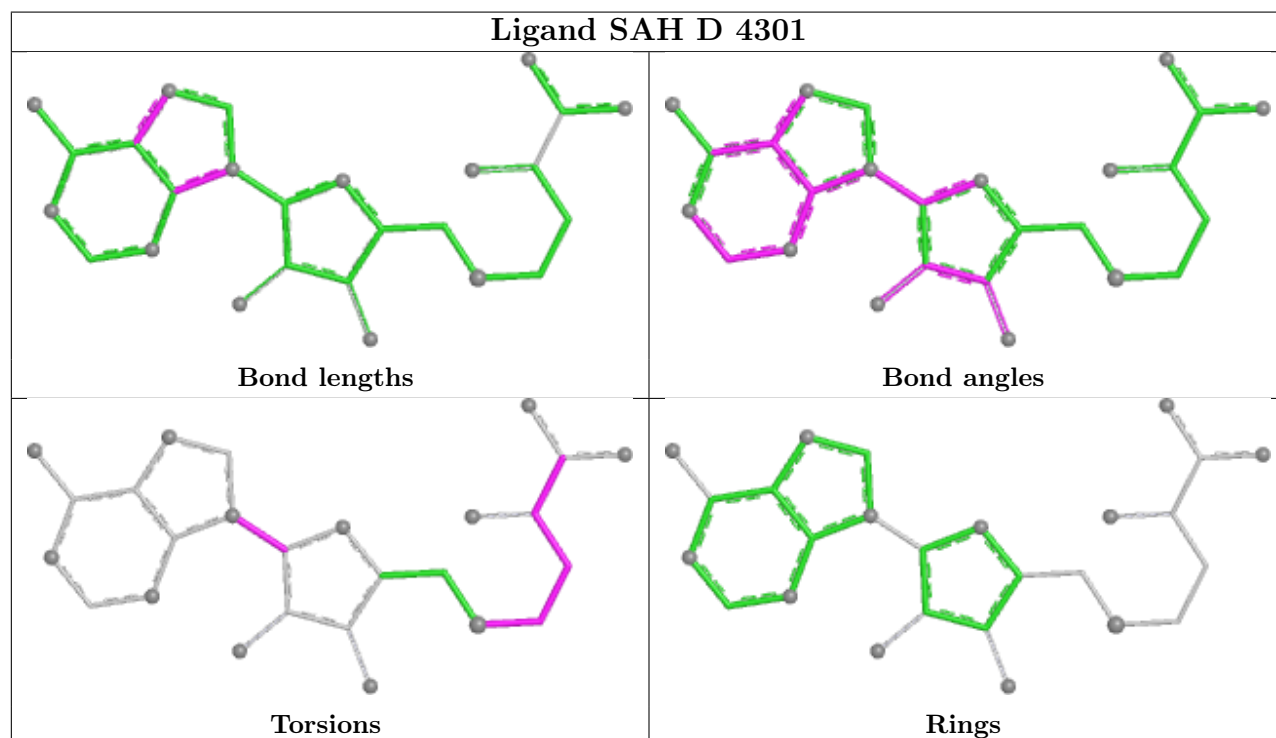
Mol	Chain	Res	Type	Atoms
2	A	1301	SAH	O4'-C4'-C5'-SD
2	A	1301	SAH	C3'-C4'-C5'-SD
2	C	3301	SAH	N-CA-CB-CG
2	C	3301	SAH	C-CA-CB-CG
2	C	3301	SAH	O-C-CA-N

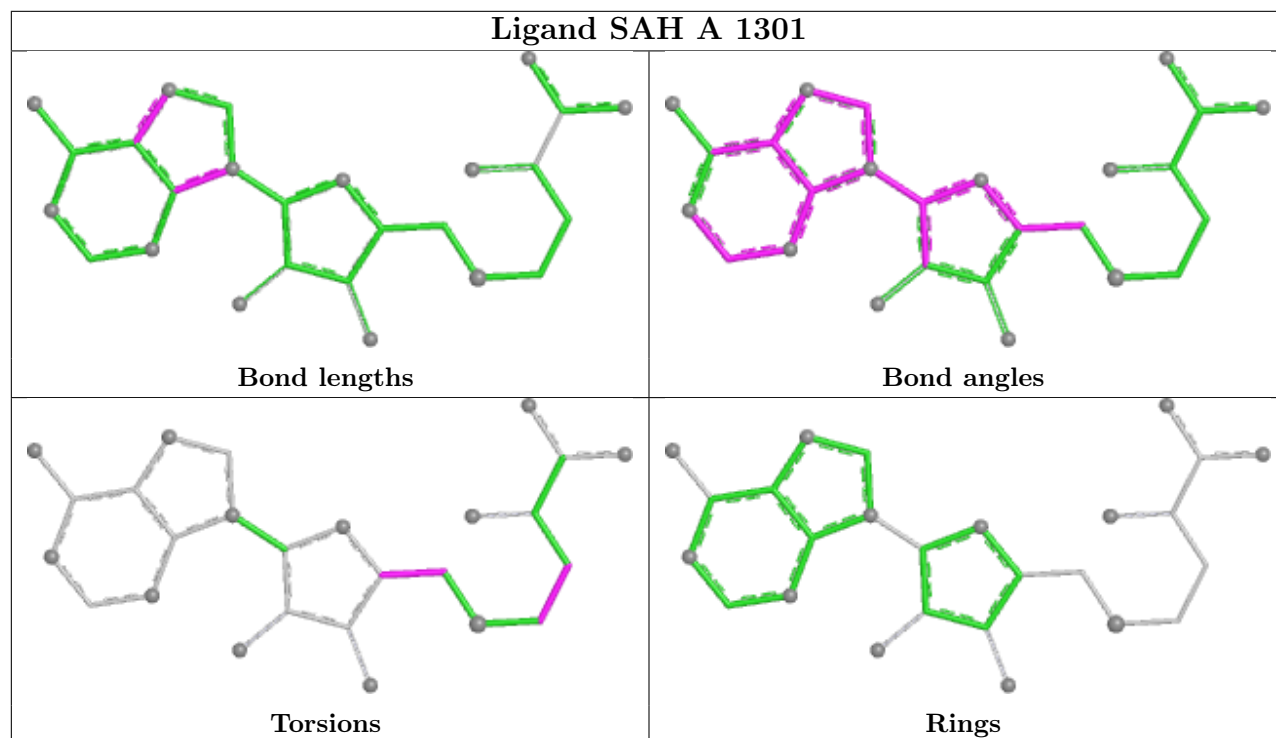
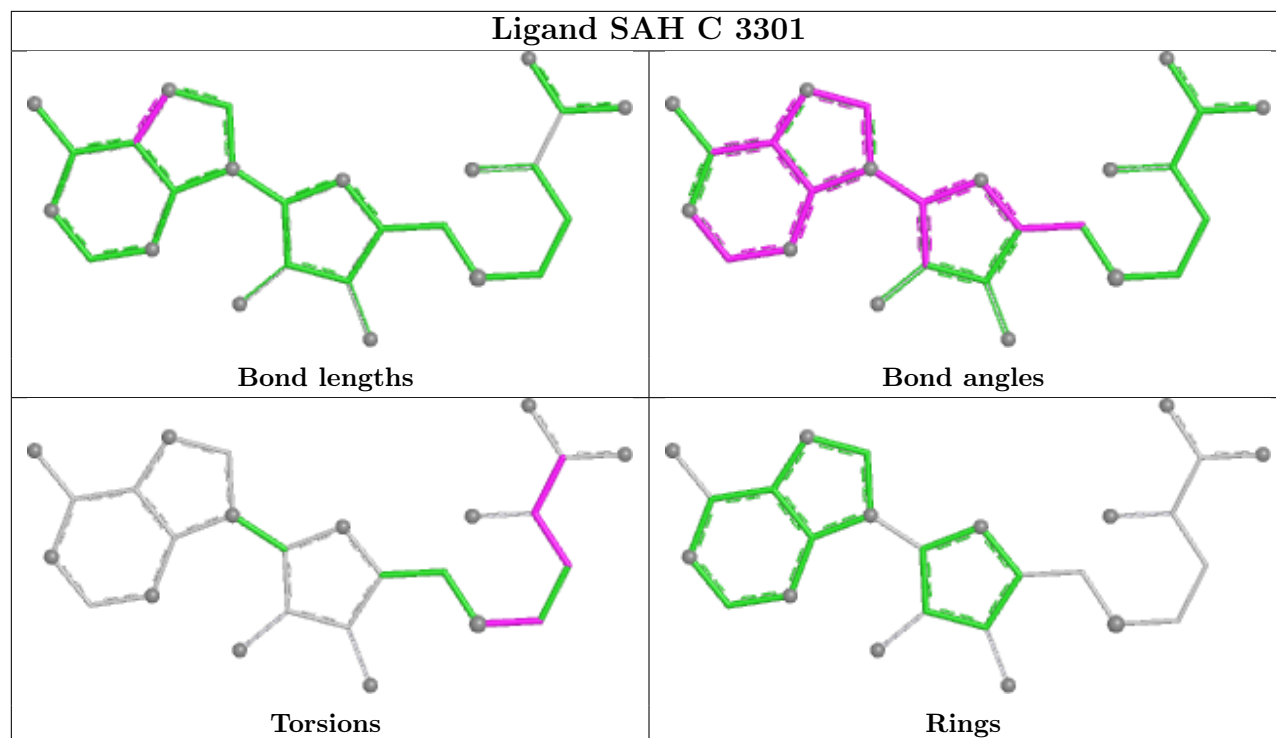
There are no ring outliers.

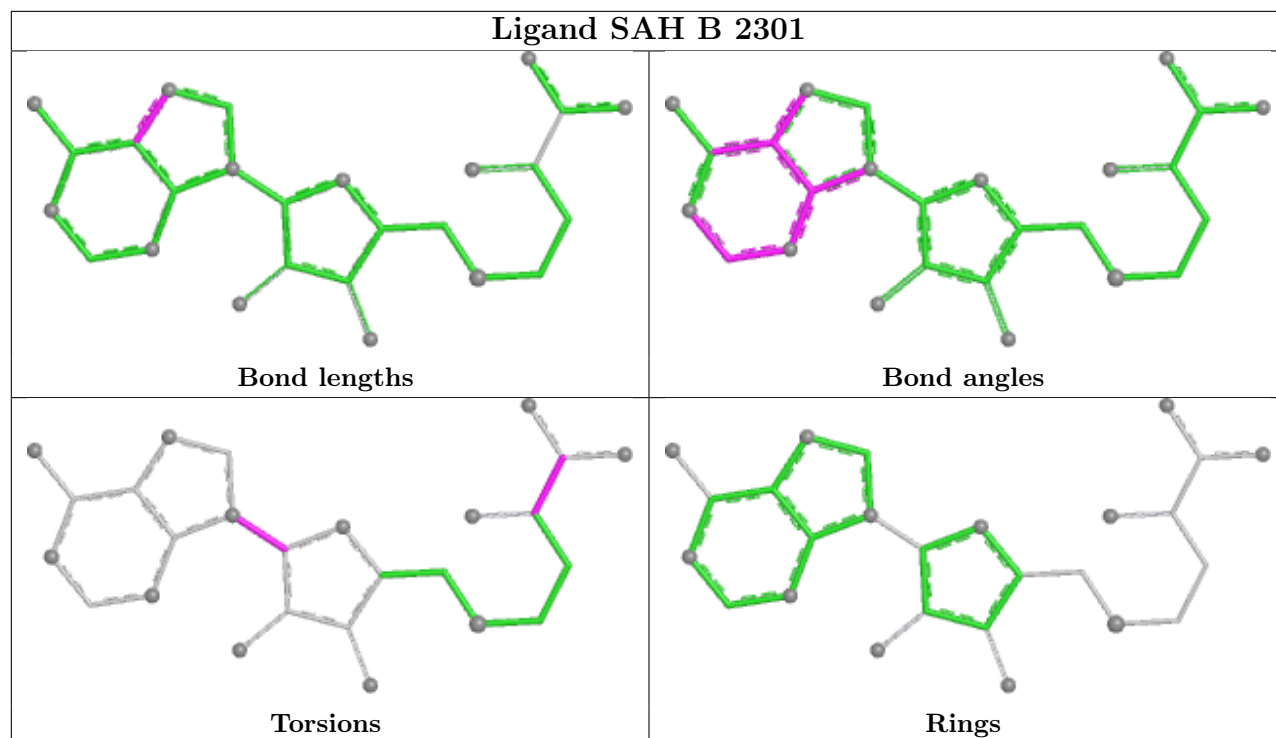
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4301	SAH	6	0
2	C	3301	SAH	5	0
2	A	1301	SAH	10	0
2	B	2301	SAH	5	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

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.