



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:41 PM UTC

PDB ID : 1YFJ / pdb_00001yfq
Title : T4Dam in Complex with AdoHcy and 15-mer Oligonucleotide Showing Semi-specific and Specific Contact
Authors : Horton, J.R.; Liebert, K.; Hattman, S.; Jeltsch, A.; Cheng, X.
Deposited on : 2005-01-02
Resolution : 2.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

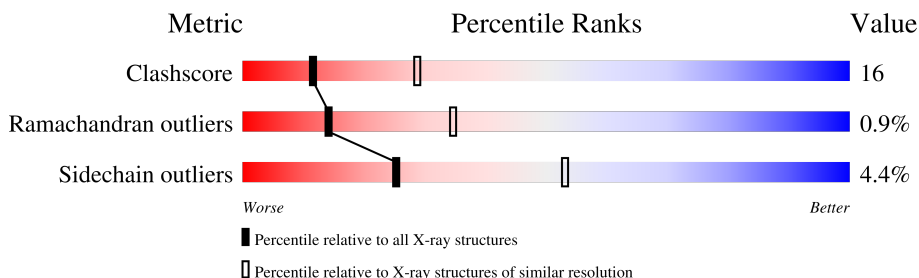
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	0	15	
1	1	15	
1	2	15	
1	3	15	
1	4	15	
1	5	15	
1	6	15	
1	7	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	15	47%47%7%
1	9	15	40%60%
2	A	259	72%25%. .
2	B	259	72%26%. .
2	C	259	75%22%. .
2	D	259	71%24%. . .
2	E	259	60%30%. .6%
2	F	259	57%34%. .6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15008 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 DNA chain called 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	2	15	Total	C	N	O	P	0	0	0
			308	146	55	92	15			
1	3	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	4	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	5	14	Total	C	N	O	P	0	0	0
			284	136	53	82	13			
1	6	15	Total	C	N	O	P	0	0	0
			290	136	50	89	15			
1	7	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	8	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	9	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	0	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			

- Molecule 2 is a protein called DNA adenine methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	259	Total	C	N	O	S	0	0	0
			2108	1362	355	386	5			
2	B	259	Total	C	N	O	S	0	0	0
			2112	1366	355	386	5			
2	C	259	Total	C	N	O	S	0	0	0
			2091	1351	353	382	5			
2	D	254	Total	C	N	O	S	0	0	0
			1981	1272	334	370	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	243	Total	C	N	O	S	0	0	0
			1833	1180	310	338	5			
2	F	243	Total	C	N	O	S	0	0	0
			1368	824	275	268	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ARG	GLN	SEE REMARK 999	UNP P04392
A	140	PHE	TYR	SEE REMARK 999	UNP P04392
A	209	LEU	GLN	SEE REMARK 999	UNP P04392
B	139	ARG	GLN	SEE REMARK 999	UNP P04392
B	140	PHE	TYR	SEE REMARK 999	UNP P04392
B	209	LEU	GLN	SEE REMARK 999	UNP P04392
C	139	ARG	GLN	SEE REMARK 999	UNP P04392
C	140	PHE	TYR	SEE REMARK 999	UNP P04392
C	209	LEU	GLN	SEE REMARK 999	UNP P04392
D	139	ARG	GLN	SEE REMARK 999	UNP P04392
D	140	PHE	TYR	SEE REMARK 999	UNP P04392
D	209	LEU	GLN	SEE REMARK 999	UNP P04392
E	139	ARG	GLN	SEE REMARK 999	UNP P04392
E	140	PHE	TYR	SEE REMARK 999	UNP P04392
E	209	LEU	GLN	SEE REMARK 999	UNP P04392
F	139	ARG	GLN	SEE REMARK 999	UNP P04392
F	140	PHE	TYR	SEE REMARK 999	UNP P04392
F	209	LEU	GLN	SEE REMARK 999	UNP P04392

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	1	Total	Cl	0	0
			1	1		
3	2	2	Total	Cl	0	0
			2	2		
3	8	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

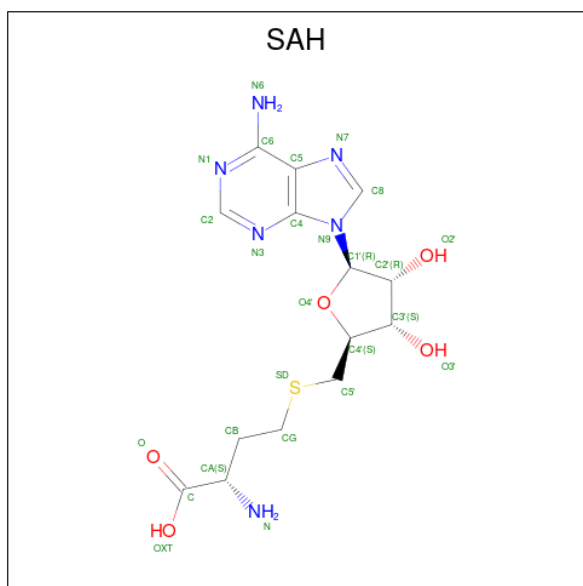
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	4	1	Total	Ca	0	0
			1	1		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	8	Total	O	0	0
			8	8		
6	2	7	Total	O	0	0
			7	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	3	8	Total 8	O 8	0	0
6	4	13	Total 13	O 13	0	0
6	5	2	Total 2	O 2	0	0
6	6	1	Total 1	O 1	0	0
6	7	1	Total 1	O 1	0	0
6	8	2	Total 2	O 2	0	0
6	A	98	Total 98	O 98	0	0
6	B	102	Total 102	O 102	0	0
6	C	60	Total 60	O 60	0	0
6	D	29	Total 29	O 29	0	0
6	E	11	Total 11	O 11	0	0
6	F	1	Total 1	O 1	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.

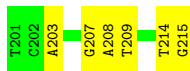
- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 1: 



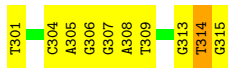
- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 2: 



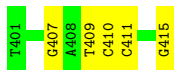
- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 3: 



- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 4: 



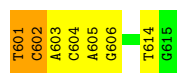
- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 5: 

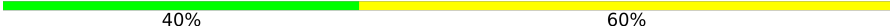


- Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 6: 

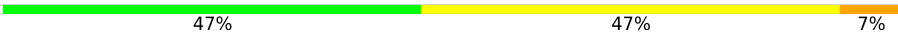


• Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 7: 



• Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 8: 



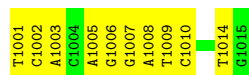
• Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 9: 



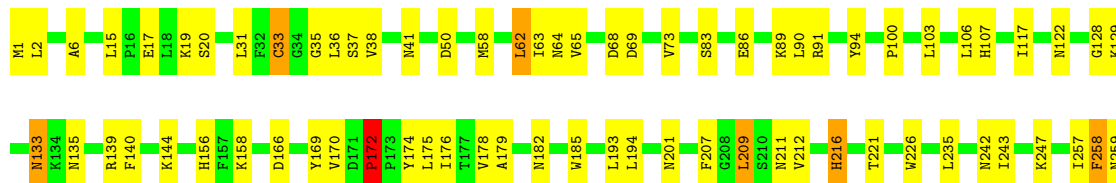
• Molecule 1: 5'-D(*TP*CP*AP*CP*AP*GP*GP*AP*TP*CP*CP*TP*GP*TP*G)-3'

Chain 0: 



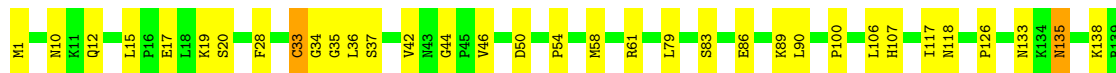
• Molecule 2: DNA adenine methylase

Chain A: 



• Molecule 2: DNA adenine methylase

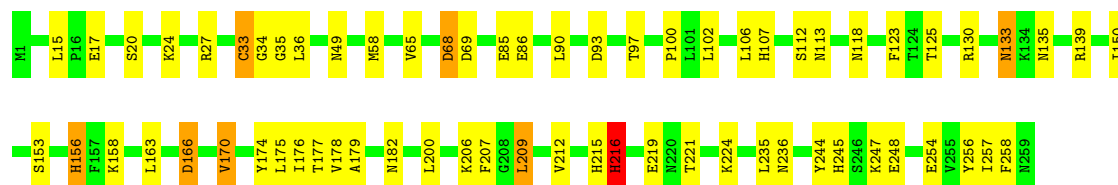
Chain B: 





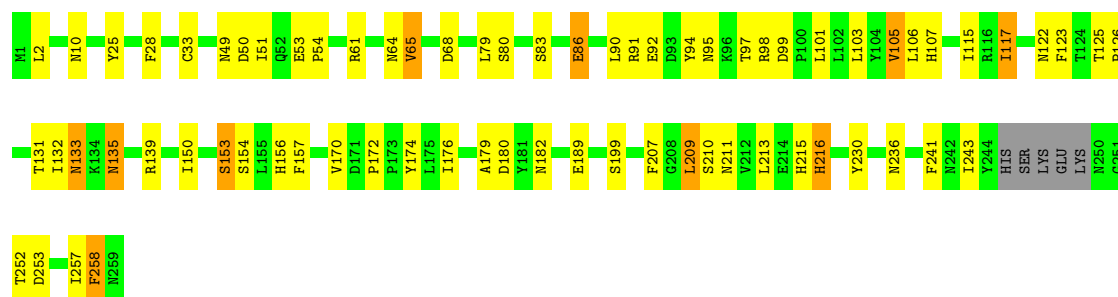
- Molecule 2: DNA adenine methylase

Chain C: 75% 22%



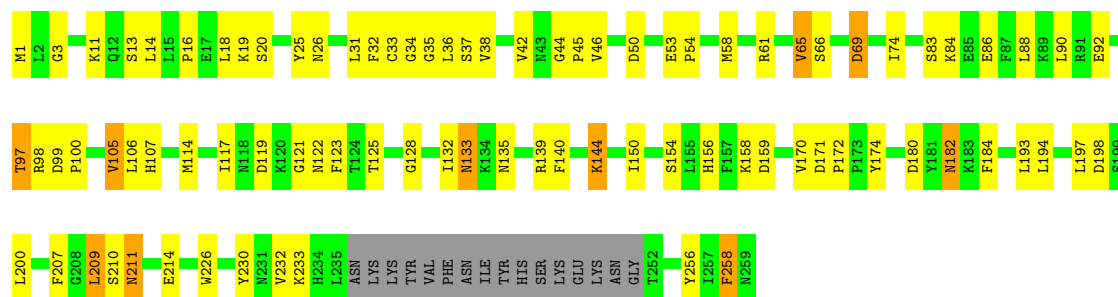
- Molecule 2: DNA adenine methylase

Chain D: 71% 24%



- Molecule 2: DNA adenine methylase

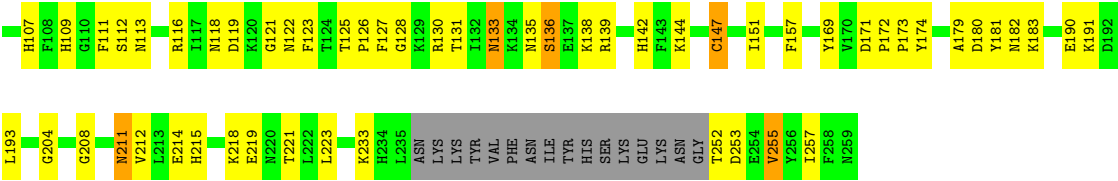
Chain E: 60% 30%



- Molecule 2: DNA adenine methylase

Chain F: 57% 34%





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 21	Depositor
Cell constants a, b, c, α , β , γ	111.20Å 133.00Å 189.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.78 – 2.69	Depositor
% Data completeness (in resolution range)	96.8 (34.78-2.69)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15008	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: SAH, CL, CA

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	0	0.34	0/340	0.72	0/523
1	1	0.43	0/340	0.88	0/523
1	2	0.48	0/344	0.93	2/527 (0.4%)
1	3	0.39	0/340	0.82	0/523
1	4	0.36	0/340	0.80	0/523
1	5	0.36	0/318	0.73	0/489
1	6	0.98	1/323 (0.3%)	1.76	6/495 (1.2%)
1	7	0.39	0/340	0.83	0/523
1	8	0.34	0/340	0.83	1/523 (0.2%)
1	9	0.32	0/340	0.73	0/523
2	A	0.71	0/2159	1.11	11/2918 (0.4%)
2	B	0.71	0/2164	1.08	4/2923 (0.1%)
2	C	0.67	0/2143	1.07	13/2898 (0.4%)
2	D	0.58	0/2028	1.06	10/2757 (0.4%)
2	E	0.54	0/1878	1.01	8/2560 (0.3%)
2	F	0.65	0/1386	1.18	7/1917 (0.4%)
All	All	0.62	1/15123 (0.0%)	1.05	62/21145 (0.3%)

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	1	0	2
1	3	0	1
1	4	0	1
1	7	0	1
1	8	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	601	DT	C3'-C2'	12.93	1.78	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	601	DT	C4'-C3'-O3'	24.69	147.04	110.00
1	6	601	DT	C2'-C3'-O3'	-18.54	83.70	111.50
2	B	150	ILE	N-CA-C	7.57	118.76	108.17
1	6	602	DC	P-O5'-C5'	-7.47	108.79	120.00
1	6	602	DC	P-O3'-C3'	-7.44	109.03	120.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	107	DG	Sidechain
1	1	112	DT	Sidechain
1	3	314	DT	Sidechain
1	4	407	DG	Sidechain
1	7	713	DG	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	0	304	0	171	16	0
1	1	304	0	171	2	0
1	2	308	0	170	6	0
1	3	304	0	171	11	0
1	4	304	0	171	6	0
1	5	284	0	159	9	0
1	6	290	0	158	11	0
1	7	304	0	171	12	0
1	8	304	0	171	7	0
1	9	304	0	171	14	0
2	A	2108	0	2058	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2112	0	2063	46	0
2	C	2091	0	2021	44	0
2	D	1981	0	1830	39	0
2	E	1833	0	1618	82	0
2	F	1368	0	745	91	0
3	1	1	0	0	0	0
3	2	2	0	0	0	0
3	8	1	0	0	0	0
4	2	1	0	0	0	0
4	4	1	0	0	0	0
5	A	26	0	19	0	0
5	B	26	0	19	1	0
5	C	26	0	19	0	0
5	D	26	0	19	1	0
5	E	26	0	19	0	0
5	F	26	0	19	7	0
6	1	8	0	0	0	0
6	2	7	0	0	0	0
6	3	8	0	0	0	0
6	4	13	0	0	0	0
6	5	2	0	0	0	0
6	6	1	0	0	0	0
6	7	1	0	0	0	0
6	8	2	0	0	0	0
6	A	98	0	0	2	0
6	B	102	0	0	2	0
6	C	60	0	0	2	0
6	D	29	0	0	0	0
6	E	11	0	0	1	0
6	F	1	0	0	0	0
All	All	15008	0	12133	427	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 16.

The worst 5 of 427 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)
1:6:601:DT:C3'	1:6:601:DT:C2'	1.78	1.32
1:6:602:DC:H2''	1:6:603:DA:OP2	1.33	1.14
1:7:703:DA:C2'	1:7:704:DC:H5''	1.75	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:SER:HB2	2:D:86:GLU:HG3	1.32	1.10
2:C:209:LEU:HD23	2:C:257:ILE:HB	1.44	0.99

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	
2	A	206/259 (80%)	194 (94%)	11 (5%)	1 (0%)	24	48
2	B	210/259 (81%)	202 (96%)	8 (4%)	0	100	100
2	C	191/259 (74%)	181 (95%)	10 (5%)	0	100	100
2	D	118/259 (46%)	106 (90%)	12 (10%)	0	100	100
2	E	217/259 (84%)	193 (89%)	21 (10%)	3 (1%)	9	23
2	F	150/259 (58%)	119 (79%)	25 (17%)	6 (4%)	2	5
All	All	1092/1554 (70%)	995 (91%)	87 (8%)	10 (1%)	14	35

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	136	SER
2	F	204	GLY
2	F	211	ASN
2	F	93	ASP
2	F	85	GLU

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	
2	A	230/242 (95%)	221 (96%)	9 (4%)	28	57
2	B	231/242 (96%)	224 (97%)	7 (3%)	36	66
2	C	226/242 (93%)	216 (96%)	10 (4%)	25	53
2	D	205/242 (85%)	193 (94%)	12 (6%)	18	42
2	E	175/242 (72%)	168 (96%)	7 (4%)	28	56
2	F	42/242 (17%)	38 (90%)	4 (10%)	8	20
All	All	1109/1452 (76%)	1060 (96%)	49 (4%)	25	53

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	68	ASP
2	D	153	SER
2	D	86	GLU
2	D	117	ILE
2	D	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	76	GLN
2	E	133	ASN
2	D	133	ASN
2	D	201	ASN
2	E	156	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SAH	B	402	-	27,28,28	1.48	3 (11%)	36,40,40	1.67	8 (22%)
5	SAH	C	403	-	27,28,28	1.50	4 (14%)	36,40,40	1.59	7 (19%)
5	SAH	E	405	-	27,28,28	1.48	5 (18%)	36,40,40	1.61	7 (19%)
5	SAH	A	401	-	27,28,28	1.65	7 (25%)	36,40,40	1.71	9 (25%)
5	SAH	F	406	-	27,28,28	1.53	4 (14%)	36,40,40	1.73	8 (22%)
5	SAH	D	404	-	27,28,28	1.58	5 (18%)	36,40,40	1.69	8 (22%)

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
5	SAH	B	402	-	-	0/15/31/31	0/3/3/3
5	SAH	C	403	-	-	1/15/31/31	0/3/3/3
5	SAH	E	405	-	-	2/15/31/31	0/3/3/3
5	SAH	A	401	-	-	1/15/31/31	0/3/3/3
5	SAH	F	406	-	-	0/15/31/31	0/3/3/3
5	SAH	D	404	-	-	0/15/31/31	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	SAH	C1'-N9	-4.84	1.33	1.46
5	B	402	SAH	C1'-N9	-4.56	1.33	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	SAH	C1'-N9	-4.40	1.34	1.46
5	F	406	SAH	C1'-N9	-4.19	1.34	1.46
5	E	405	SAH	C1'-N9	-4.07	1.35	1.46

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	SAH	O4'-C1'-C2'	-5.30	95.27	106.62
5	B	402	SAH	O4'-C1'-C2'	-4.74	96.47	106.62
5	D	404	SAH	O4'-C1'-C2'	-4.57	96.84	106.62
5	C	403	SAH	O4'-C1'-C2'	-4.46	97.08	106.62
5	F	406	SAH	O4'-C1'-C2'	-4.35	97.31	106.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	405	SAH	CA-CB-CG-SD
5	E	405	SAH	C2'-C1'-N9-C8
5	A	401	SAH	C2'-C1'-N9-C8
5	C	403	SAH	C2'-C1'-N9-C8

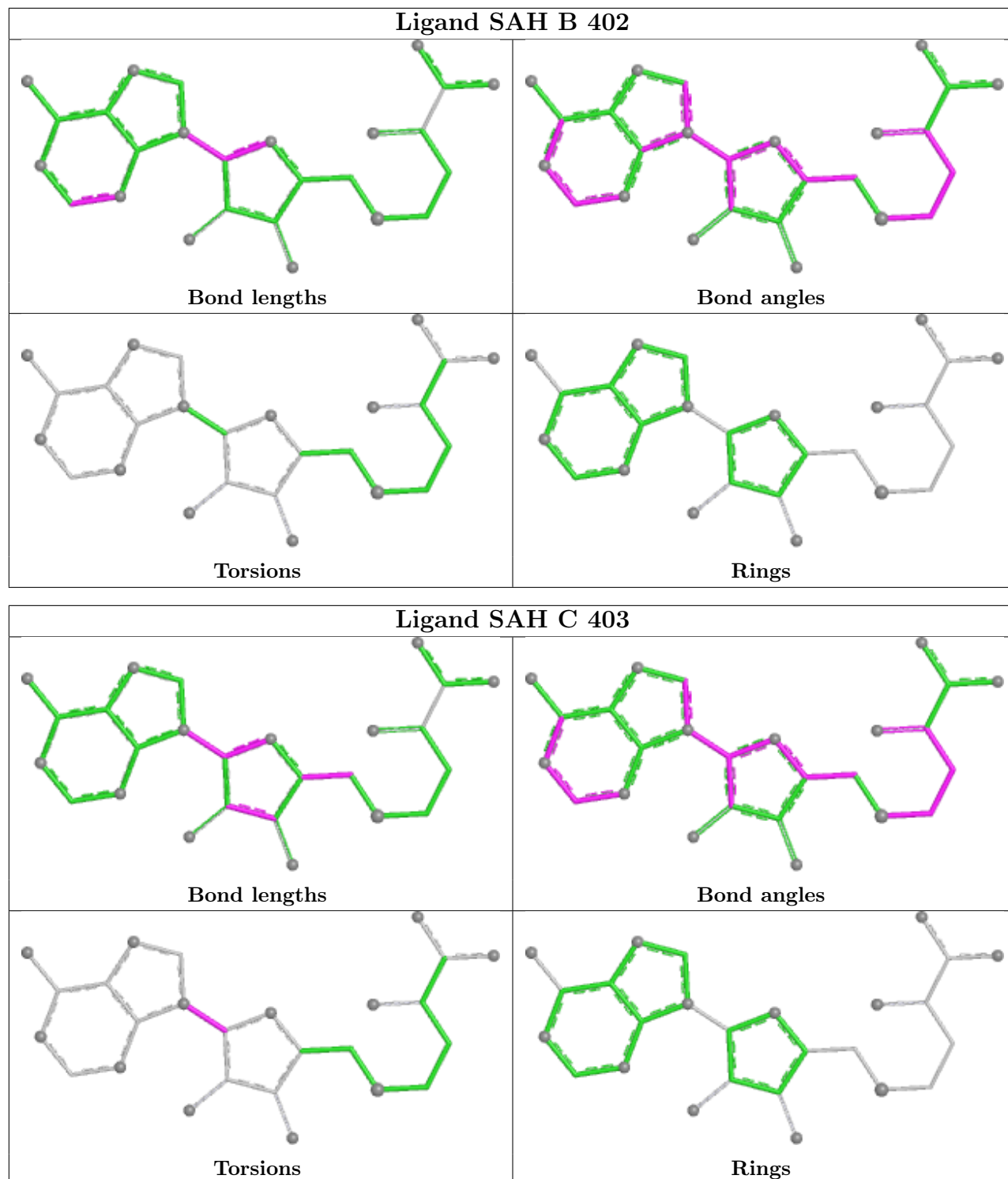
There are no ring outliers.

3 monomers are involved in 9 short contacts:

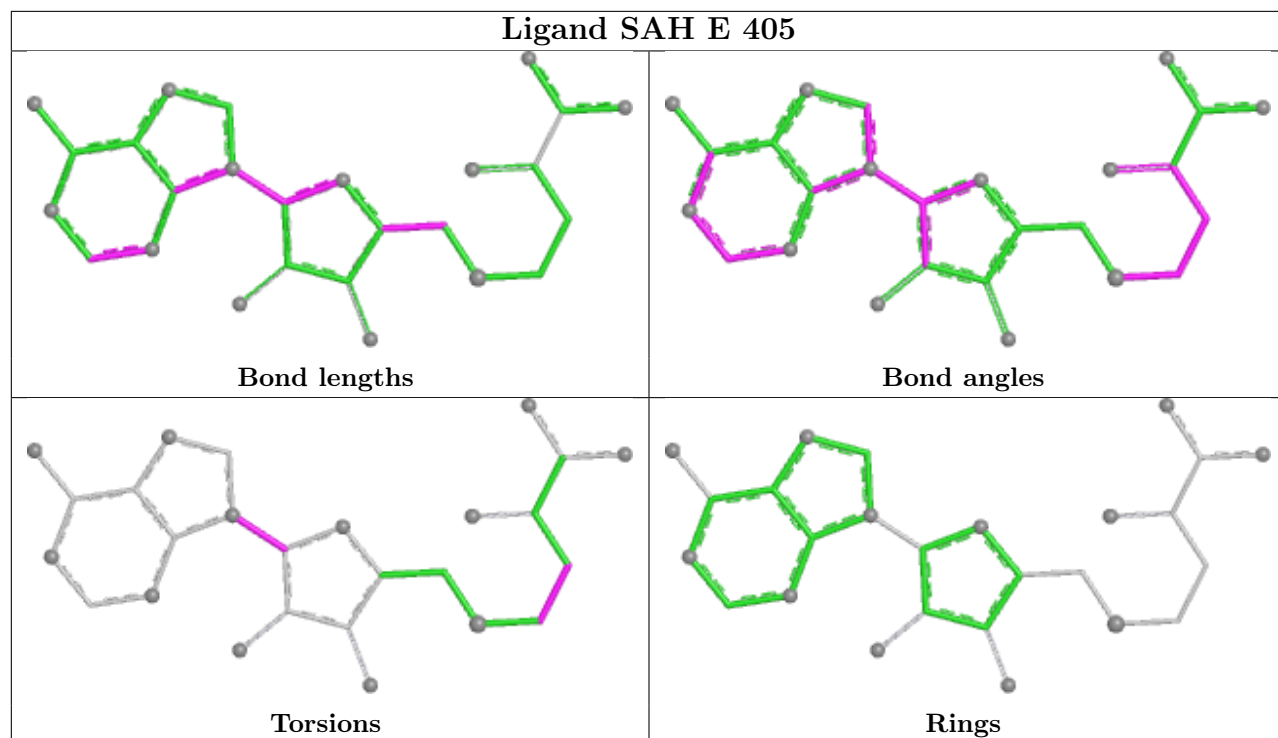
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	SAH	1	0
5	F	406	SAH	7	0
5	D	404	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

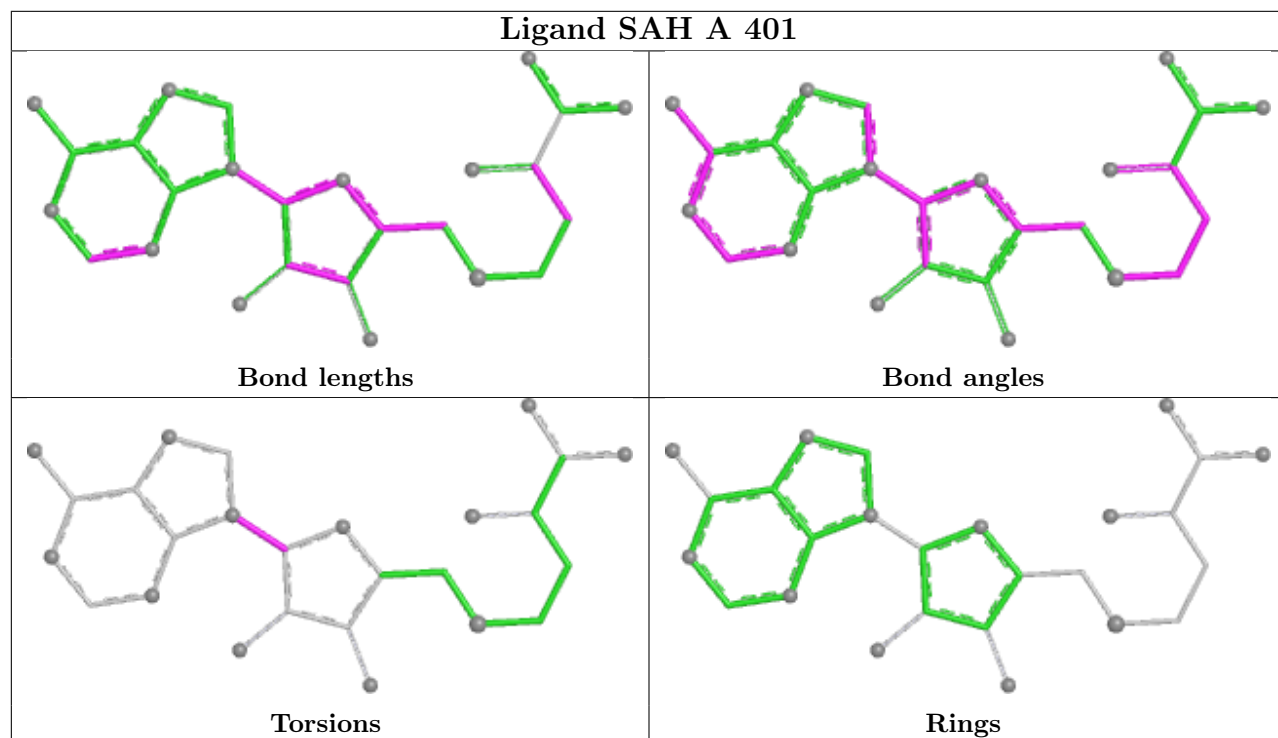
equivalents in the CSD to analyse the geometry.

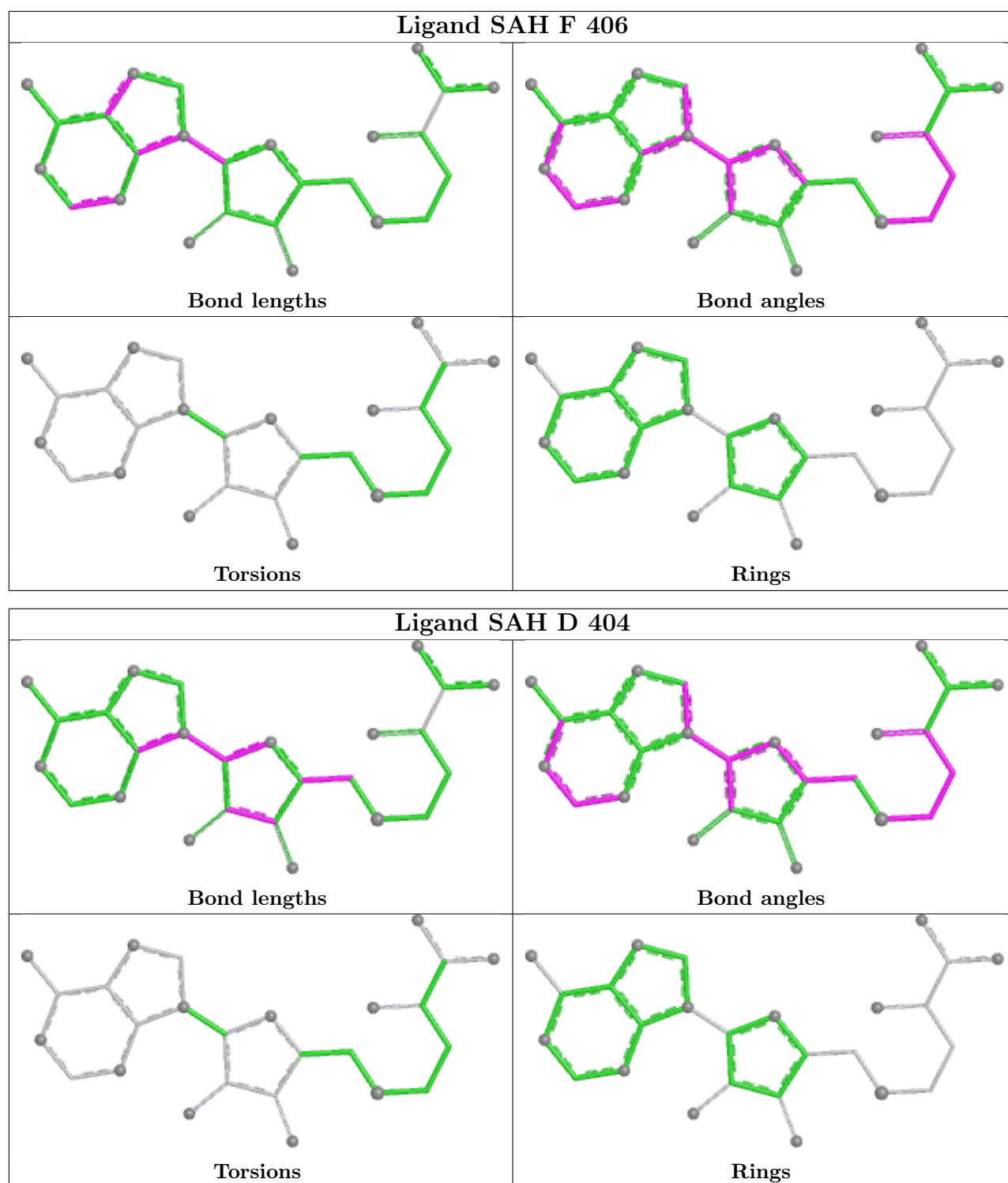


Ligand SAH E 405



Ligand SAH A 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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.