Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:20 PM BST

PDB ID : 1AK0
Title : P1 NUCLEASE IN COMPLEX WITH A SUBSTRATE ANALOG
Authors : Romier, C.; Suck, D.
Deposited on : 1997-05-28
Resolution : 1.80 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

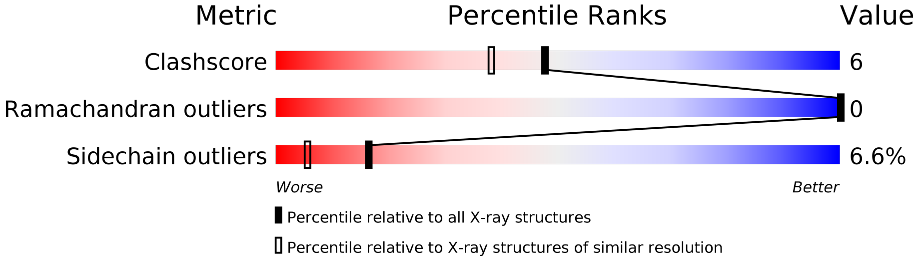
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 on 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	270	
2	B	2	

2 Entry composition ⓘ

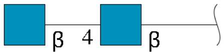
There are 7 unique types of molecules in this entry. The entry contains 2313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P1 NUCLEASE.

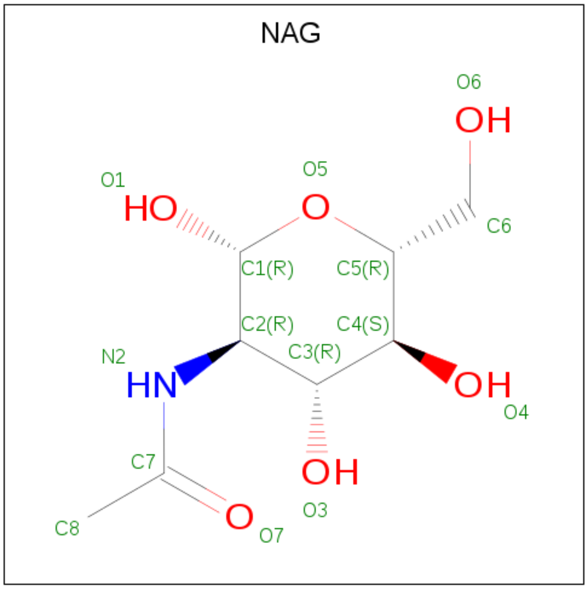
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2021	1267	342	405	7	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

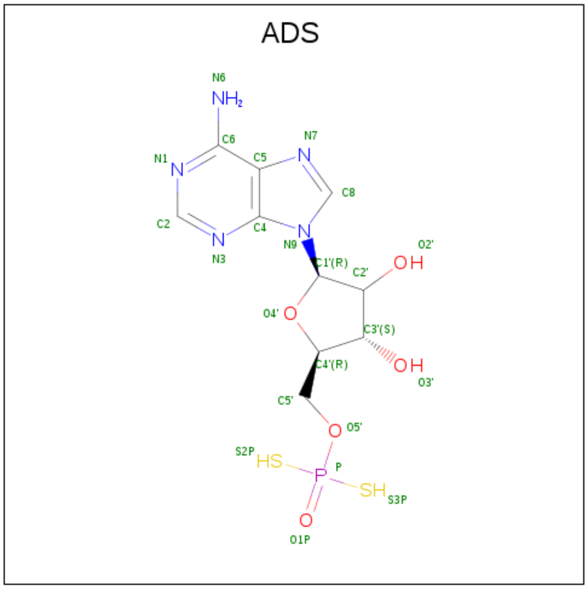


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

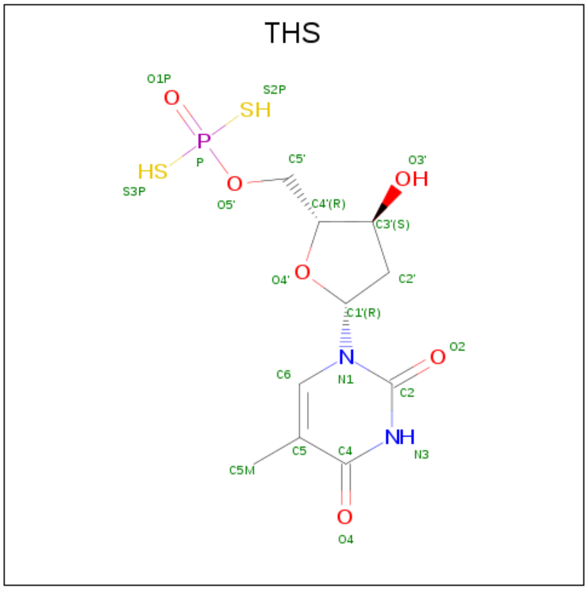
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	4	4	4	0	0

- Molecule 5 is ADENOSINE-5'-(DITHIO)PHOSPHATE (three-letter code: ADS) (formula: $C_{10}H_{14}N_5O_5PS_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	18	10	5	3	0	0

- Molecule 6 is THYMIDINE-5'-(DITHIO)PHOSPHATE (three-letter code: THS) (formula: $C_{10}H_{15}N_2O_6PS_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P S 20 10 2 5 1 2	0	0
6	A	1	Total C N O P S 20 10 2 5 1 2	0	0
6	A	1	Total C N O P S 20 10 2 5 1 2	0	0

- Molecule 7 is water.

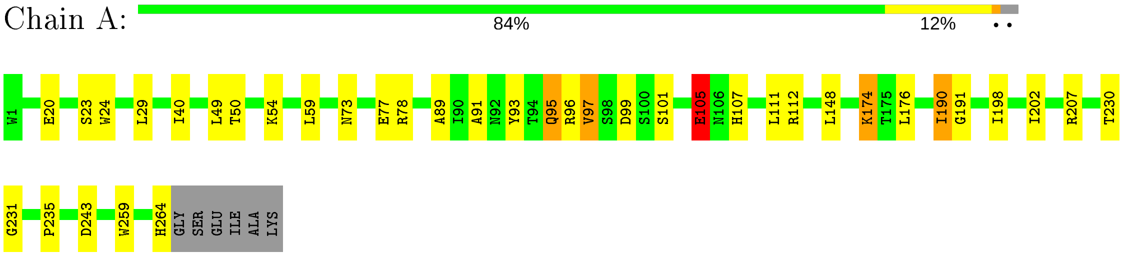
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	154	Total O 154 154	0	0

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: P1 NUCLEASE



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	41.98Å 74.04Å 102.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	89.1 (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.207 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2313	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: ZN, THS, NAG, ADS

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	0.56	1/2075 (0.0%)	0.77	3/2838 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TRP	CB-CG	5.02	1.59	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	GLU	CB-CA-C	6.60	123.61	110.40
1	A	23	SER	CB-CA-C	5.95	121.41	110.10
1	A	231	GLY	N-CA-C	-5.20	100.11	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2021	0	1873	19	0
2	B	28	0	25	0	0
3	A	28	0	26	3	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	9	3	0
6	A	60	0	36	3	0
7	A	154	0	0	6	0
All	All	2313	0	1969	25	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 6.

All (25) 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)
5:A:292:ADS:C5'	6:A:293:THS:HM51	2.17	0.74
5:A:292:ADS:H5'2	6:A:293:THS:HM51	1.69	0.74
1:A:73:ASN:HD21	1:A:78:ARG:HH12	1.33	0.74
3:A:287:NAG:C7	7:A:552:HOH:O	2.37	0.73
1:A:59:LEU:HD22	1:A:89:ALA:HB2	1.72	0.71
1:A:93:TYR:O	1:A:97:VAL:HG22	2.01	0.60
1:A:174:LYS:O	1:A:174:LYS:HD3	2.02	0.60
3:A:287:NAG:C8	7:A:552:HOH:O	2.49	0.60
5:A:292:ADS:O5'	6:A:293:THS:HM51	2.04	0.58
1:A:190:ILE:HG13	1:A:191:GLY:N	2.22	0.54
1:A:174:LYS:C	1:A:174:LYS:HD3	2.30	0.52
1:A:95:GLN:HG3	1:A:96:ARG:N	2.25	0.52
1:A:99:ASP:O	1:A:107:HIS:HE1	1.94	0.51
3:A:287:NAG:O7	7:A:552:HOH:O	2.19	0.50
1:A:207:ARG:HH11	1:A:207:ARG:HG3	1.76	0.49
1:A:105:GLU:HB2	7:A:492:HOH:O	2.13	0.47
1:A:190:ILE:HG23	7:A:534:HOH:O	2.15	0.45
1:A:99:ASP:O	1:A:107:HIS:CE1	2.70	0.44
1:A:243:ASP:HB2	7:A:427:HOH:O	2.17	0.43
1:A:91:ALA:HB2	1:A:202:ILE:CD1	2.48	0.43
1:A:20:GLU:H	1:A:20:GLU:CD	2.22	0.43
1:A:40:ILE:HD13	1:A:112:ARG:HG2	2.00	0.42
1:A:20:GLU:HB3	1:A:264:HIS:HE1	1.85	0.42
1:A:198:ILE:HA	1:A:259:TRP:CH2	2.56	0.41
1:A:50:THR:O	1:A:54:LYS:HG2	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	262/270 (97%)	253 (97%)	9 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	211/215 (98%)	197 (93%)	14 (7%)	16 5

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	49	LEU
1	A	77	GLU
1	A	95	GLN
1	A	97	VAL
1	A	101	SER
1	A	105	GLU
1	A	111	LEU
1	A	148	LEU
1	A	174	LYS
1	A	176	LEU
1	A	190	ILE
1	A	230	THR

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Mol	Chain	Res	Type
1	A	235	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	67	ASN
1	A	73	ASN
1	A	107	HIS
1	A	179	ASN

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

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.35	0	17,19,21	1.06	2 (11%)
2	NAG	B	2	2	14,14,15	0.61	0	17,19,21	0.86	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C2-N2-C7	-2.20	119.77	122.90
2	B	1	NAG	C4-C3-C2	-2.15	107.87	111.02

There are no chirality outliers.

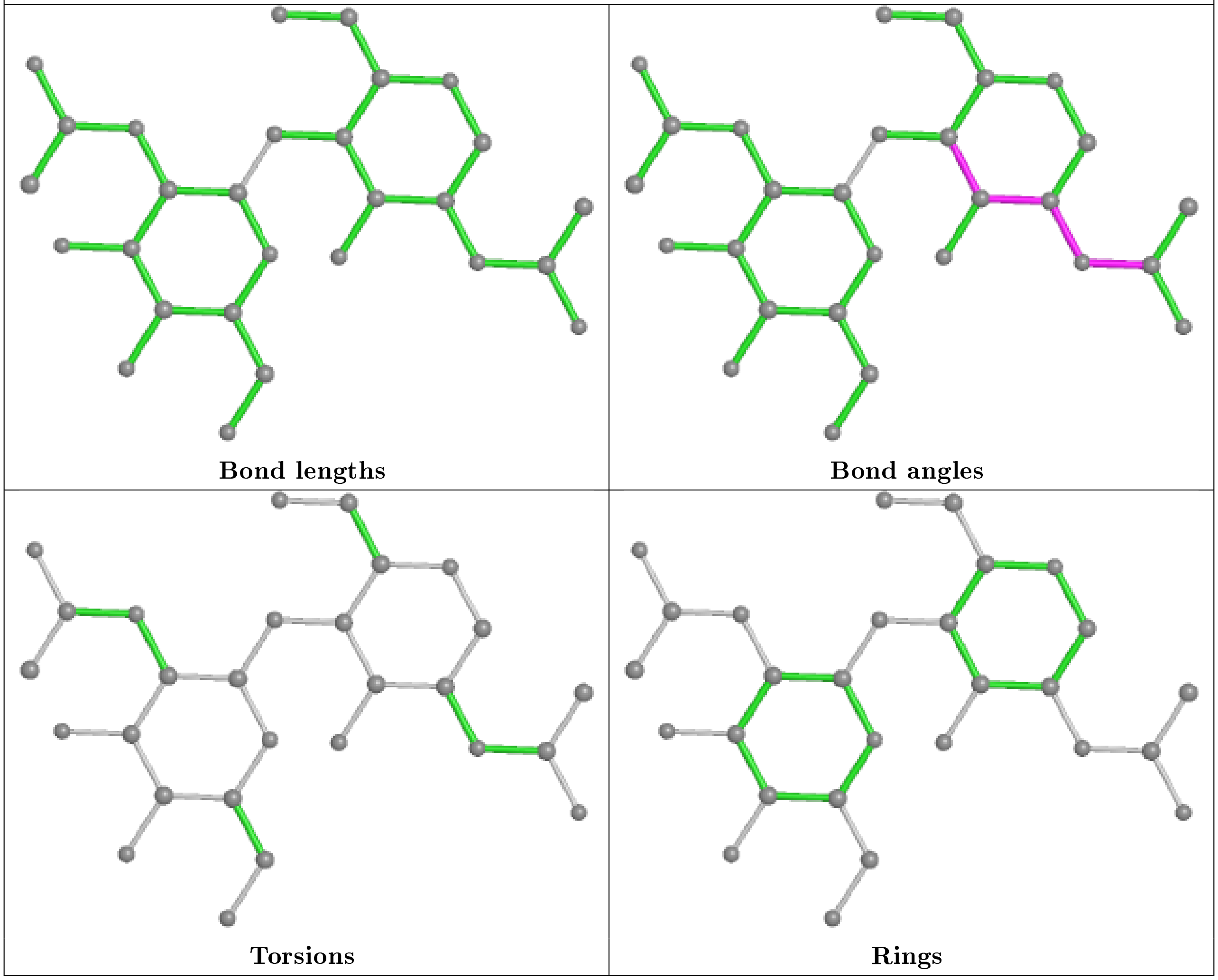
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain B



Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	NAG	A	285	1	14,14,15	1.01	2 (14%)	17,19,21	2.34	7 (41%)
6	THS	A	293	5,6	15,21,22	1.98	4 (26%)	15,30,33	4.20	3 (20%)
3	NAG	A	287	1	14,14,15	1.42	3 (21%)	17,19,21	3.32	8 (47%)

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	THS	A	295	4,6	15,21,22	1.77	3 (20%)	15,30,33	3.48	1 (6%)
5	ADS	A	292	6	18,20,25	1.04	0	17,29,38	1.39	3 (17%)
6	THS	A	294	6	15,21,22	1.20	1 (6%)	15,30,33	3.79	5 (33%)

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	NAG	A	285	1	-	2/6/23/26	0/1/1/1
6	THS	A	293	5,6	-	0/3/21/22	0/2/2/2
3	NAG	A	287	1	-	0/6/23/26	0/1/1/1
6	THS	A	295	4,6	-	2/3/21/22	0/2/2/2
5	ADS	A	292	6	-	2/2/18/26	0/3/3/3
6	THS	A	294	6	-	1/3/21/22	0/2/2/2

All (13) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
6	A	293	THS	C4-N3	4.69	1.41	1.33
6	A	295	THS	C4-N3	4.67	1.41	1.33
6	A	293	THS	C4-C5	3.58	1.49	1.41
6	A	293	THS	C5M-C5	3.02	1.56	1.51
3	A	287	NAG	C3-C2	-2.96	1.46	1.52
3	A	287	NAG	C1-C2	-2.89	1.48	1.52
3	A	285	NAG	O5-C5	2.74	1.49	1.43
6	A	295	THS	C5M-C5	2.67	1.56	1.51
6	A	294	THS	C4-N3	2.42	1.37	1.33
6	A	293	THS	O5'-C5'	-2.31	1.38	1.44
3	A	285	NAG	C4-C5	2.21	1.57	1.53
6	A	295	THS	C4-C5	2.21	1.46	1.41
3	A	287	NAG	C2-N2	-2.04	1.42	1.46

All (27) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
6	A	293	THS	C4-N3-C2	15.39	128.13	115.14
6	A	294	THS	C4-N3-C2	13.57	126.60	115.14
6	A	295	THS	C4-N3-C2	12.95	126.07	115.14
3	A	287	NAG	C4-C3-C2	-6.79	101.06	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	287	NAG	O7-C7-C8	6.27	133.71	122.06
3	A	285	NAG	C4-C3-C2	-5.95	102.30	111.02
3	A	287	NAG	C2-N2-C7	-5.88	114.53	122.90
3	A	287	NAG	C1-O5-C5	4.92	118.86	112.19
3	A	287	NAG	O7-C7-N2	-3.99	114.61	121.95
3	A	285	NAG	C1-C2-N2	3.71	116.83	110.49
3	A	285	NAG	C8-C7-N2	-3.33	110.46	116.10
3	A	285	NAG	C1-O5-C5	3.00	116.26	112.19
3	A	287	NAG	C8-C7-N2	-2.99	111.04	116.10
3	A	287	NAG	C6-C5-C4	-2.91	106.18	113.00
3	A	285	NAG	O5-C1-C2	-2.81	106.85	111.29
6	A	294	THS	O3'-C3'-C4'	-2.71	99.73	110.10
5	A	292	ADS	O5'-C5'-C4'	-2.55	102.55	111.29
6	A	294	THS	C5M-C5-C4	-2.51	116.88	121.37
6	A	294	THS	C2'-C3'-C4'	2.47	107.91	102.76
3	A	287	NAG	O5-C5-C4	2.44	116.75	110.83
5	A	292	ADS	O4'-C4'-C3'	2.34	111.14	105.67
6	A	293	THS	O4'-C4'-C5'	-2.31	101.78	109.37
6	A	294	THS	C5-C6-N1	-2.15	119.88	122.19
3	A	285	NAG	C6-C5-C4	-2.07	108.15	113.00
6	A	293	THS	C2'-C1'-N1	2.04	118.97	114.27
5	A	292	ADS	O3'-C3'-C4'	-2.02	102.37	110.10
3	A	285	NAG	O7-C7-C8	2.01	125.79	122.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	295	THS	O4'-C1'-N1-C6
6	A	294	THS	O4'-C1'-N1-C6
5	A	292	ADS	O4'-C4'-C5'-O5'
5	A	292	ADS	C3'-C4'-C5'-O5'
6	A	295	THS	C3'-C4'-C5'-O5'
3	A	285	NAG	C1-C2-N2-C7
3	A	285	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	293	THS	3	0

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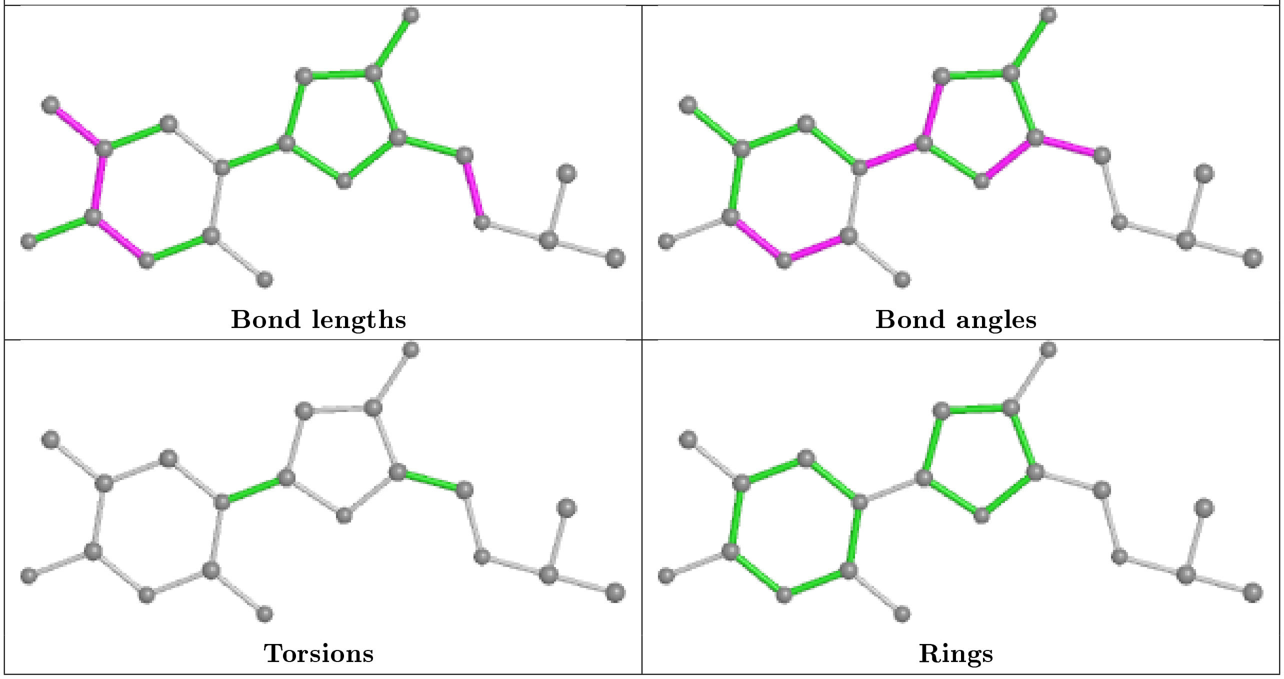
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	287	NAG	3	0
5	A	292	ADS	3	0

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.

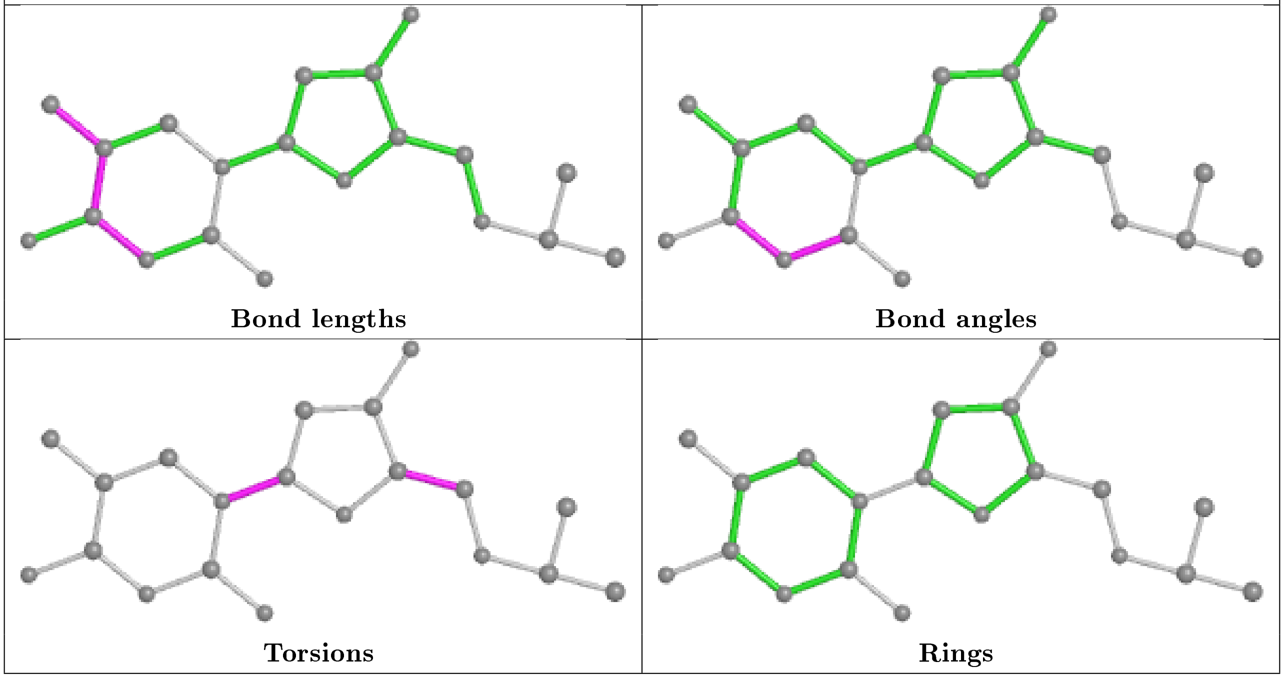
Ligand THS A 293



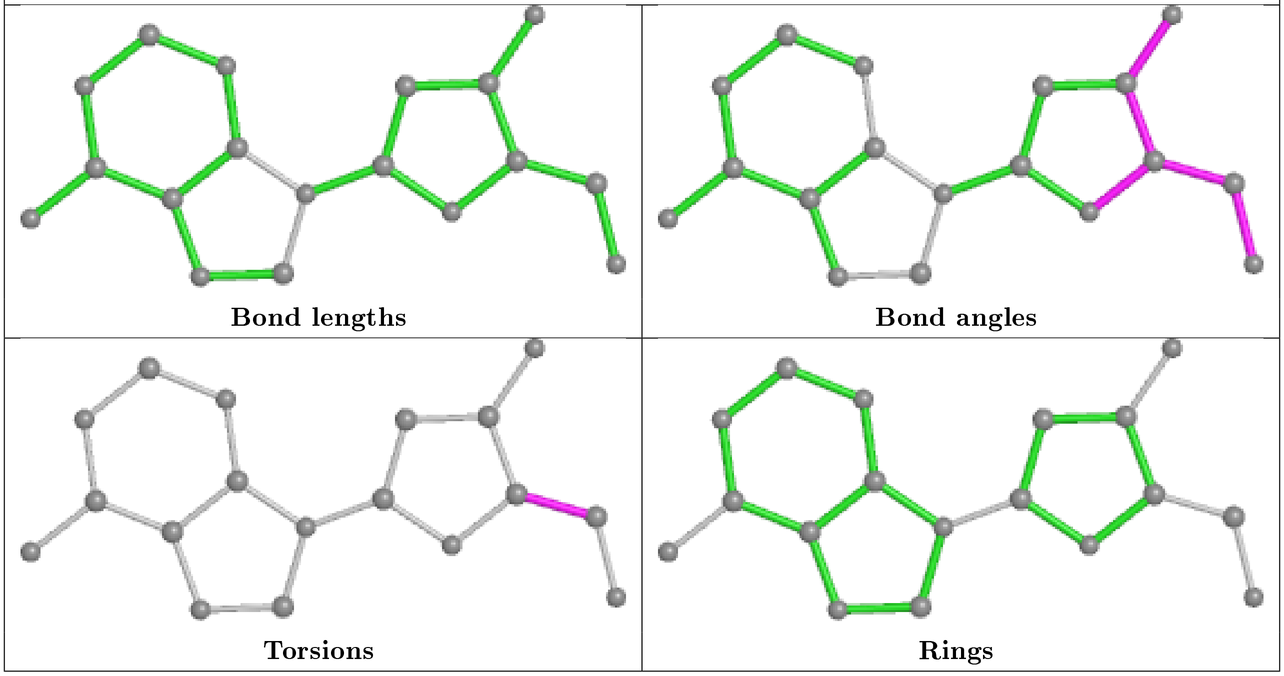
Bond lengths **Bond angles**

Torsions **Rings**

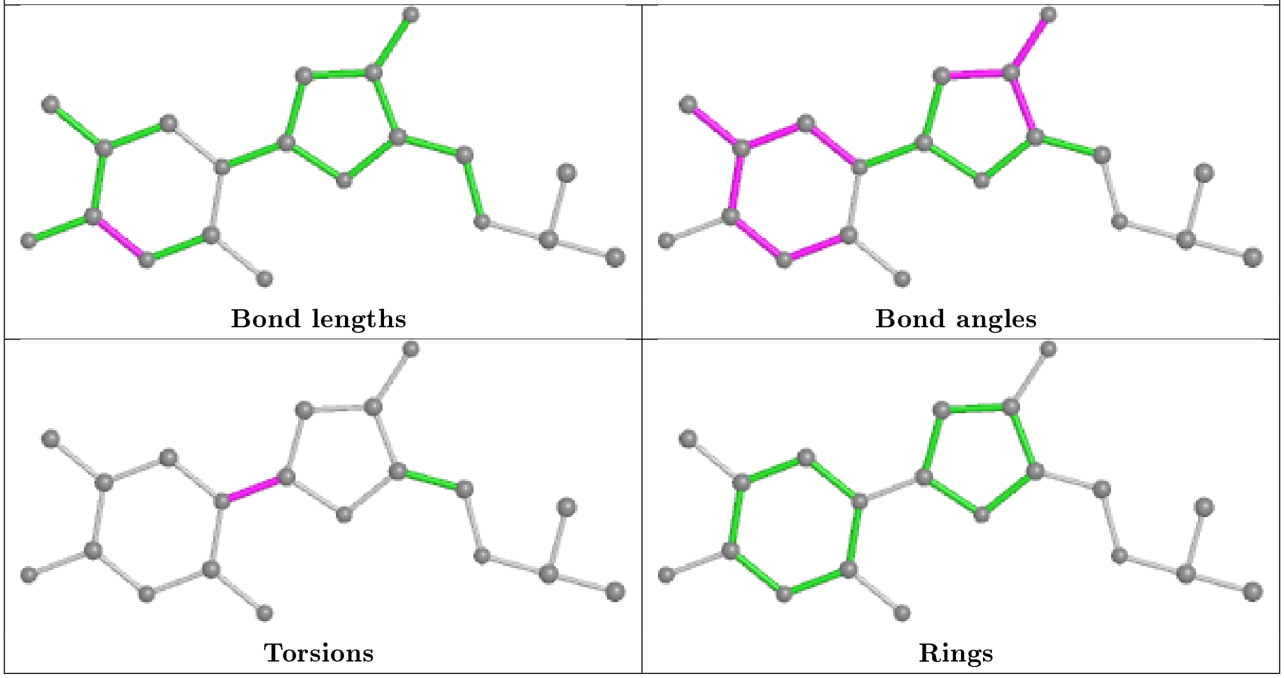
Ligand THS A 295



Ligand ADS A 292



Ligand THS A 294



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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.