wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 07:28 PM EDT

PDB ID	:	6NBE
Title	:	Ternary Complex of Ac-Alpha-Actin with Profilin and CoA-NAA80
Authors	:	Rebowski, G.; Boczkowska, M.; Dominguez, R.
Deposited on	:	2018-12-07
Resolution	:	2.00 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 (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:

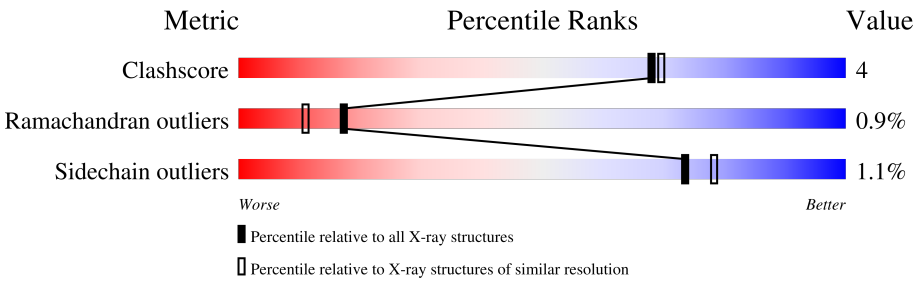
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 >=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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	375	91% 7% •
2	N	235	71% 9% 21%
3	P	140	93% 6% •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11587 atoms, of which 5541 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	370	5831	1854	2899	493	565	20	0	5	0

- Molecule 2 is a protein called N-alpha-acetyltransferase 80.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	N	186	2971	937	1494	277	256	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	74	ALA	-	expression tag	UNP Q93015
N	75	GLY	-	expression tag	UNP Q93015
N	76	HIS	-	expression tag	UNP Q93015
N	77	MET	-	expression tag	UNP Q93015

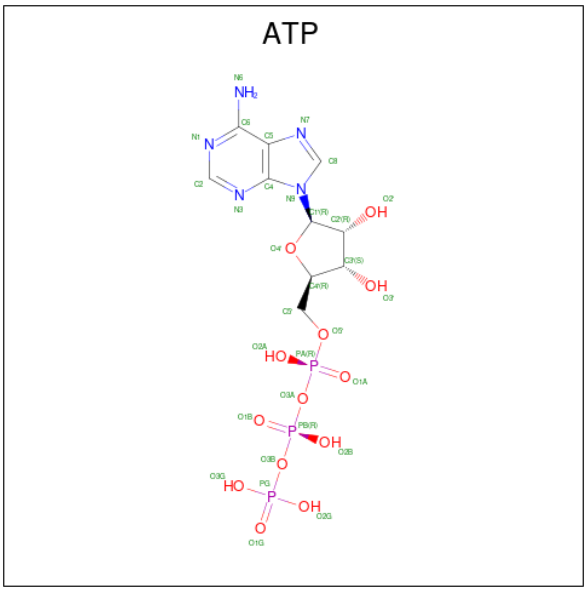
- Molecule 3 is a protein called Profilin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	P	138	2081	654	1040	179	201	7	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

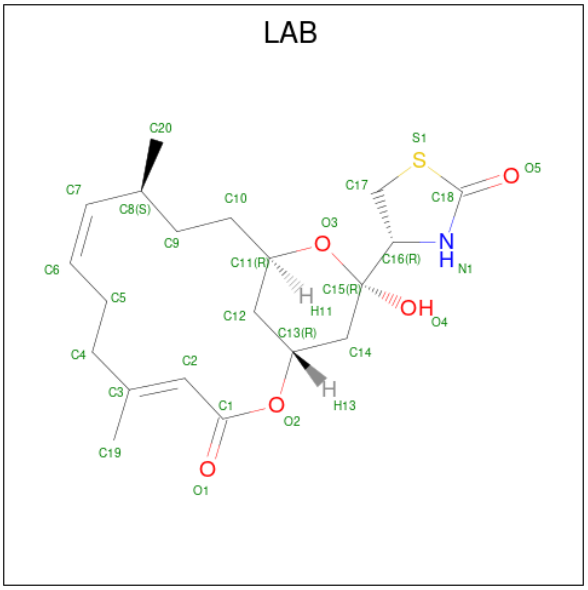
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



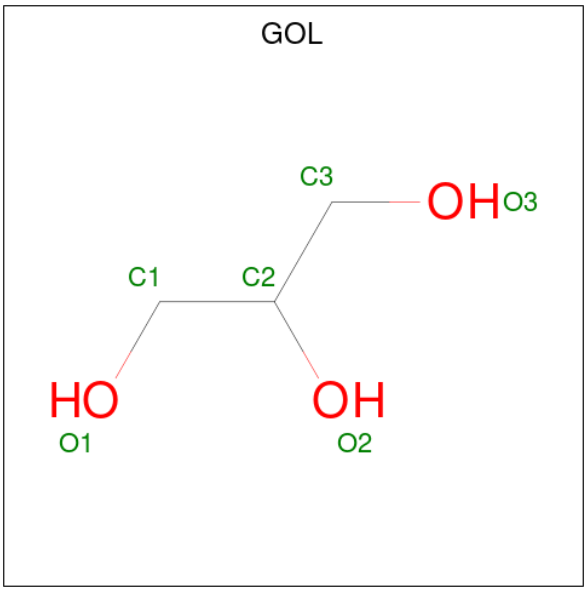
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
5	A	1	42	10	11	5	13	3	0	0

- Molecule 6 is LATRUNCULIN B (three-letter code: LAB) (formula: $C_{20}H_{29}NO_5S$).



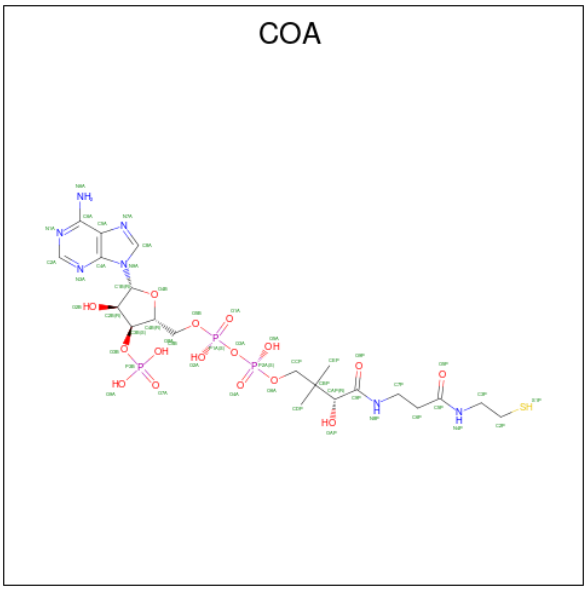
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
6	A	1	56	20	29	1	5	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



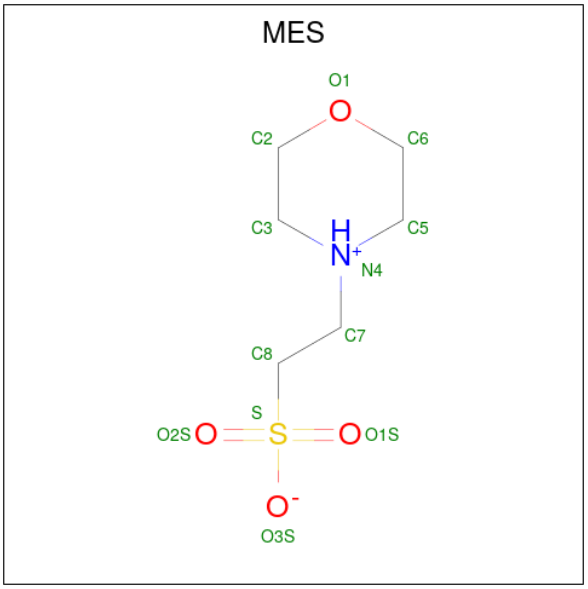
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	14	3	8	3	0	0
			Total	C	H	O		
7	A	1	13	3	7	3	0	0
			Total	C	H	O		
7	N	1	14	3	8	3	0	0

- Molecule 8 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
8	N	1	80	21	32	7	16	3	1	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	N	1	25	6	13	1	4	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	266	266	266	0	0
			Total	O		
10	N	122	122	122	0	0
			Total	O		
10	P	71	71	71	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.

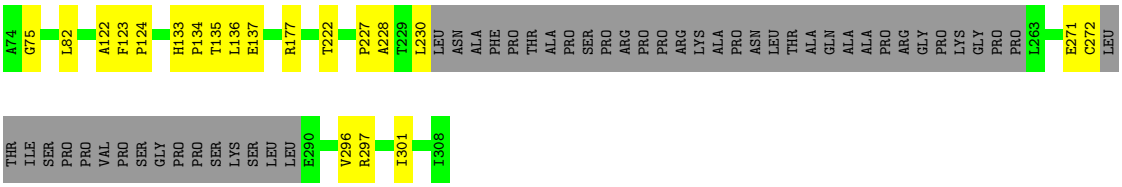
Note EDS failed to run properly.

• Molecule 1: Actin, alpha skeletal muscle

Chain A:

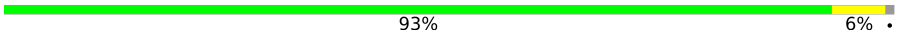
• Molecule 2: N-alpha-acetyltransferase 80

Chain N:



• Molecule 3: Profilin-1

Chain P:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.47Å 115.89Å 132.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.35 – 2.00	Depositor
% Data completeness (in resolution range)	99.6 (33.35-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.45 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.159 , 0.184	Depositor
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.588	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11587	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, COA, HIC, MES, LAB, GOL, KKD, ATP

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	0.38	0/2985	0.52	0/4040
2	N	0.42	0/1514	0.58	0/2056
3	P	0.35	0/1059	0.55	0/1430
All	All	0.39	0/5558	0.54	0/7526

There are no bond length outliers.

There are no bond angle outliers.

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	2932	2899	2892	18	0
2	N	1477	1494	1492	15	0
3	P	1041	1040	1040	7	0
4	A	1	0	0	0	0
5	A	31	11	12	1	0
6	A	27	29	29	5	0
7	A	12	15	16	1	0
7	N	6	8	8	0	0
8	N	48	32	32	0	0
9	N	12	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	266	0	0	2	0
10	N	122	0	0	1	0
10	P	71	0	0	0	0
All	All	6046	5541	5534	42	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 4.

The worst 5 of 42 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)
2:N:296:VAL:HG23	2:N:297:ARG:HG3	1.72	0.71
3:P:136:ARG:HG2	3:P:136:ARG:HH21	1.55	0.71
6:A:402:LAB:O1	6:A:402:LAB:H142	1.98	0.64
1:A:206:ARG:HD3	6:A:402:LAB:S1	2.40	0.61
1:A:180:LEU:HD11	1:A:260:THR:HG22	1.86	0.58

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	109/375 (29%)	105 (96%)	3 (3%)	1 (1%)	17 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	GLN

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	93/316 (29%)	92 (99%)	1 (1%)	73 78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HIC	A	73	1	8,11,12	1.62	1 (12%)	6,14,16	1.15	1 (16%)
1	KKD	A	1	1	9,10,11	1.38	1 (11%)	11,12,14	1.42	1 (9%)

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
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1
1	KKD	A	1	1	-	3/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	3.95	1.42	1.36
1	A	1	KKD	CT1-N	2.80	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	KKD	O-C-CA	-2.16	119.13	124.78
1	A	73	HIC	CB-CA-C	-2.15	107.43	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	KKD	CB-CA-N-CT1
1	A	1	KKD	C-CA-N-CT1
1	A	1	KKD	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	ATP	A	401	4	26,33,33	4.23	8 (30%)	31,52,52	2.13	4 (12%)
7	GOL	A	403	-	5,5,5	0.58	0	5,5,5	1.05	0
6	LAB	A	402	-	28,29,29	1.59	2 (7%)	30,41,41	1.64	8 (26%)
7	GOL	A	404	-	5,5,5	0.97	0	5,5,5	0.91	0
9	MES	N	401	-	12,12,12	1.51	3 (25%)	14,16,16	2.06	3 (21%)
8	COA	N	400	-	41,50,50	3.95	14 (34%)	52,75,75	2.05	12 (23%)
7	GOL	N	402	-	5,5,5	0.56	0	5,5,5	0.73	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
5	ATP	A	401	4	-	2/18/38/38	0/3/3/3
7	GOL	A	403	-	-	2/4/4/4	-
6	LAB	A	402	-	-	3/21/49/49	0/2/3/3
7	GOL	A	404	-	-	2/4/4/4	-
9	MES	N	401	-	-	0/6/14/14	0/1/1/1
8	COA	N	400	-	-	9/44/64/64	0/3/3/3
7	GOL	N	402	-	-	4/4/4/4	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	400	COA	O4B-C1B	15.60	1.62	1.41
5	A	401	ATP	C2'-C1'	-15.13	1.30	1.53
8	N	400	COA	C2B-C1B	-12.87	1.34	1.53
5	A	401	ATP	O4'-C1'	12.57	1.58	1.41
8	N	400	COA	C5P-N4P	6.85	1.49	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	400	COA	C5A-C6A-N6A	8.29	132.95	120.35
5	A	401	ATP	C5-C6-N6	7.78	132.17	120.35
8	N	400	COA	N6A-C6A-N1A	-5.81	106.52	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	400	COA	N3A-C2A-N1A	-5.24	120.49	128.68
5	A	401	ATP	N3-C2-N1	-5.21	120.53	128.68

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	ATP	PB-O3B-PG-O3G
6	A	402	LAB	C14-C13-O2-C1
7	A	403	GOL	O1-C1-C2-C3
7	A	404	GOL	C1-C2-C3-O3
7	N	402	GOL	O1-C1-C2-C3

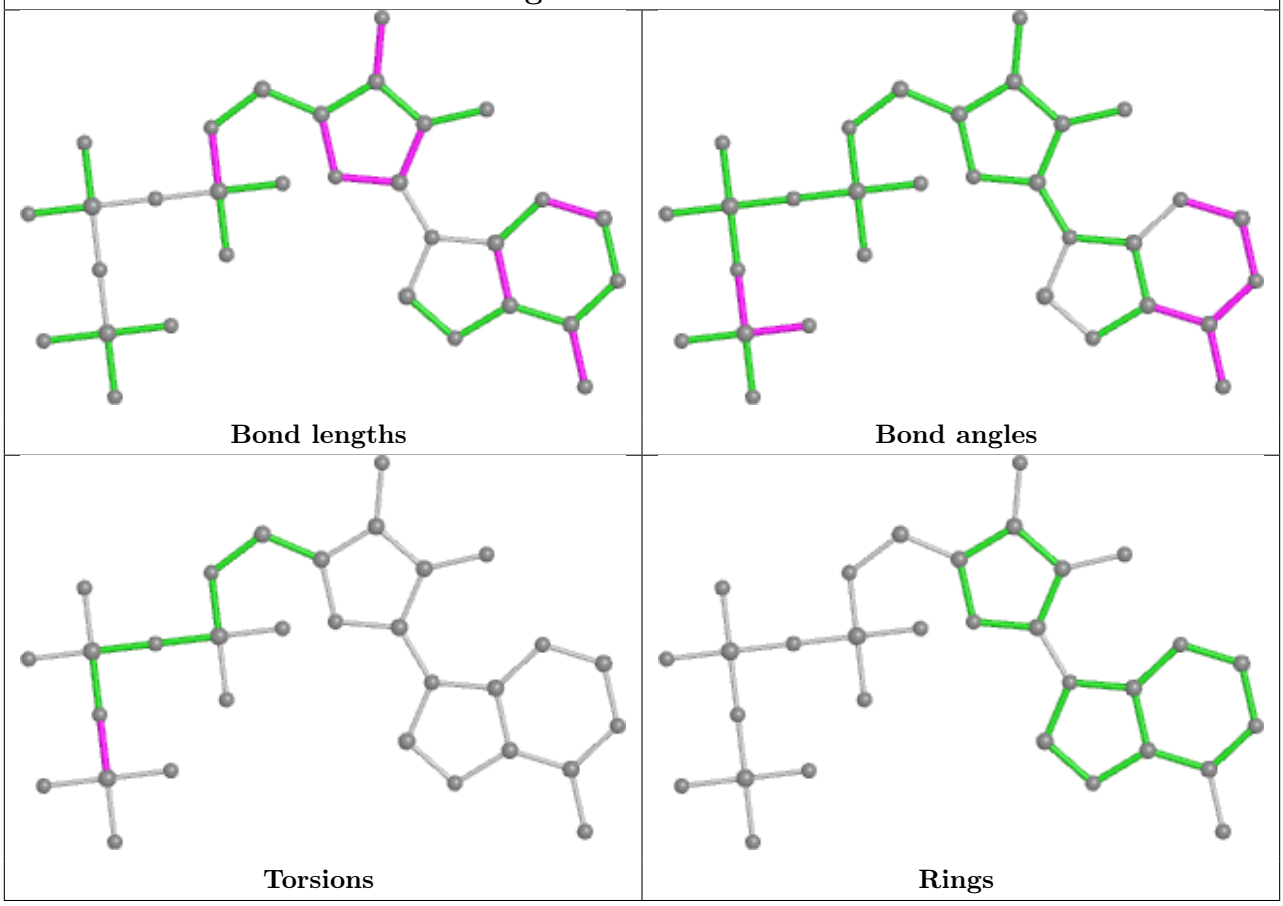
There are no ring outliers.

3 monomers are involved in 7 short contacts:

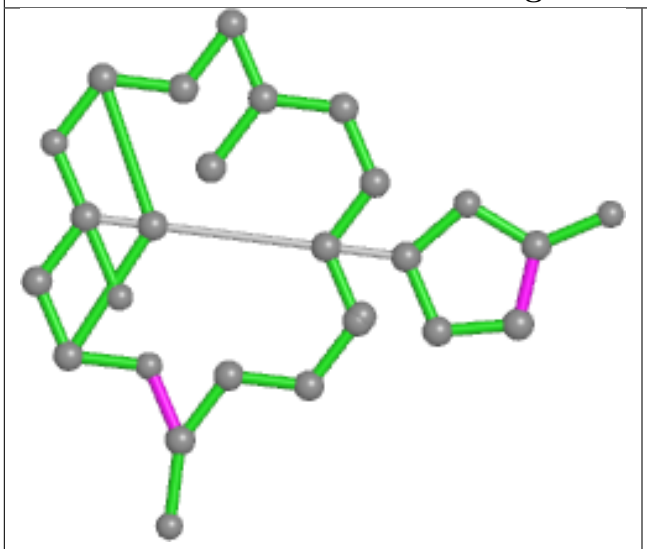
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	ATP	1	0
7	A	403	GOL	1	0
6	A	402	LAB	5	0

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 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.

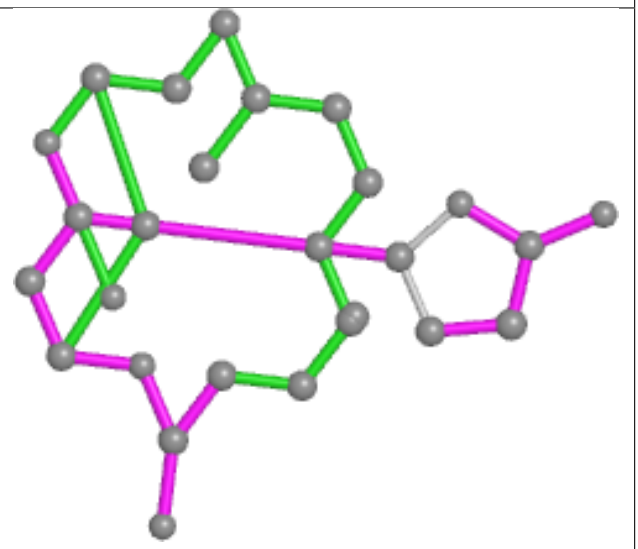
Ligand ATP A 401



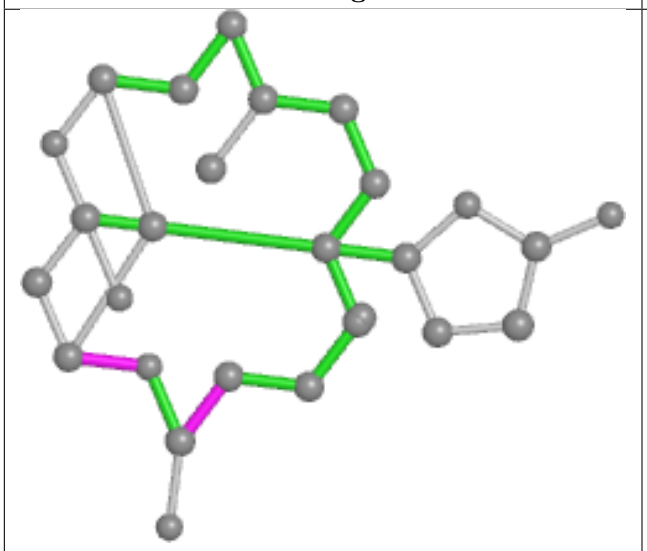
Ligand LAB A 402



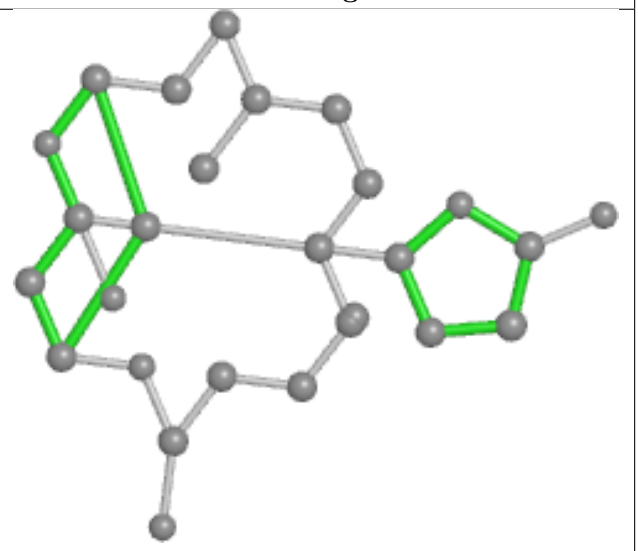
Bond lengths



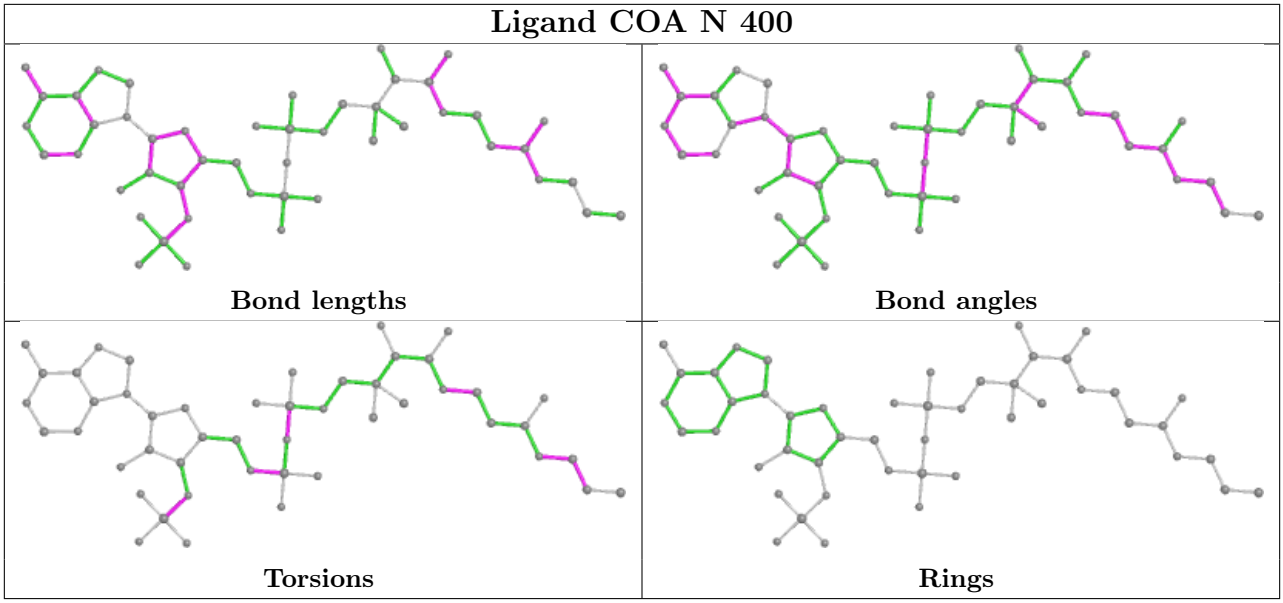
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.