



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:47 AM UTC

PDB ID : 6NAS / pdb_00006nas
Title : Ternary Complex of Ac-Alpha-Actin with Profilin and AcCoA-NAA80
Authors : Rebowski, G.; Boczkowska, M.; Dominguez, R.
Deposited on : 2018-12-06
Resolution : 2.90 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

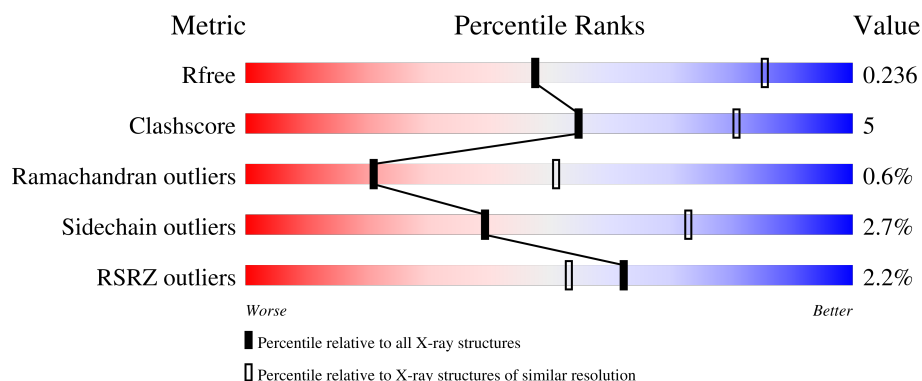
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	% 86% 12% ..
2	N	235	5% 64% 12% 23%
3	P	140	86% 12% ..

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10993 atoms, of which 5464 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
1	A	370	Total	C	H	N	O	S	0	0	0
			5769	1838	2862	488	561	20			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	N	180	Total	C	H	N	O	S	0	0	0
			2885	911	1450	271	247	6			

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

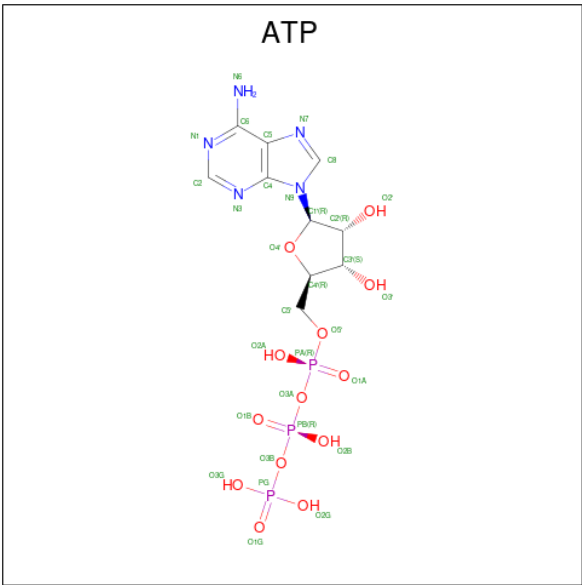
- Molecule 3 is a protein called Profilin-1.

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

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

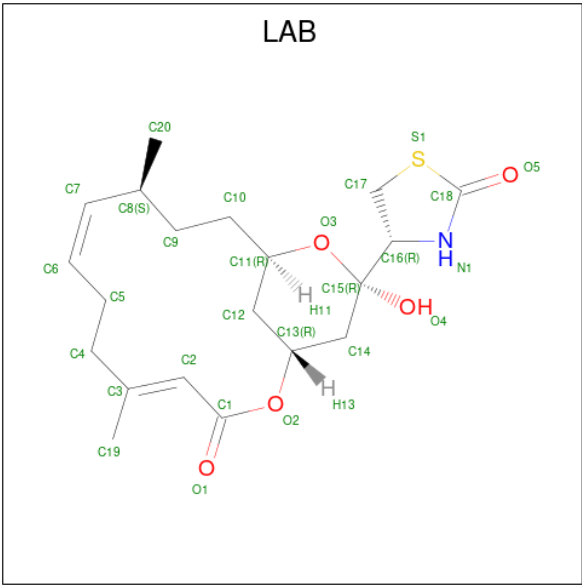
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



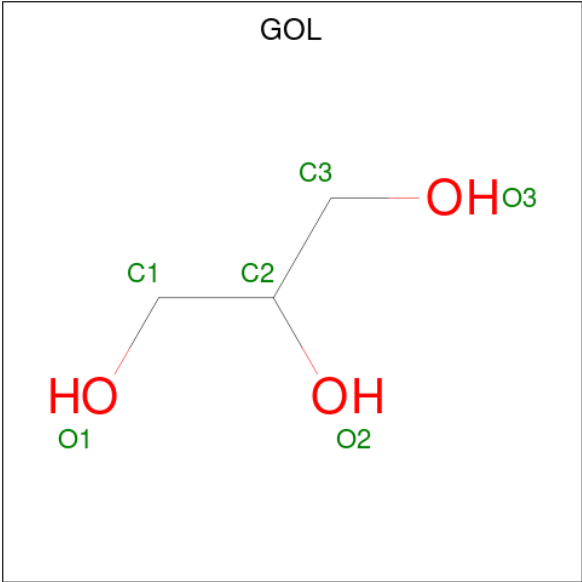
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 6 is LATRUNCULIN B (CCD ID: LAB) (formula: C₂₀H₂₉NO₅S).



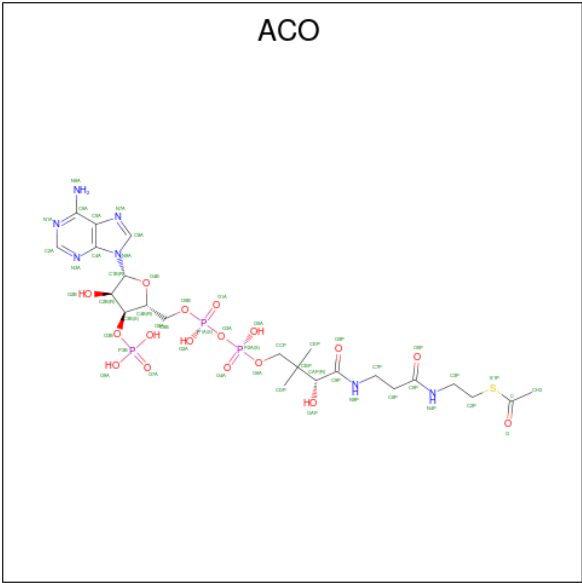
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			56	20	29	1	5	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



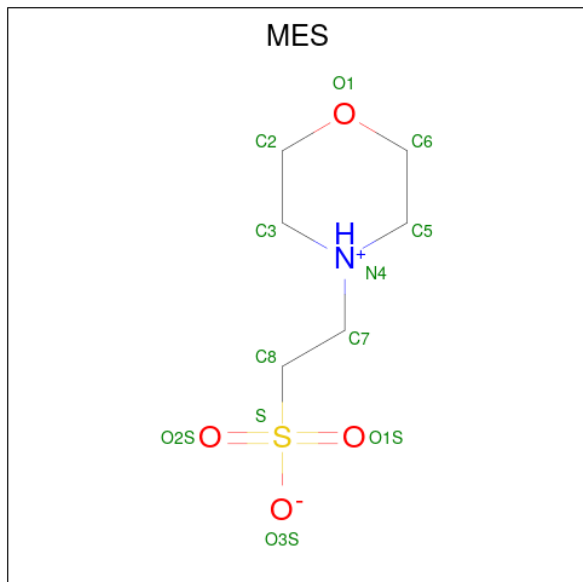
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	N	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	N	1	Total	C	H	N	O	P	S	0	0
			85	23	34	7	17	3	1		

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



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	6	Total	O	0	0
			6	6		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.83Å 114.89Å 132.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.72 – 2.90 28.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.72-2.90) 99.0 (28.72-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.239 0.187 , 0.236	Depositor DCC
R_{free} test set	1774 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10993	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ATP, LAB, MES, KKD, ACO, CA, HIC, GOL

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	0.19	0/2945	0.40	0/3986
2	N	0.36	1/1470 (0.1%)	0.48	0/1993
3	P	0.18	0/1059	0.43	0/1430
All	All	0.24	1/5474 (0.0%)	0.43	0/7409

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	95	ASP	C-O	-5.14	1.18	1.24

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	2907	2862	2855	25	0
2	N	1435	1450	1450	15	0
3	P	1041	1040	1040	11	0
4	A	1	0	0	0	0
5	A	31	12	12	2	0
6	A	27	29	28	4	0
7	A	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	6	8	8	0	0
8	N	51	34	34	1	0
9	N	12	13	13	0	0
10	A	6	0	0	0	0
All	All	5529	5464	5456	53	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 5.

All (53) 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)
6:A:402:LAB:C16	6:A:402:LAB:N1	1.73	1.36
8:N:400:ACO:O4B	8:N:400:ACO:C1B	1.67	1.19
1:A:180:LEU:HD11	1:A:260:THR:HG22	1.72	0.70
2:N:78:SER:OG	2:N:177:ARG:NH1	2.35	0.60
3:P:47:VAL:O	3:P:51:VAL:HG22	2.04	0.58
1:A:41:GLN:O	1:A:41:GLN:HG3	2.02	0.57
1:A:272:ALA:HB1	1:A:276:GLU:HB2	1.86	0.57
1:A:157:ASP:OD1	5:A:401:ATP:O3'	2.22	0.56
2:N:87:VAL:HA	2:N:128:MET:HE2	1.88	0.55
3:P:17:GLN:NE2	3:P:113:MET:SD	2.70	0.55
1:A:366:GLY:O	1:A:369:ILE:HG22	2.06	0.54
2:N:139:ALA:HB1	2:N:140:PRO:CD	2.38	0.54
2:N:78:SER:OG	2:N:177:ARG:HD2	2.08	0.54
1:A:213:LYS:NZ	5:A:401:ATP:O2'	2.41	0.53
1:A:180:LEU:C	1:A:180:LEU:HD23	2.34	0.52
2:N:229:THR:HG22	2:N:229:THR:O	2.08	0.52
1:A:207:GLU:OE2	6:A:402:LAB:O4	2.28	0.51
1:A:152:VAL:HG23	1:A:165:ILE:HD12	1.93	0.51
6:A:402:LAB:O2	6:A:402:LAB:H42	2.11	0.50
3:P:101:THR:HG21	3:P:124:ASN:HA	1.94	0.50
1:A:286:ASP:OD1	3:P:90:LYS:NZ	2.39	0.50
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.94	0.50
2:N:212:LEU:HD23	2:N:304:MET:HE3	1.92	0.49
1:A:220:ALA:O	1:A:312:ARG:NH1	2.45	0.48
1:A:233:SER:OG	1:A:234:SER:N	2.42	0.48
3:P:130:MET:HE3	3:P:130:MET:HA	1.95	0.48
6:A:402:LAB:N1	6:A:402:LAB:C15	2.64	0.48
3:P:63:LEU:C	3:P:63:LEU:HD12	2.39	0.48
1:A:153:LEU:HD21	1:A:274:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:13:ASP:OD1	3:P:13:ASP:N	2.46	0.47
1:A:303:THR:HG22	1:A:303:THR:O	2.14	0.47
2:N:82:LEU:HD13	2:N:129:LEU:HD21	1.99	0.44
1:A:192:ILE:HD12	1:A:253:GLU:HG3	1.99	0.44
1:A:359:LYS:O	1:A:359:LYS:HD2	2.17	0.44
2:N:77:MET:HE3	2:N:77:MET:HA	2.00	0.44
1:A:345:ILE:HD11	2:N:227:PRO:HD2	1.99	0.44
2:N:211:GLN:O	2:N:304:MET:HA	2.18	0.44
2:N:215:PRO:HG2	2:N:292:GLN:HB2	1.99	0.44
1:A:213:LYS:HE2	1:A:306:TYR:OH	2.17	0.44
1:A:352:PHE:CE1	1:A:355:MET:HE2	2.53	0.43
3:P:58:PHE:CD1	3:P:72:VAL:HG21	2.53	0.43
1:A:330:ILE:HG22	1:A:332:PRO:HD3	2.00	0.43
1:A:172:PRO:HA	1:A:175:ILE:HD12	2.00	0.42
2:N:270:PRO:O	2:N:271:GLU:C	2.63	0.42
3:P:7:ILE:O	3:P:11:MET:HG2	2.20	0.42
2:N:226:LEU:O	2:N:227:PRO:C	2.63	0.42
1:A:180:LEU:HD23	1:A:181:ALA:N	2.35	0.41
3:P:16:CYS:SG	3:P:112:LEU:HD22	2.61	0.41
3:P:18:ASP:OD1	3:P:19:ALA:N	2.54	0.41
2:N:194:LEU:O	2:N:305:GLU:HA	2.21	0.41
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.02	0.40
1:A:190:MET:HG2	1:A:209:VAL:HG11	2.02	0.40
2:N:178:LEU:O	2:N:182:LEU:HG	2.22	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	365/375 (97%)	351 (96%)	13 (4%)	1 (0%)	36 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	172/235 (73%)	161 (94%)	8 (5%)	3 (2%)	7	26
3	P	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
All	All	673/750 (90%)	642 (95%)	27 (4%)	4 (1%)	21	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
2	N	132	PRO
2	N	123	PHE
2	N	270	PRO

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	313/316 (99%)	302 (96%)	11 (4%)	32	66
2	N	156/201 (78%)	152 (97%)	4 (3%)	40	73
3	P	113/114 (99%)	112 (99%)	1 (1%)	70	90
All	All	582/631 (92%)	566 (97%)	16 (3%)	39	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET
1	A	49	GLN
1	A	61	LYS
1	A	176	MET
1	A	224	GLU
1	A	297	ASN
1	A	320	LEU
1	A	323	SER
1	A	324	THR
1	A	359	LYS

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Mol	Chain	Res	Type
1	A	368	SER
2	N	115	SER
2	N	224	ARG
2	N	230	LEU
2	N	301	ILE
3	P	13	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	41	GLN
1	A	246	GLN
1	A	297	ASN
2	N	133	HIS
2	N	153	ASN
3	P	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	KKD	A	1	1	9,10,11	2.31	2 (22%)	11,12,14	1.36	1 (9%)
1	HIC	A	73	1	10,11,12	1.52	1 (10%)	9,14,16	1.25	1 (11%)

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	KKD	A	1	1	-	4/9/10/12	-
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	KKD	CT1-N	6.00	1.53	1.34
1	A	73	HIC	CD2-CG	3.10	1.41	1.36
1	A	1	KKD	CB-CG	2.49	1.57	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-2.89	111.56	112.66
1	A	1	KKD	OD1-CG-CB	-2.07	116.47	122.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
8	ACO	N	400	-	51,53,53	3.12	20 (39%)	73,79,79	1.57	14 (19%)
7	GOL	N	402	-	5,5,5	0.73	0	5,5,5	0.86	0
7	GOL	A	403	-	5,5,5	0.77	0	5,5,5	1.18	1 (20%)
7	GOL	A	404	-	5,5,5	0.79	0	5,5,5	1.05	0
9	MES	N	401	-	12,12,12	2.17	1 (8%)	15,16,16	1.41	2 (13%)
6	LAB	A	402	-	28,29,29	5.71	16 (57%)	29,41,41	4.36	9 (31%)
5	ATP	A	401	4	32,33,33	1.54	8 (25%)	48,52,52	1.84	10 (20%)

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
8	ACO	N	400	-	-	11/51/67/67	0/3/3/3
7	GOL	N	402	-	-	4/4/4/4	-
7	GOL	A	403	-	-	2/4/4/4	-
7	GOL	A	404	-	-	2/4/4/4	-
9	MES	N	401	-	-	1/6/14/14	0/1/1/1
6	LAB	A	402	-	-	5/21/49/49	0/2/3/3
5	ATP	A	401	4	-	3/22/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	LAB	C16-N1	21.29	1.73	1.46
6	A	402	LAB	C2-C3	12.12	1.55	1.33
8	N	400	ACO	O4B-C1B	10.83	1.67	1.42
9	N	401	MES	C8-S	-7.21	1.67	1.77
6	A	402	LAB	C7-C6	6.73	1.59	1.31
8	N	400	ACO	C2B-C1B	-6.68	1.32	1.53
8	N	400	ACO	P2A-O3A	6.59	1.66	1.59
8	N	400	ACO	C5P-N4P	6.45	1.48	1.33
8	N	400	ACO	O4B-C4B	-6.41	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	LAB	C18-S1	-6.35	1.64	1.77
8	N	400	ACO	P1A-O3A	6.12	1.66	1.59
6	A	402	LAB	C12-C11	5.62	1.65	1.52
6	A	402	LAB	C10-C11	-5.59	1.34	1.51
6	A	402	LAB	O2-C1	5.23	1.45	1.34
6	A	402	LAB	C17-S1	-5.13	1.69	1.81
6	A	402	LAB	C15-C16	-4.82	1.45	1.54
8	N	400	ACO	C9P-N8P	4.76	1.44	1.33
5	A	401	ATP	C5-C4	4.73	1.47	1.39
8	N	400	ACO	C6A-N6A	4.43	1.45	1.34
6	A	402	LAB	O3-C11	4.08	1.53	1.44
8	N	400	ACO	C6P-C5P	4.07	1.59	1.51
6	A	402	LAB	C2-C1	3.96	1.56	1.46
6	A	402	LAB	C9-C10	3.91	1.63	1.53
8	N	400	ACO	O3B-C3B	-3.64	1.31	1.44
8	N	400	ACO	P3B-O3B	3.54	1.65	1.59
6	A	402	LAB	C17-C16	-3.17	1.45	1.52
8	N	400	ACO	O9P-C9P	-3.09	1.17	1.23
8	N	400	ACO	CEP-CBP	2.93	1.59	1.53
8	N	400	ACO	C3B-C4B	2.93	1.60	1.52
5	A	401	ATP	PB-O3B	2.71	1.62	1.59
5	A	401	ATP	C5-C6	2.70	1.48	1.41
5	A	401	ATP	C8-N7	2.64	1.36	1.31
5	A	401	ATP	C5-N7	-2.58	1.34	1.39
6	A	402	LAB	O3-C15	2.56	1.47	1.43
6	A	402	LAB	C4-C3	2.47	1.56	1.51
8	N	400	ACO	O2B-C2B	2.40	1.48	1.43
8	N	400	ACO	C5A-C4A	-2.39	1.34	1.39
5	A	401	ATP	C4-N9	-2.31	1.32	1.37
6	A	402	LAB	C14-C13	-2.27	1.46	1.51
8	N	400	ACO	C-S1P	2.22	1.87	1.75
8	N	400	ACO	C5A-N7A	-2.12	1.35	1.39
8	N	400	ACO	O5P-C5P	-2.12	1.19	1.23
5	A	401	ATP	PB-O3A	2.07	1.61	1.59
5	A	401	ATP	PA-O3A	2.05	1.61	1.59
8	N	400	ACO	C4A-N9A	-2.03	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	LAB	C17-S1-C18	21.18	104.31	92.04
8	N	400	ACO	N3A-C2A-N1A	-5.60	120.11	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	ATP	C5-C4-N3	-5.39	119.29	126.72
6	A	402	LAB	O3-C11-C12	-5.21	99.86	109.02
8	N	400	ACO	C5A-C4A-N3A	-4.96	119.89	126.72
5	A	401	ATP	N3-C4-N9	4.55	134.90	127.17
5	A	401	ATP	C4-N9-C8	3.99	109.92	105.74
5	A	401	ATP	N3-C2-N1	-3.85	122.75	128.58
8	N	400	ACO	N9A-C8A-N7A	-3.72	108.66	113.94
5	A	401	ATP	C2-N3-C4	3.71	120.88	111.83
5	A	401	ATP	C4-C5-N7	-3.64	106.42	110.58
8	N	400	ACO	C2A-N3A-C4A	3.42	120.18	111.83
6	A	402	LAB	C12-C13-C14	3.42	117.75	111.02
9	N	401	MES	C5-N4-C3	3.07	115.45	108.84
5	A	401	ATP	C5-N7-C8	2.92	108.04	103.45
5	A	401	ATP	N9-C8-N7	-2.91	109.81	113.94
6	A	402	LAB	C4-C5-C6	-2.83	106.41	112.57
6	A	402	LAB	C19-C3-C4	2.79	120.07	115.23
8	N	400	ACO	N3A-C4A-N9A	2.69	131.75	127.17
8	N	400	ACO	C5A-N7A-C8A	2.60	107.53	103.45
5	A	401	ATP	C6-C5-N7	2.54	136.99	132.09
6	A	402	LAB	O4-C15-O3	-2.45	105.23	110.00
6	A	402	LAB	C9-C10-C11	-2.45	109.59	114.06
8	N	400	ACO	C3B-C2B-C1B	2.43	105.23	99.89
8	N	400	ACO	C5A-C4A-N9A	2.34	108.36	105.81
5	A	401	ATP	C2-N1-C6	2.33	122.56	118.73
8	N	400	ACO	O6A-CCP-CBP	-2.28	106.89	110.55
9	N	401	MES	O3S-S-C8	2.26	110.43	106.00
6	A	402	LAB	O2-C1-C2	2.24	116.39	111.20
8	N	400	ACO	C4A-C5A-N7A	-2.22	108.05	110.58
8	N	400	ACO	P3B-O3B-C3B	-2.19	117.58	123.43
8	N	400	ACO	CDP-CBP-CAP	2.15	112.44	108.77
8	N	400	ACO	N6A-C6A-N1A	-2.11	113.69	118.38
7	A	403	GOL	C3-C2-C1	-2.06	104.23	111.80
8	N	400	ACO	C2P-C3P-N4P	-2.04	108.16	112.41
6	A	402	LAB	O5-C18-S1	2.00	126.64	123.06

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	ATP	PB-O3B-PG-O3G
6	A	402	LAB	O3-C15-C16-C17
7	A	404	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	N	402	GOL	O1-C1-C2-C3
8	N	400	ACO	C5B-O5B-P1A-O1A
8	N	400	ACO	C5B-O5B-P1A-O2A
8	N	400	ACO	C5B-O5B-P1A-O3A
8	N	400	ACO	C2P-C3P-N4P-C5P
8	N	400	ACO	S1P-C2P-C3P-N4P
8	N	400	ACO	O-C-S1P-C2P
8	N	400	ACO	CH3-C-S1P-C2P
6	A	402	LAB	C14-C13-O2-C1
7	N	402	GOL	O1-C1-C2-O2
8	N	400	ACO	C4B-C3B-O3B-P3B
7	A	403	GOL	O1-C1-C2-C3
7	N	402	GOL	C1-C2-C3-O3
7	A	404	GOL	O2-C2-C3-O3
7	N	402	GOL	O2-C2-C3-O3
7	A	403	GOL	O1-C1-C2-O2
8	N	400	ACO	C2B-C3B-O3B-P3B
8	N	400	ACO	C6P-C7P-N8P-C9P
9	N	401	MES	C8-C7-N4-C3
6	A	402	LAB	C12-C13-O2-C1
6	A	402	LAB	O2-C1-C2-C3
5	A	401	ATP	PB-O3B-PG-O2G
6	A	402	LAB	O1-C1-C2-C3
5	A	401	ATP	PB-O3B-PG-O1G
8	N	400	ACO	P1A-O3A-P2A-O5A

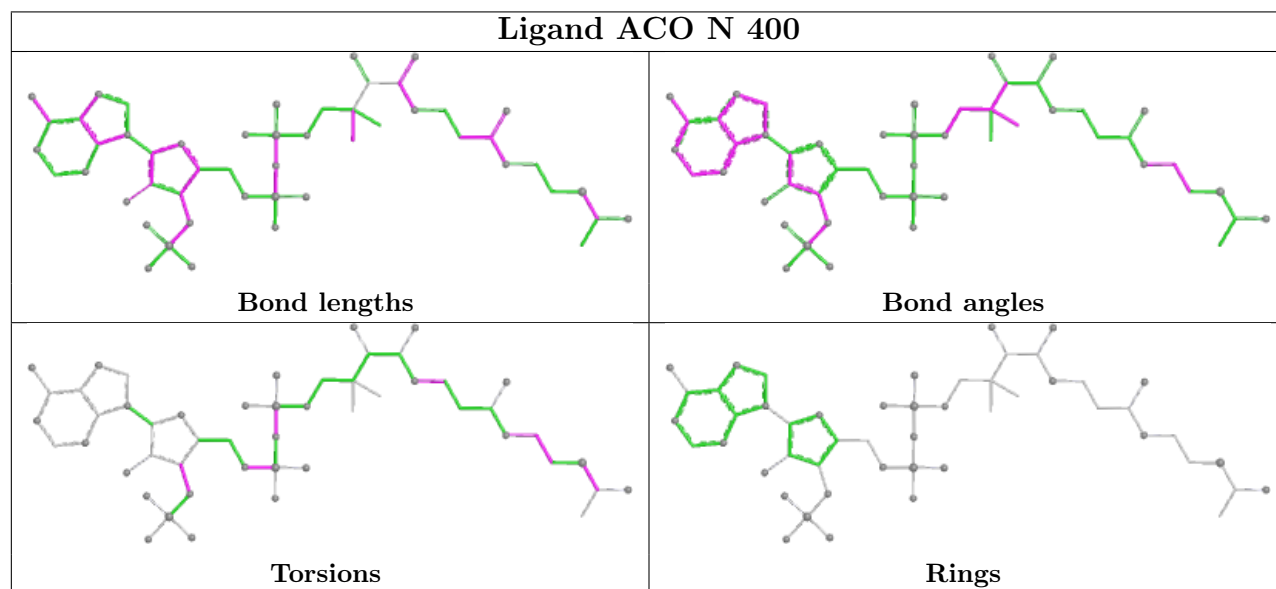
There are no ring outliers.

3 monomers are involved in 7 short contacts:

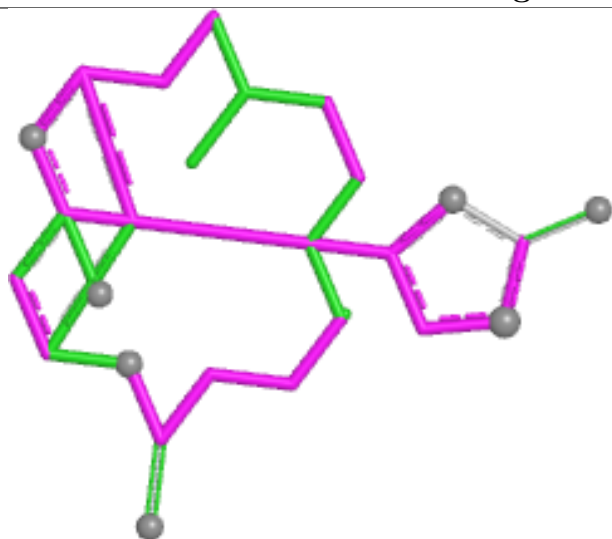
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	400	ACO	1	0
6	A	402	LAB	4	0
5	A	401	ATP	2	0

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

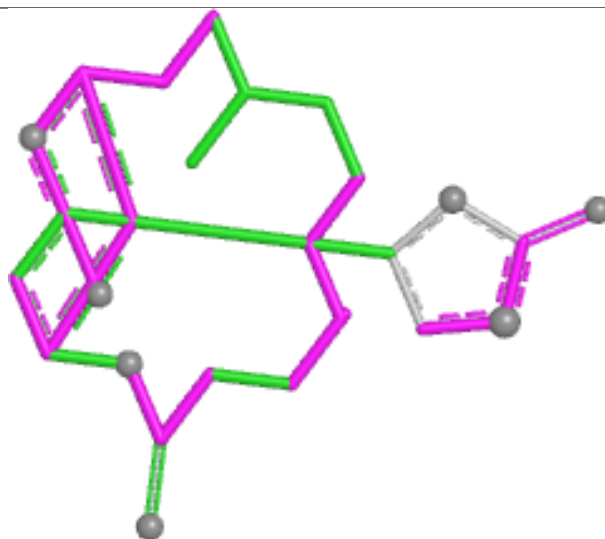
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



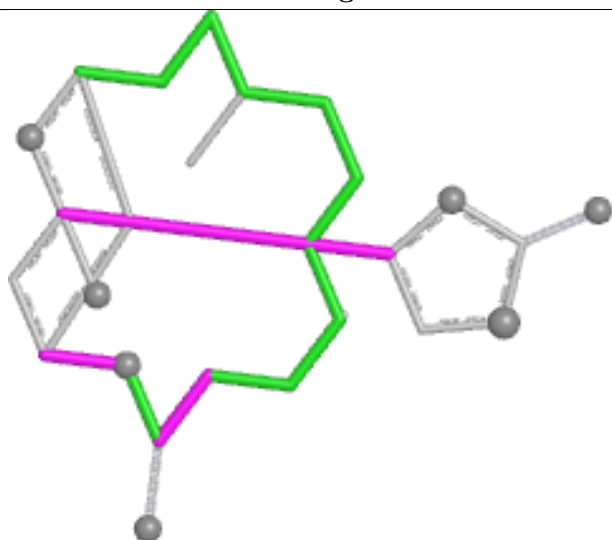
Ligand LAB A 402



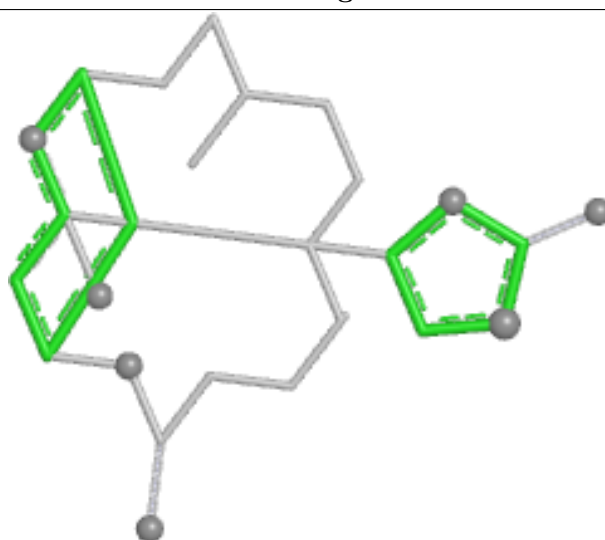
Bond lengths



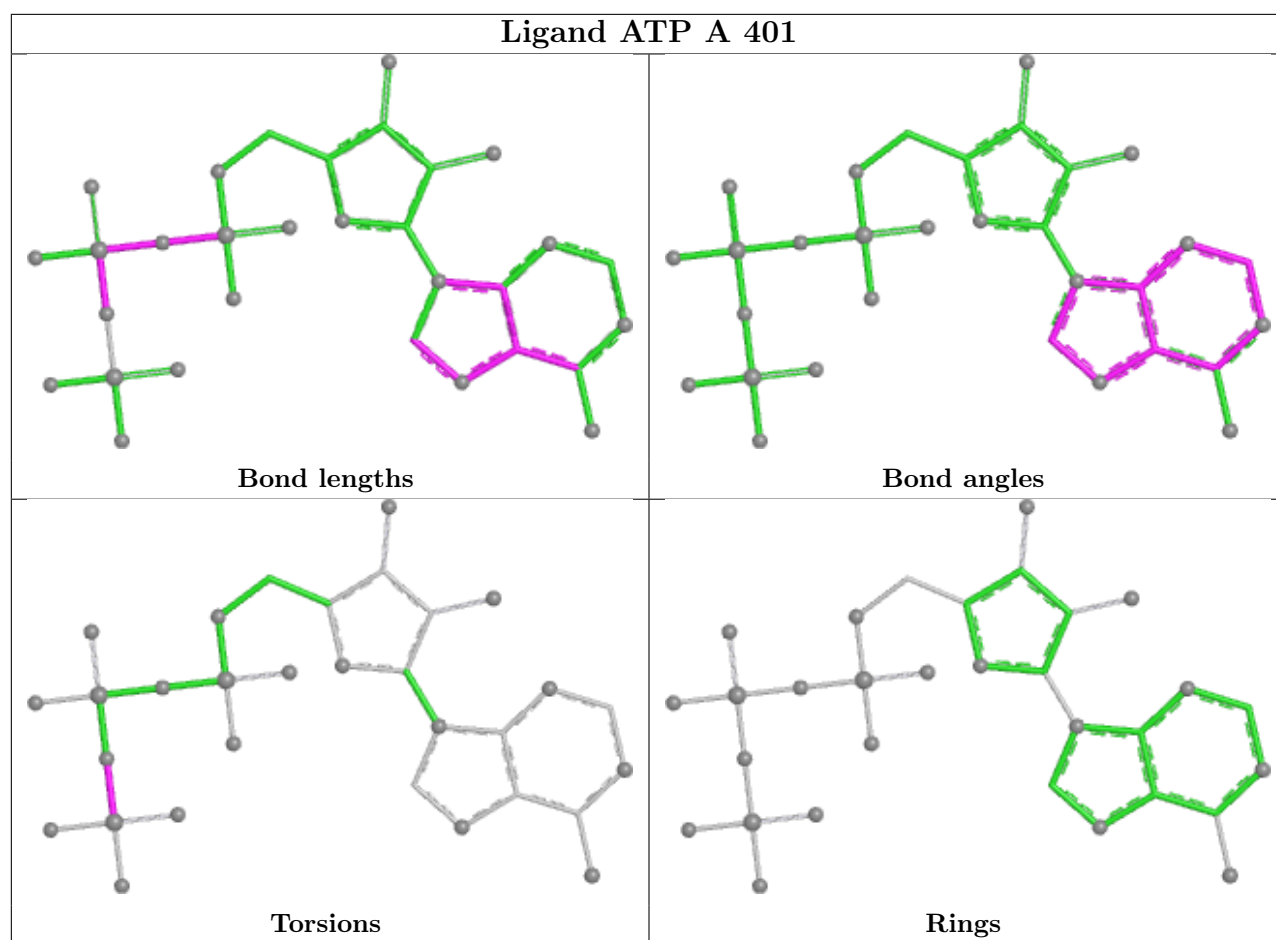
Bond angles



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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/375 (98%)	-0.31	4 (1%) 78 71	25, 37, 58, 102	0
2	N	180/235 (76%)	-0.01	11 (6%) 27 21	26, 35, 98, 121	0
3	P	138/140 (98%)	0.04	0 100 100	35, 51, 84, 100	0
All	All	686/750 (91%)	-0.16	15 (2%) 62 53	25, 39, 82, 121	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	138	ALA	4.6
2	N	133	HIS	4.3
2	N	75	GLY	3.7
2	N	76	HIS	3.1
2	N	291	THR	3.1
2	N	269	LEU	2.8
2	N	296	VAL	2.7
1	A	48	GLY	2.6
2	N	299	ARG	2.6
1	A	47	MET	2.5
2	N	294	GLN	2.5
1	A	41	GLN	2.3
2	N	132	PRO	2.2
1	A	51	ASP	2.1
2	N	270	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KKD	A	1	11/12	0.93	0.10	26,38,51,55	0
1	HIC	A	73	11/12	0.96	0.08	26,32,39,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

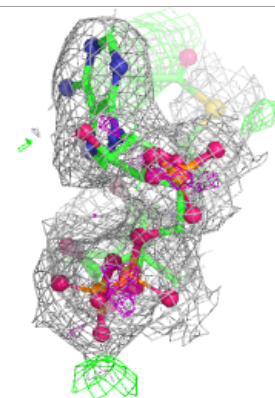
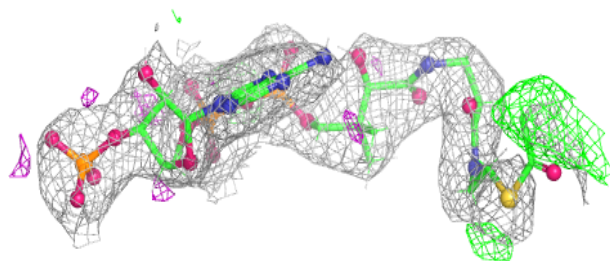
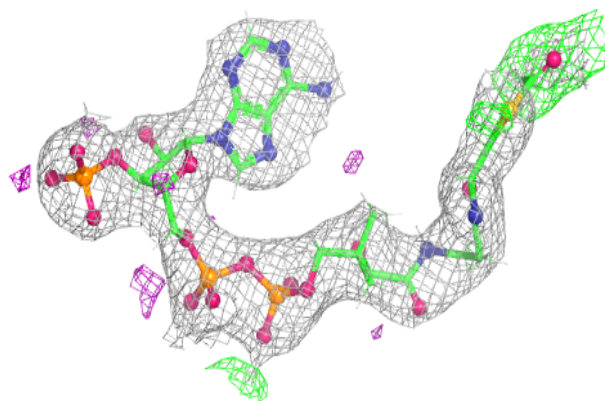
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	N	402	6/6	0.82	0.26	40,48,56,57	0
7	GOL	A	404	6/6	0.88	0.09	41,49,55,60	0
9	MES	N	401	12/12	0.89	0.14	39,49,64,74	0
7	GOL	A	403	6/6	0.92	0.14	39,50,60,60	0
8	ACO	N	400	51/51	0.92	0.10	23,34,51,54	6
4	CA	A	400	1/1	0.92	0.12	34,34,34,34	0
6	LAB	A	402	27/27	0.96	0.08	19,27,33,36	0
5	ATP	A	401	31/31	0.97	0.07	20,26,35,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

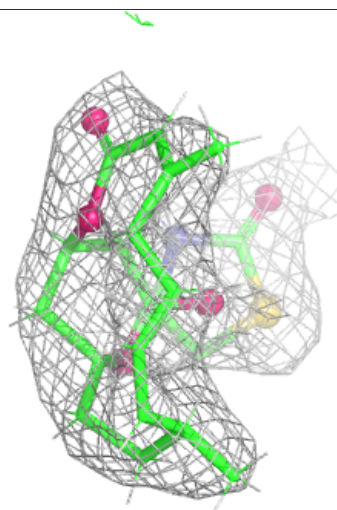
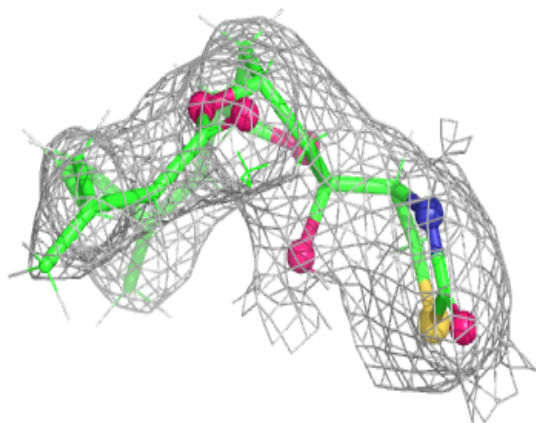
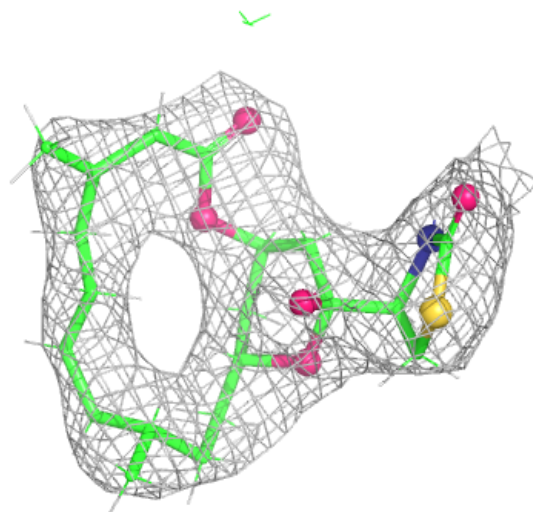
Electron density around ACO N 400:

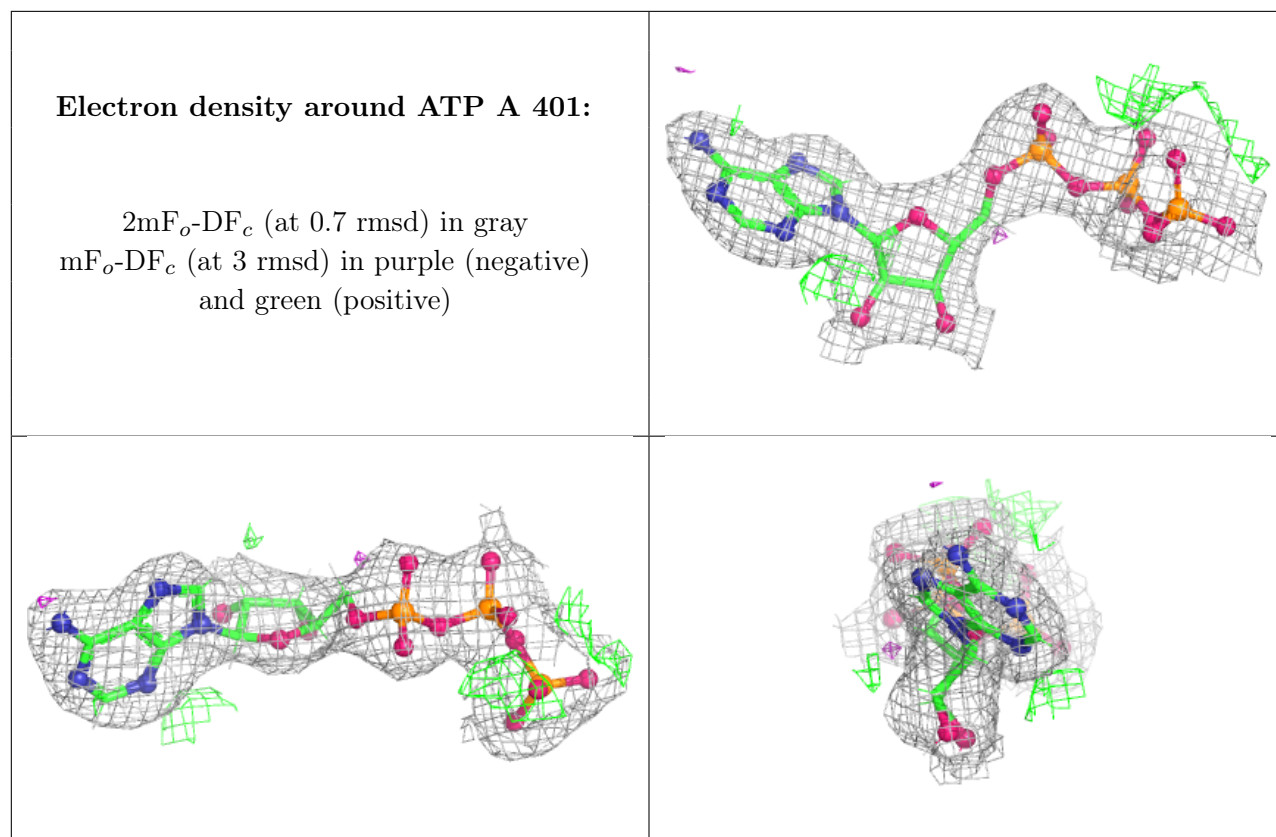
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LAB A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.