



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:17 PM BST

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 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 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) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

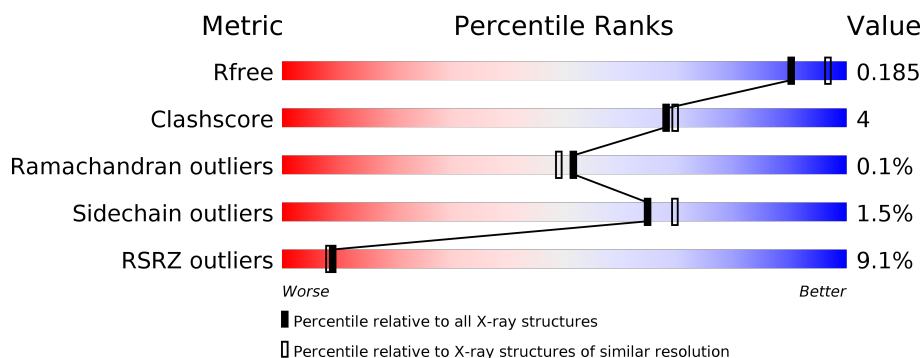
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 $\leq 5\%$. 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	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
2	N	235	<div> <div>16%</div> <div> <div></div> <div>69%</div> <div>9%</div> <div>•</div> <div>21%</div> </div> </div>
3	P	140	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>••</div> </div> </div>

2 Entry composition

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
1	A	370	Total	C	H	N	O	S	0	5	0
			5831	1854	2899	493	565	20			

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

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

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

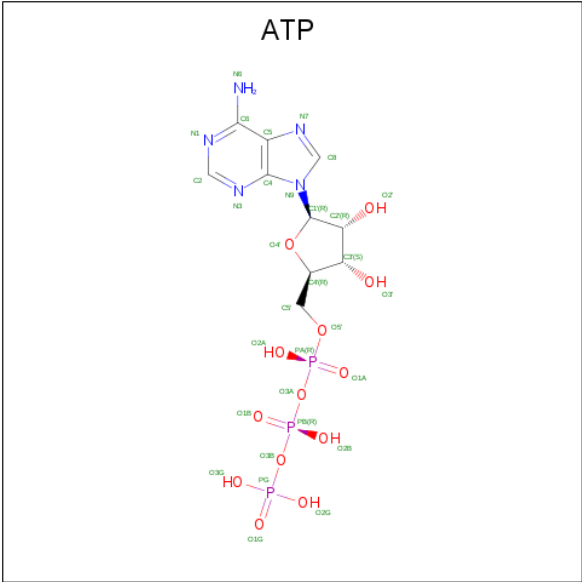
- Molecule 3 is a protein called Profilin-1.

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 (three-letter code: CA) (formula: Ca).

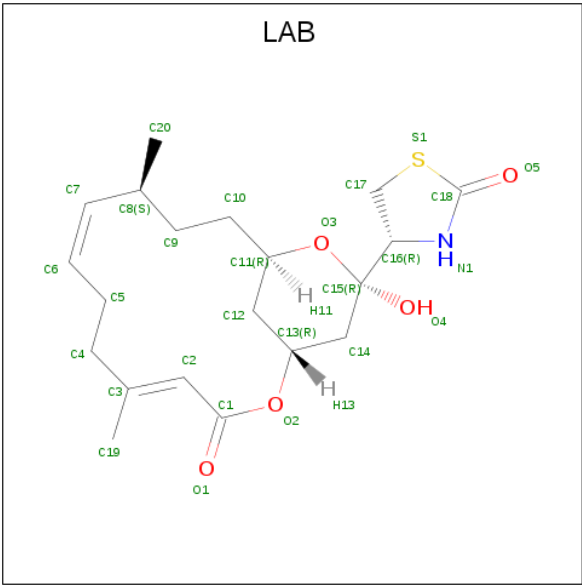
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



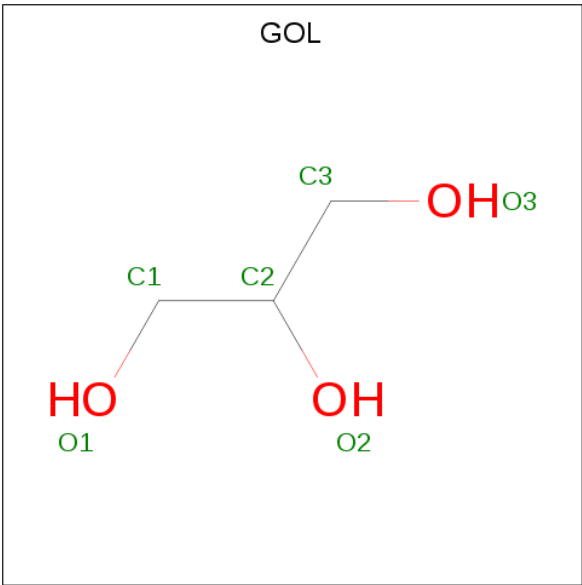
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		

- Molecule 6 is LATRUNCULIN B (three-letter code: LAB) (formula: C₂₀H₂₉NO₅S).



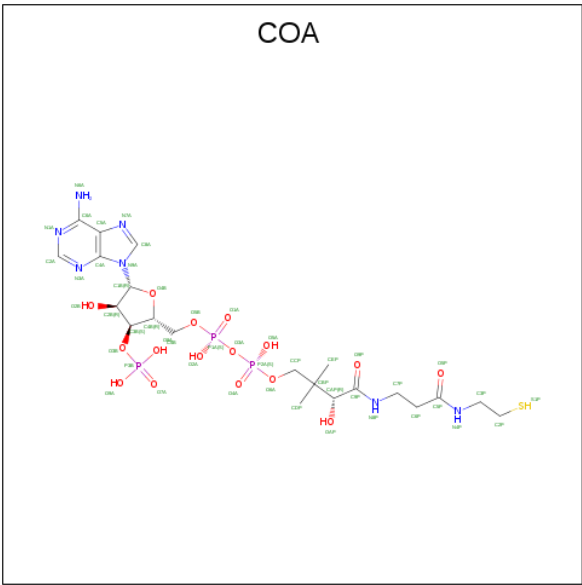
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			56	20	29	1	5	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



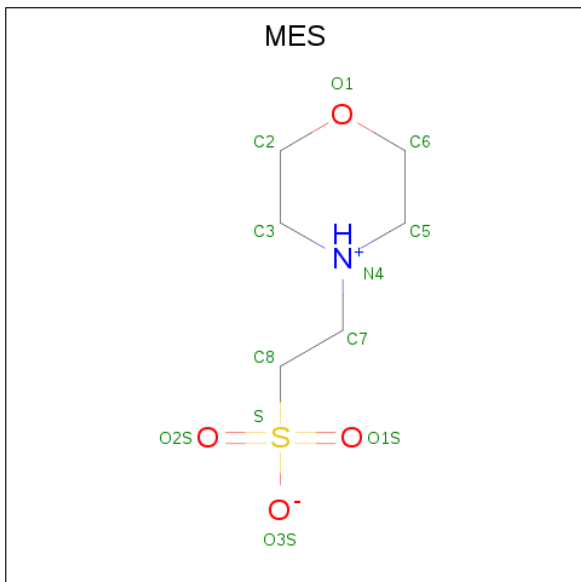
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			13	3	7	3		
7	N	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

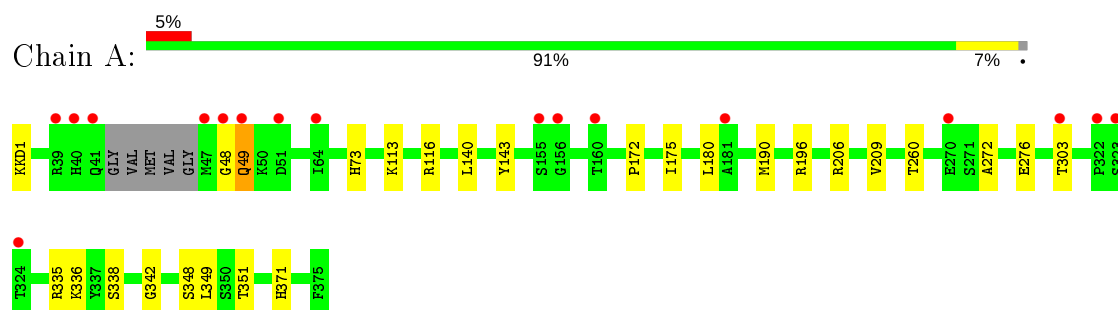
- Molecule 10 is water.

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

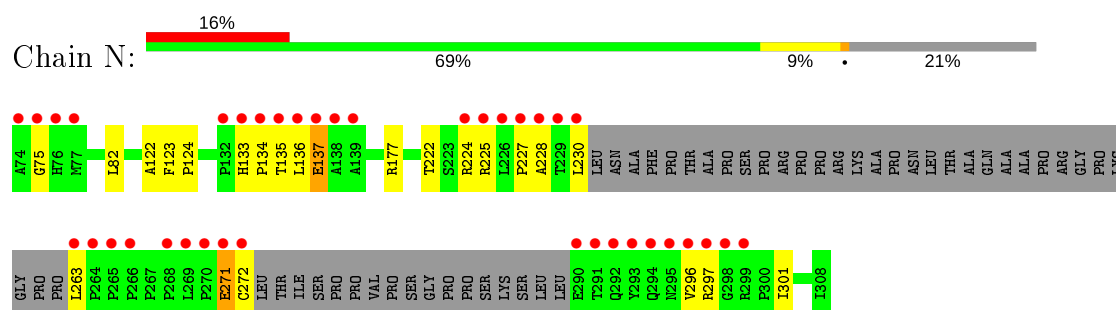
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

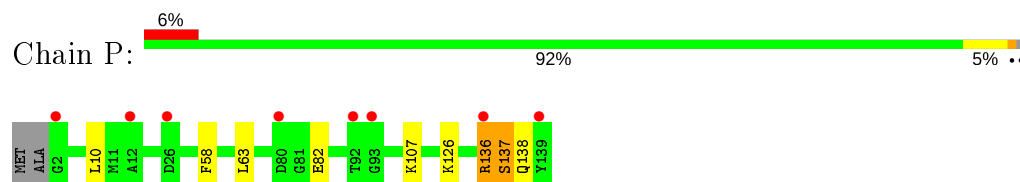
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: N-alpha-acetyltransferase 80



- Molecule 3: Profilin-1



4 Data and refinement statistics

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 33.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.35-2.00) 99.6 (33.35-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.159 , 0.184 0.161 , 0.185	Depositor DCC
R_{free} test set	2000 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ATP, CA, LAB, COA, HIC, MES, KKD

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

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.

All (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:HH21	3:P:136:ARG:HG2	1.55	0.71
6:A:402:LAB:H142	6:A:402:LAB:O1	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
1:A:206:ARG:NH1	10:A:504:HOH:O	2.38	0.57
2:N:301:ILE:HD12	2:N:301:ILE:O	2.05	0.57
6:A:402:LAB:O2	6:A:402:LAB:H42	2.05	0.56
1:A:196:ARG:O	1:A:196:ARG:HG2	2.07	0.54
2:N:133:HIS:C	2:N:135:THR:H	2.12	0.53
1:A:113:LYS:HG2	1:A:371:HIS:CE1	2.46	0.50
1:A:348:SER:HB3	2:N:222:THR:HG22	1.93	0.49
1:A:180:LEU:C	1:A:180:LEU:HD23	2.33	0.48
6:A:402:LAB:H51	6:A:402:LAB:H11	1.96	0.47
2:N:271:GLU:O	2:N:272:CYS:CB	2.61	0.47
2:N:122:ALA:O	2:N:123:PHE:HB2	2.14	0.47
3:P:136:ARG:HH21	3:P:136:ARG:CG	2.24	0.47
1:A:336:LYS:HE3	5:A:401:ATP:N7	2.30	0.46
3:P:137:SER:O	3:P:138:GLN:HB2	2.15	0.46
2:N:133:HIS:HB2	2:N:135:THR:H	1.81	0.45
3:P:107:LYS:NZ	3:P:138:GLN:O	2.46	0.44
1:A:349:LEU:HB3	1:A:351:THR:HG22	2.00	0.44
1:A:113:LYS:NZ	3:P:82:GLU:OE2	2.46	0.44
1:A:48:GLY:O	1:A:49:GLN:CB	2.66	0.43
1:A:335:ARG:HA	1:A:338:SER:HB3	1.99	0.43
3:P:63:LEU:C	3:P:63:LEU:HD12	2.39	0.43
1:A:143:TYR:HD1	2:N:230:LEU:HD13	1.84	0.43
3:P:10:LEU:O	3:P:126:LYS:HE3	2.19	0.43
2:N:134:PRO:HD2	2:N:136:LEU:O	2.19	0.42
2:N:123:PHE:HA	2:N:124:PRO:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:O	1:A:342:GLY:HA3	2.20	0.42
2:N:82:LEU:HD12	2:N:177:ARG:CZ	2.50	0.42
6:A:402:LAB:H51	6:A:402:LAB:H8	1.87	0.42
2:N:134:PRO:O	2:N:135:THR:OG1	2.36	0.41
2:N:133:HIS:HB3	2:N:137:GLU:O	2.20	0.41
7:A:403:GOL:H12	10:A:512:HOH:O	2.20	0.41
1:A:303:THR:HG22	1:A:303:THR:O	2.19	0.41
1:A:172:PRO:HA	1:A:175:ILE:HD12	2.03	0.40
1:A:272:ALA:HB1	1:A:276:GLU:HB2	2.02	0.40
2:N:227:PRO:O	2:N:228:ALA:HB3	2.21	0.40
1:A:190:MET:HG2	1:A:209:VAL:HG21	2.03	0.40
2:N:75:GLY:O	10:N:501:HOH:O	2.22	0.40

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	370/375 (99%)	363 (98%)	6 (2%)	1 (0%)	41	37
2	N	180/235 (77%)	173 (96%)	7 (4%)	0	100	100
3	P	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
All	All	686/750 (92%)	667 (97%)	18 (3%)	1 (0%)	51	49

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	318/316 (101%)	317 (100%)	1 (0%)	92	95
2	N	161/201 (80%)	156 (97%)	5 (3%)	40	40
3	P	113/114 (99%)	110 (97%)	3 (3%)	44	46
All	All	592/631 (94%)	583 (98%)	9 (2%)	65	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
2	N	137	GLU
2	N	224	ARG
2	N	225	ARG
2	N	263	LEU
2	N	271	GLU
3	P	58	PHE
3	P	136	ARG
3	P	137	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	N	154	GLN

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	KKD	A	1	1	6,10,11	1.47	1 (16%)	8,12,14	1.41	1 (12%)
1	HIC	A	73	1	8,11,12	1.62	1 (12%)	6,14,16	1.15	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KKD	A	1	1	-	4/7/10/12	-
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

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(°)	Ideal(°)
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 (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	KKD	N-CA-CB-CG
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	$\# Z > 2$
6	LAB	A	402	-	28,29,29	1.59	2 (7%)	30,41,41	1.64	8 (26%)
8	COA	N	400	-	41,50,50	3.95	14 (34%)	52,75,75	2.05	12 (23%)
9	MES	N	401	-	12,12,12	1.51	3 (25%)	14,16,16	2.06	3 (21%)
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
7	GOL	N	402	-	5,5,5	0.56	0	5,5,5	0.73	0
7	GOL	A	404	-	5,5,5	0.97	0	5,5,5	0.91	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
6	LAB	A	402	-	-	3/21/49/49	0/2/3/3
8	COA	N	400	-	-	9/44/64/64	0/3/3/3
9	MES	N	401	-	-	0/6/14/14	0/1/1/1
5	ATP	A	401	4	-	2/18/38/38	0/3/3/3
7	GOL	A	403	-	-	2/4/4/4	-
7	GOL	N	402	-	-	4/4/4/4	-
7	GOL	A	404	-	-	2/4/4/4	-

All (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
6	A	402	LAB	O2-C1	5.52	1.46	1.34
8	N	400	COA	C2A-N3A	5.49	1.40	1.32
8	N	400	COA	O4B-C4B	-5.46	1.32	1.45
8	N	400	COA	C9P-N8P	5.28	1.45	1.33
6	A	402	LAB	C18-S1	-4.92	1.66	1.77
5	A	401	ATP	O4'-C4'	-4.91	1.34	1.45
8	N	400	COA	C6A-N6A	3.52	1.46	1.34
8	N	400	COA	P3B-O3B	3.46	1.65	1.59
8	N	400	COA	C6P-C5P	2.95	1.57	1.51
5	A	401	ATP	C6-N6	2.91	1.44	1.34
5	A	401	ATP	C5-C4	-2.87	1.33	1.40
9	N	401	MES	C8-S	2.87	1.81	1.77
8	N	400	COA	O9P-C9P	-2.80	1.17	1.23
5	A	401	ATP	PA-O5'	2.70	1.70	1.59
5	A	401	ATP	C2-N3	2.57	1.36	1.32
9	N	401	MES	O1S-S	2.46	1.52	1.45
8	N	400	COA	C3B-C4B	2.43	1.59	1.52
8	N	400	COA	O5P-C5P	-2.41	1.18	1.23
8	N	400	COA	C5A-C4A	-2.37	1.34	1.40
9	N	401	MES	O2S-S	2.37	1.52	1.45
5	A	401	ATP	O3'-C3'	-2.17	1.37	1.43
8	N	400	COA	O3B-C3B	-2.15	1.36	1.44

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
5	A	401	ATP	N6-C6-N1	-4.95	108.31	118.57
9	N	401	MES	O2S-S-C8	4.81	112.71	106.92
8	N	400	COA	C1B-N9A-C4A	-4.48	118.76	126.64
9	N	401	MES	O1S-S-C8	4.46	112.29	106.92
6	A	402	LAB	O2-C1-C2	4.13	120.97	111.27
8	N	400	COA	C2P-C3P-N4P	3.69	120.74	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	400	COA	C3P-N4P-C5P	2.81	128.06	122.84
6	A	402	LAB	O1-C1-C2	-2.75	119.29	126.23
9	N	401	MES	O2S-S-O1S	-2.73	104.50	113.95
8	N	400	COA	C6P-C5P-N4P	-2.57	112.09	116.42
8	N	400	COA	C7P-C6P-C5P	2.53	116.57	112.36
6	A	402	LAB	O5-C18-N1	-2.53	124.05	126.81
8	N	400	COA	C3B-C2B-C1B	2.52	105.46	99.89
8	N	400	COA	CDP-CBP-CAP	2.47	113.11	108.82
6	A	402	LAB	O2-C1-O1	-2.22	119.73	123.35
6	A	402	LAB	O3-C15-C16	2.22	107.09	104.25
6	A	402	LAB	C17-S1-C18	2.17	93.17	92.00
6	A	402	LAB	O2-C13-C14	2.17	113.00	107.59
8	N	400	COA	C6P-C7P-N8P	-2.14	107.57	111.90
6	A	402	LAB	C14-C15-C16	-2.12	109.62	113.75
8	N	400	COA	P2A-O3A-P1A	-2.06	125.76	132.83
5	A	401	ATP	O3G-PG-O3B	2.02	111.40	104.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	LAB	C14-C13-O2-C1
8	N	400	COA	C3B-O3B-P3B-O7A
8	N	400	COA	C5B-O5B-P1A-O1A
8	N	400	COA	C5B-O5B-P1A-O2A
8	N	400	COA	C2P-C3P-N4P-C5P
5	A	401	ATP	PB-O3B-PG-O3G
7	A	403	GOL	O1-C1-C2-C3
7	N	402	GOL	O1-C1-C2-C3
7	A	404	GOL	C1-C2-C3-O3
7	A	404	GOL	O2-C2-C3-O3
7	N	402	GOL	C1-C2-C3-O3
7	N	402	GOL	O1-C1-C2-O2
7	N	402	GOL	O2-C2-C3-O3
7	A	403	GOL	O1-C1-C2-O2
8	N	400	COA	C3B-O3B-P3B-O8A
8	N	400	COA	C5B-O5B-P1A-O3A
6	A	402	LAB	O2-C1-C2-C3
8	N	400	COA	C6P-C7P-N8P-C9P
5	A	401	ATP	PB-O3B-PG-O1G
8	N	400	COA	S1P-C2P-C3P-N4P
6	A	402	LAB	O1-C1-C2-C3

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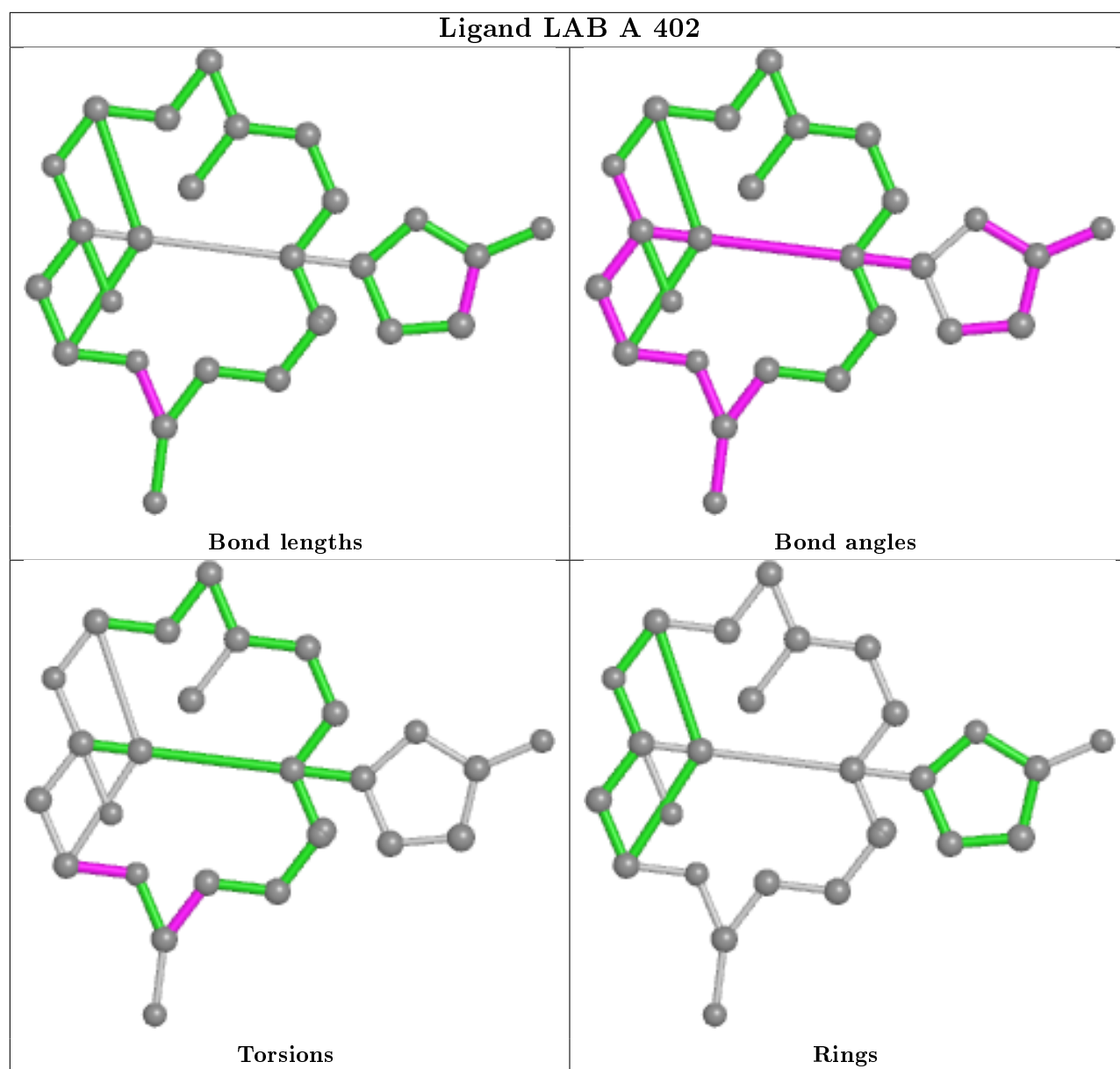
Mol	Chain	Res	Type	Atoms
8	N	400	COA	P1A-O3A-P2A-O5A

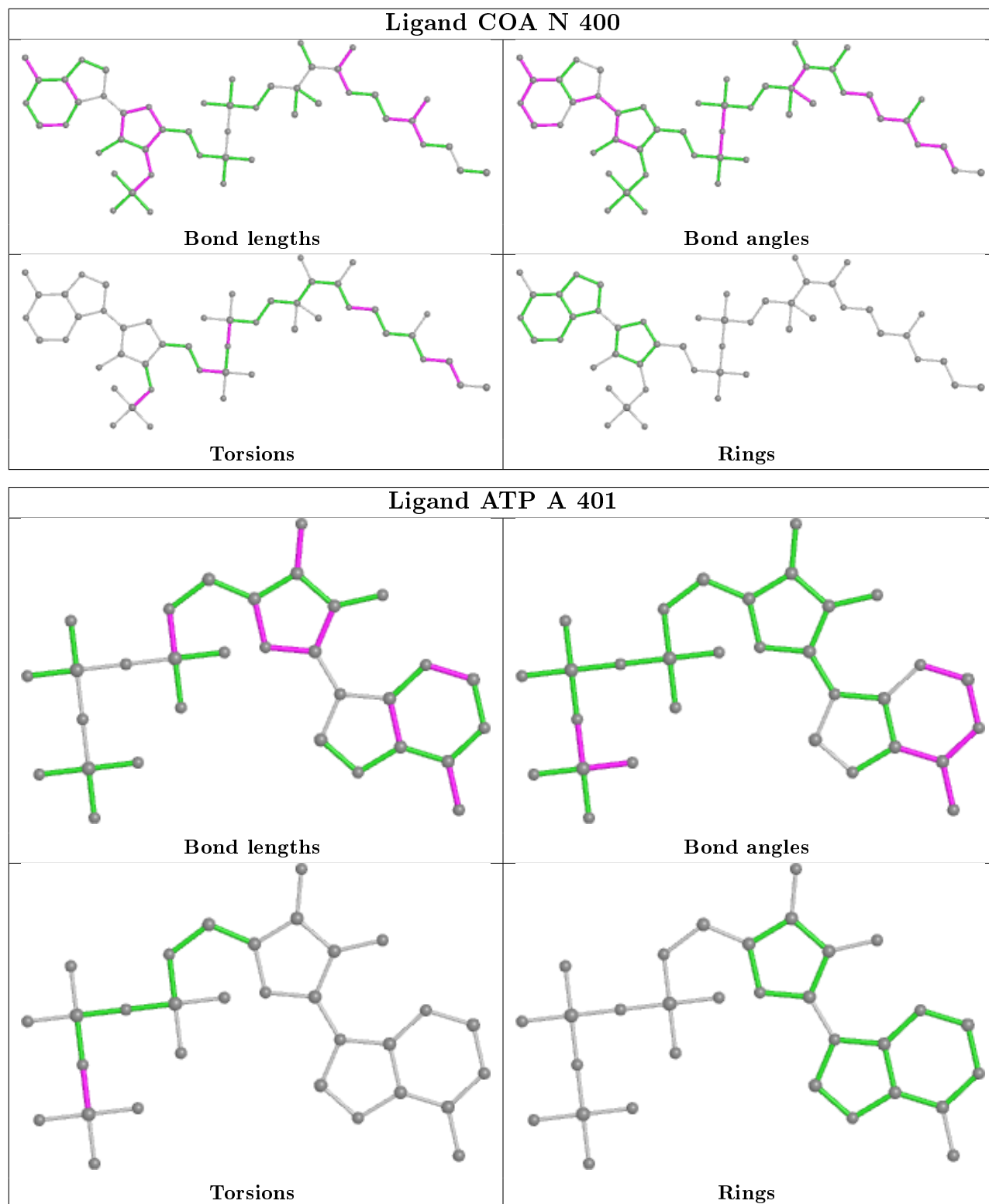
There are no ring outliers.

3 monomers are involved in 7 short contacts:

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





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

6.1 Protein, DNA and RNA chains

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%)	0.14	17 (4%) 32 31	17, 27, 44, 97	0
2	N	186/235 (79%)	0.88	38 (20%) 1 0	18, 27, 80, 98	0
3	P	138/140 (98%)	0.21	8 (5%) 23 22	25, 36, 63, 75	0
All	All	692/750 (92%)	0.35	63 (9%) 9 8	17, 29, 67, 98	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	272	CYS	13.7
2	N	136	LEU	12.8
2	N	269	LEU	9.0
1	A	47	MET	8.9
2	N	134	PRO	8.1
2	N	270	PRO	7.9
2	N	135	THR	7.8
2	N	138	ALA	6.6
1	A	41	GLN	6.5
2	N	137	GLU	6.4
2	N	271	GLU	6.3
2	N	74	ALA	6.1
2	N	297	ARG	5.8
2	N	268	PRO	5.7
1	A	48	GLY	5.7
2	N	290	GLU	5.3
2	N	293	TYR	5.1
2	N	139	ALA	5.1
2	N	299	ARG	4.9
2	N	296	VAL	4.9
2	N	291	THR	4.5
2	N	133	HIS	4.3
1	A	40	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
2	N	227	PRO	4.1
2	N	292	GLN	3.9
2	N	75	GLY	3.9
1	A	49	GLN	3.8
2	N	225	ARG	3.7
2	N	294	GLN	3.7
2	N	265	PRO	3.7
2	N	264	PRO	3.4
2	N	132	PRO	3.3
2	N	298	GLY	3.3
2	N	226	LEU	3.2
2	N	230	LEU	3.1
3	P	26	ASP	3.1
2	N	263	LEU	3.0
2	N	266	PRO	3.0
2	N	229	THR	2.9
3	P	2	GLY	2.7
3	P	93	GLY	2.7
1	A	322	PRO	2.7
1	A	39	ARG	2.6
1	A	156	GLY	2.6
1	A	64	ILE	2.6
3	P	80	ASP	2.5
2	N	228	ALA	2.5
3	P	12	ALA	2.4
1	A	181	ALA	2.4
1	A	303	THR	2.4
2	N	224	ARG	2.4
1	A	51	ASP	2.4
1	A	155	SER	2.3
3	P	139	TYR	2.3
1	A	270	GLU	2.2
1	A	160	THR	2.2
1	A	324	THR	2.2
3	P	92	THR	2.2
1	A	323	SER	2.2
2	N	77	MET	2.2
2	N	76	HIS	2.1
2	N	295	ASN	2.1
3	P	136	ARG	2.1

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(Å ²)	Q<0.9
1	KKD	A	1	11/12	0.94	0.15	19,27,36,36	0
1	HIC	A	73	11/12	0.98	0.15	18,23,32,32	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

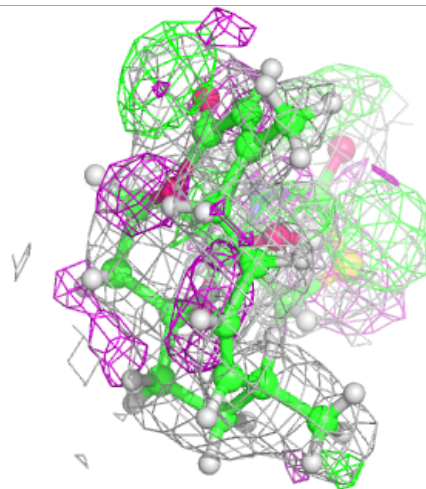
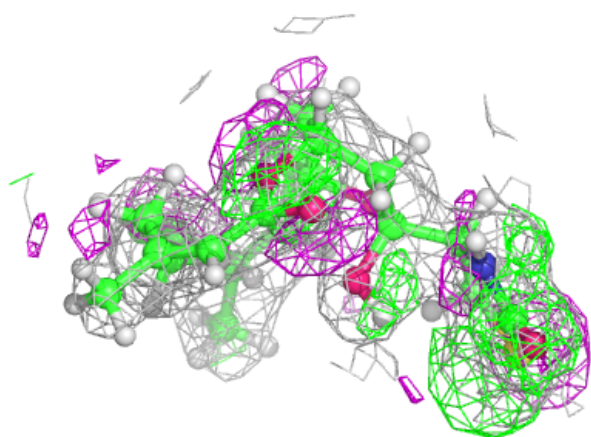
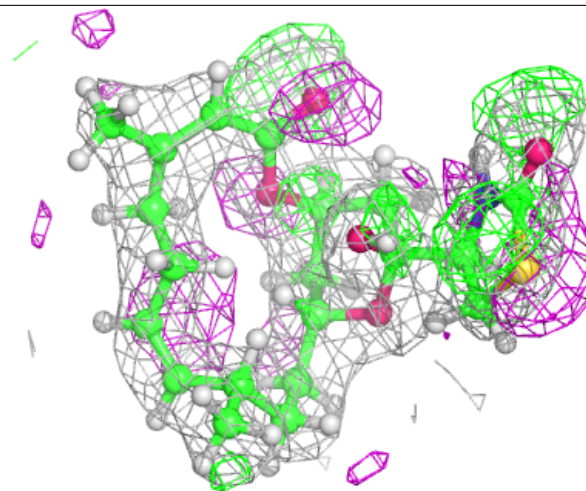
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MES	N	401	12/12	0.74	0.28	34,53,71,74	0
7	GOL	N	402	6/6	0.80	0.39	41,50,67,80	0
6	LAB	A	402	27/27	0.82	0.21	18,23,30,35	0
7	GOL	A	403	6/6	0.91	0.21	34,41,60,72	0
7	GOL	A	404	6/6	0.93	0.28	43,51,54,60	0
8	COA	N	400	48/48	0.97	0.11	19,27,48,54	0
5	ATP	A	401	31/31	0.98	0.18	17,21,27,29	0
4	CA	A	400	1/1	1.00	0.16	21,21,21,21	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.

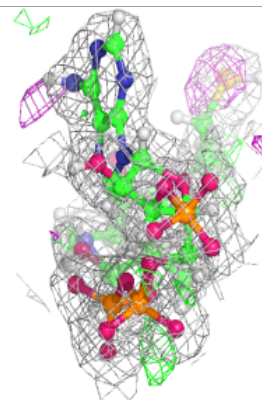
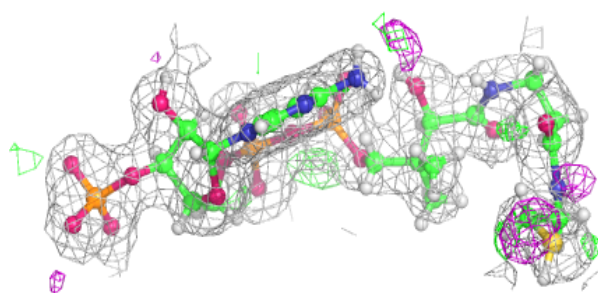
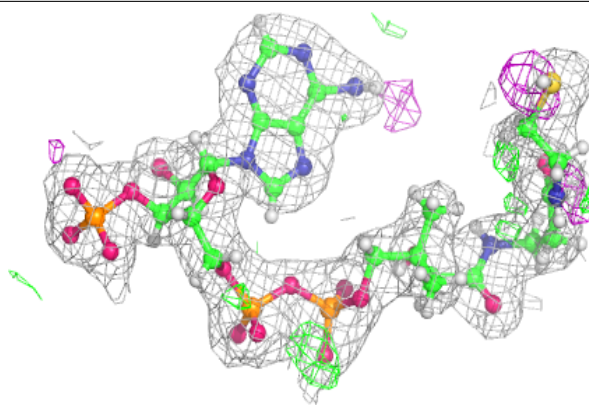
Electron density around LAB A 402:

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

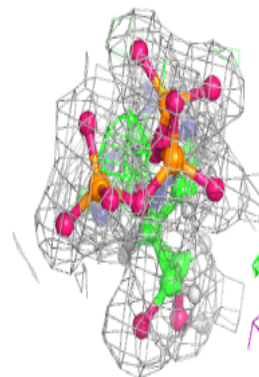
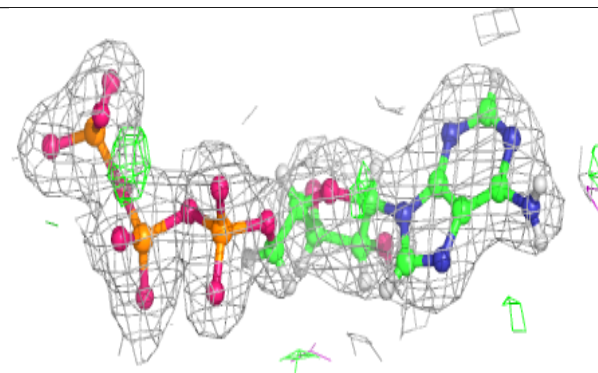
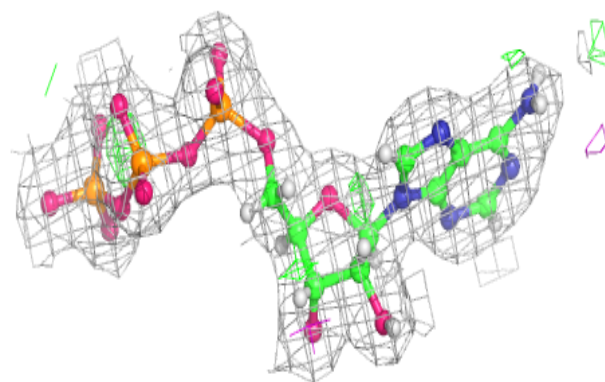


Electron density around COA N 400:

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

**Electron density around ATP A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.