



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:34 AM JST

PDB ID : 7C2F  
Title : Crystal Structure of the Thorarchaeota ProGel/rabbit actin complex  
Authors : Robinson, R.C.; Akil, C.  
Deposited on : 2020-05-07  
Resolution : 2.03 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](mailto: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>.

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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 : 2.36  
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) : 2.36

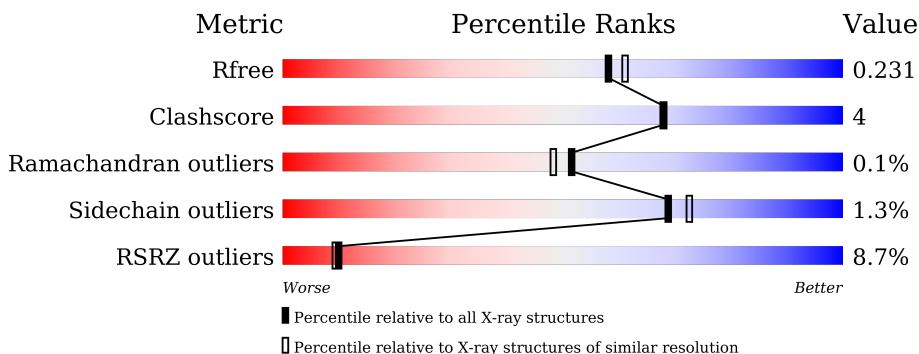
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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  $\geq 3$ , 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	 4% 91% 6% .
1	C	375	 6% 89% 7% .
2	B	94	 18% 79% 15% 6%
2	D	94	 26% 77% 17% 6%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15009 atoms, of which 7192 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	362	5692	1808	2835	483	547	19	0	6	0
1	C	361	5673	1804	2826	479	545	19	0	5	0

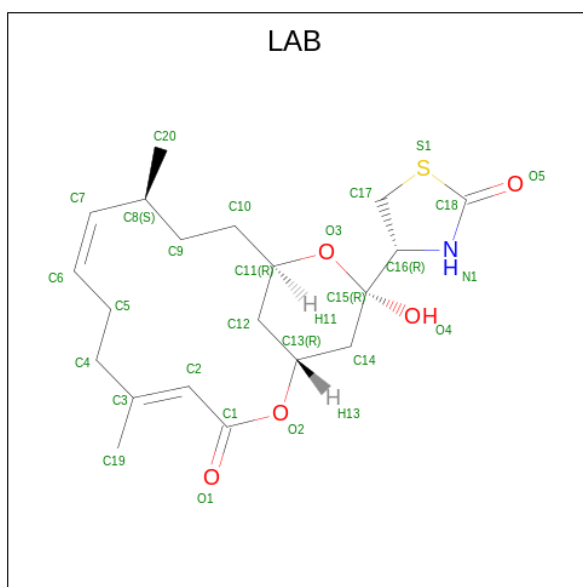
- Molecule 2 is a protein called Gelsolin-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	88	1459	465	738	120	133	3	0	4	0
2	D	88	1434	455	727	118	131	3	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

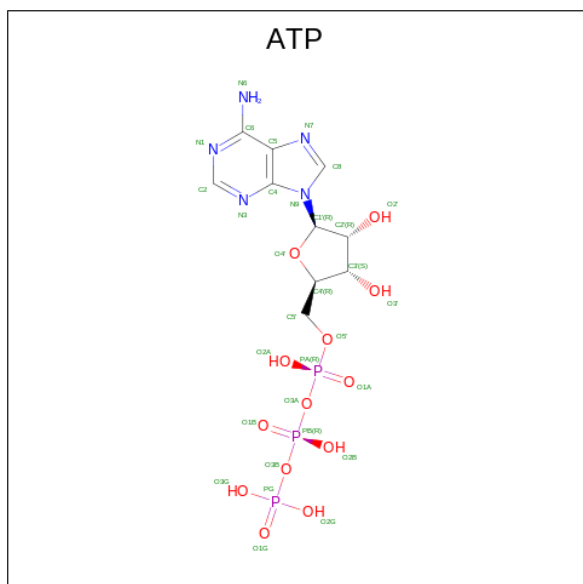
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A135VMT5
B	0	PRO	-	expression tag	UNP A0A135VMT5
D	-1	GLY	-	expression tag	UNP A0A135VMT5
D	0	PRO	-	expression tag	UNP A0A135VMT5

- Molecule 3 is LATRUNCULIN B (three-letter code: LAB) (formula: C<sub>20</sub>H<sub>29</sub>NO<sub>5</sub>S).



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

- Molecule 4 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		
4	A	1	Total	C	H	N	O	P	0	0
			35	10	4	5	13	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	P	0	0
			35	10	4	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

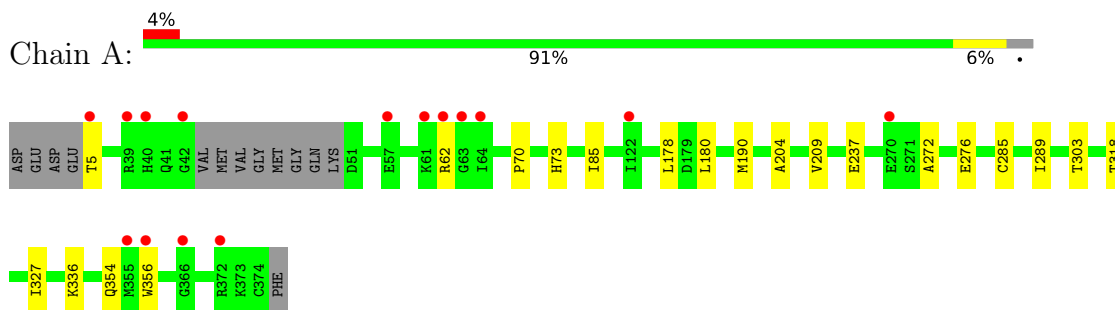
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total	O	0	0
			281	281		
6	B	23	Total	O	0	0
			23	23		
6	C	245	Total	O	0	0
			245	245		
6	D	18	Total	O	0	0
			18	18		

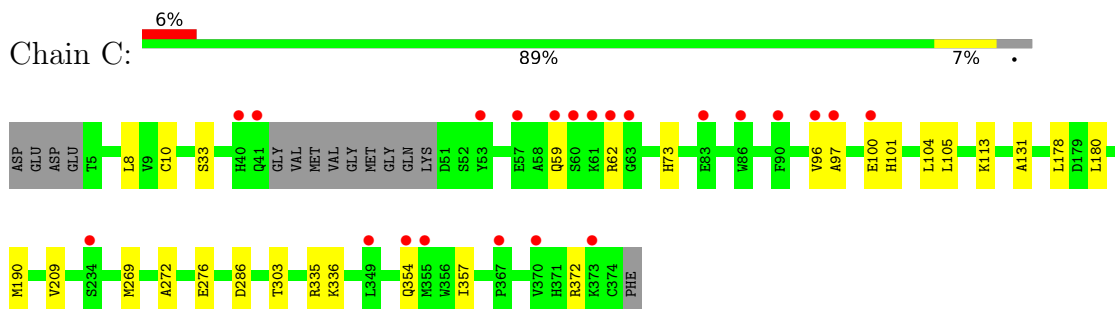
### 3 Residue-property plots [i](#)

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.

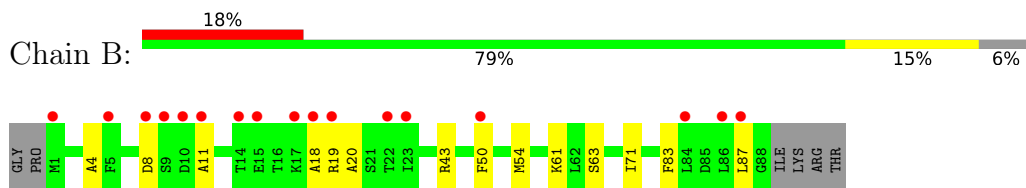
- Molecule 1: Actin, alpha skeletal muscle



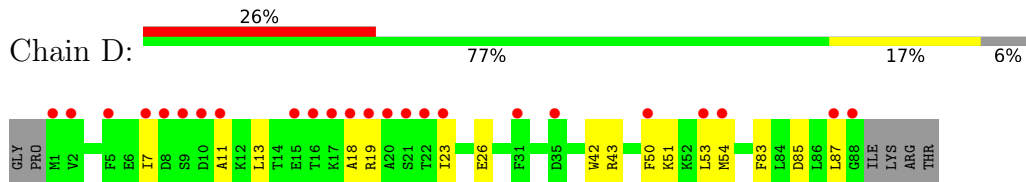
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Gelsolin-like domain-containing protein



- Molecule 2: Gelsolin-like domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.43Å 108.63Å 167.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.03 48.59 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.59-2.03) 99.5 (48.59-2.03)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.03Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.199 , 0.231 0.200 , 0.231	Depositor DCC
$R_{free}$ test set	3415 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtrriage
Anisotropy	0.568	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3214e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ATP, LAB, HIC

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	0.26	0/2925	0.47	0/3962
1	C	0.26	0/2912	0.48	0/3946
2	B	0.27	0/748	0.51	0/1005
2	D	0.27	0/723	0.52	0/973
All	All	0.26	0/7308	0.48	0/9886

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	2857	2835	2822	13	0
1	C	2847	2826	2812	20	0
2	B	721	738	722	11	0
2	D	707	727	729	8	0
3	A	27	29	29	3	0
3	C	27	29	29	3	0
4	A	31	4	12	0	0
4	C	31	4	12	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	A	281	0	0	4	0
6	B	23	0	0	1	0
6	C	245	0	0	6	0
6	D	18	0	0	2	0
All	All	7817	7192	7167	55	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 (55) 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)
3:C:401:LAB:N1	3:C:401:LAB:C16	1.71	1.32
3:A:401:LAB:C16	3:A:401:LAB:N1	1.71	1.28
1:A:5:THR:N	6:A:503:HOH:O	2.09	0.85
1:C:269:MET:SD	6:C:719:HOH:O	2.34	0.84
2:D:53:LEU:O	6:D:101:HOH:O	1.97	0.83
1:A:237:GLU:OE1	6:A:501:HOH:O	1.98	0.81
1:C:113:LYS:NZ	6:C:502:HOH:O	2.14	0.79
2:D:7:ILE:O	6:D:102:HOH:O	2.03	0.76
1:A:356:TRP:O	6:A:502:HOH:O	2.09	0.69
1:A:336:LYS:NZ	6:A:505:HOH:O	2.30	0.65
1:C:286:ASP:OD1	6:C:501:HOH:O	2.14	0.64
1:C:97:ALA:HB3	1:C:100:GLU:OE2	1.98	0.63
1:C:10:CYS:HB3	1:C:105:LEU:HD23	1.81	0.62
2:B:11:ALA:HA	2:B:54[B]:MET:SD	2.41	0.61
2:B:19:ARG:NH1	6:B:101:HOH:O	2.35	0.60
3:A:401:LAB:N1	3:A:401:LAB:C15	2.61	0.58
2:B:54[A]:MET:SD	1:C:372:ARG:NH2	2.78	0.56
1:C:62:ARG:NH2	6:C:507:HOH:O	2.39	0.55
1:C:100:GLU:HB2	1:C:101:HIS:CD2	2.41	0.55
3:C:401:LAB:N1	3:C:401:LAB:C15	2.61	0.55
2:B:50[B]:PHE:N	2:B:50[B]:PHE:HD2	2.06	0.54
2:B:50[B]:PHE:N	2:B:50[B]:PHE:CD2	2.75	0.53
1:A:272:ALA:HB1	1:A:276:GLU:HB3	1.90	0.53
2:D:18:ALA:O	2:D:19:ARG:HG3	2.10	0.52
1:A:178:LEU:HG	1:A:180:LEU:HB3	1.91	0.51
1:C:59:GLN:HA	1:C:62:ARG:HB3	1.93	0.51
2:B:61:LYS:HZ1	1:C:372:ARG:HG3	1.78	0.49
1:C:336:LYS:NZ	6:C:513:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.96	0.48
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.96	0.48
1:A:62:ARG:HE	1:A:204:ALA:HB2	1.79	0.47
2:D:7:ILE:CG2	2:D:54[B]:MET:HE3	2.44	0.47
1:C:8:LEU:HD11	1:C:96:VAL:HG21	1.97	0.46
2:B:83:PHE:O	2:B:87:LEU:HD12	2.15	0.46
1:C:303:THR:HG22	1:C:303:THR:O	2.15	0.46
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.97	0.45
3:C:401:LAB:N1	3:C:401:LAB:C14	2.80	0.44
1:A:303:THR:HG22	1:A:303:THR:O	2.17	0.44
2:D:11:ALA:HA	2:D:54[B]:MET:SD	2.58	0.44
1:C:131:ALA:HA	1:C:357:ILE:O	2.18	0.44
3:A:401:LAB:N1	3:A:401:LAB:C14	2.81	0.44
2:D:26:GLU:O	2:D:51:LYS:NZ	2.49	0.43
2:D:83:PHE:O	2:D:87:LEU:HD12	2.18	0.43
1:C:272:ALA:HB1	1:C:276:GLU:HB3	2.00	0.43
2:B:50[B]:PHE:HD2	2:B:50[B]:PHE:H	1.67	0.43
1:C:335:ARG:NH2	6:C:520:HOH:O	2.52	0.42
1:C:303:THR:O	1:C:303:THR:CG2	2.68	0.41
1:C:190:MET:HG2	1:C:209:VAL:HG21	2.01	0.41
1:A:303:THR:O	1:A:303:THR:CG2	2.69	0.41
2:B:4:ALA:HB2	2:B:18:ALA:HB2	2.01	0.41
2:B:61:LYS:NZ	1:C:372:ARG:HG3	2.35	0.40
1:A:318:THR:HA	1:A:327:ILE:CD1	2.51	0.40
2:B:63:SER:CB	2:B:71:ILE:HD11	2.51	0.40
1:C:178:LEU:HG	1:C:180:LEU:HB3	2.04	0.40
2:D:23:ILE:HG23	2:D:42:TRP:CH2	2.57	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	363/375 (97%)	358 (99%)	5 (1%)	0	100	100
1	C	361/375 (96%)	355 (98%)	6 (2%)	0	100	100
2	B	90/94 (96%)	85 (94%)	4 (4%)	1 (1%)	14	7
2	D	87/94 (93%)	83 (95%)	4 (5%)	0	100	100
All	All	901/938 (96%)	881 (98%)	19 (2%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	ALA

### 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	312/317 (98%)	311 (100%)	1 (0%)	92	94
1	C	311/317 (98%)	307 (99%)	4 (1%)	69	72
2	B	77/79 (98%)	75 (97%)	2 (3%)	46	46
2	D	75/79 (95%)	71 (95%)	4 (5%)	22	17
All	All	775/792 (98%)	764 (99%)	11 (1%)	69	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
2	B	8	ASP
2	B	43	ARG
1	C	33[A]	SER
1	C	33[B]	SER
1	C	104	LEU
1	C	354	GLN
2	D	13	LEU
2	D	43	ARG
2	D	50	PHE

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Mol	Chain	Res	Type
2	D	85	ASP

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	C	73	1	8,11,12	1.66	1 (12%)	6,14,16	1.03	0
1	HIC	A	73	1	8,11,12	1.63	1 (12%)	6,14,16	1.03	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
1	HIC	C	73	1	-	0/5/6/8	0/1/1/1
1	HIC	A	73	1	-	1/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	HIC	CD2-CG	3.71	1.41	1.36
1	A	73	HIC	CD2-CG	3.59	1.41	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-ND1

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	ATP	C	402	5	26,33,33	0.91	1 (3%)	31,52,52	1.36	4 (12%)
4	ATP	A	402	5	26,33,33	0.93	1 (3%)	31,52,52	1.35	4 (12%)
3	LAB	A	401	-	28,29,29	5.12	15 (53%)	30,41,41	4.30	5 (16%)
3	LAB	C	401	-	28,29,29	5.13	15 (53%)	30,41,41	4.41	6 (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
4	ATP	C	402	5	-	2/18/38/38	0/3/3/3
4	ATP	A	402	5	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LAB	A	401	-	-	3/21/49/49	0/2/3/3
3	LAB	C	401	-	-	3/21/49/49	0/2/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	LAB	C16-N1	18.17	1.71	1.46
3	A	401	LAB	C16-N1	18.09	1.71	1.46
3	A	401	LAB	C2-C3	11.10	1.54	1.33
3	C	401	LAB	C2-C3	11.08	1.54	1.33
3	C	401	LAB	C7-C6	6.13	1.58	1.31
3	A	401	LAB	C7-C6	6.12	1.57	1.31
3	A	401	LAB	C17-S1	-5.91	1.69	1.81
3	C	401	LAB	C17-S1	-5.82	1.69	1.81
3	C	401	LAB	C18-S1	-5.79	1.64	1.77
3	A	401	LAB	C18-S1	-5.55	1.65	1.77
3	C	401	LAB	O2-C1	5.52	1.46	1.34
3	A	401	LAB	O2-C1	5.38	1.45	1.34
3	A	401	LAB	C18-N1	4.94	1.40	1.34
3	C	401	LAB	C18-N1	4.82	1.40	1.34
3	C	401	LAB	C12-C11	4.48	1.63	1.52
3	C	401	LAB	C10-C11	-4.47	1.36	1.51
3	A	401	LAB	C10-C11	-4.47	1.36	1.51
3	A	401	LAB	C12-C11	4.45	1.63	1.52
3	A	401	LAB	C17-C16	-4.45	1.45	1.53
3	C	401	LAB	C17-C16	-4.42	1.45	1.53
3	A	401	LAB	C2-C1	3.95	1.56	1.46
3	C	401	LAB	C2-C1	3.95	1.56	1.46
3	A	401	LAB	O3-C11	3.50	1.52	1.44
3	C	401	LAB	O3-C11	3.48	1.52	1.44
3	C	401	LAB	C4-C3	2.90	1.57	1.51
3	A	401	LAB	C4-C3	2.88	1.57	1.51
3	C	401	LAB	C9-C10	2.83	1.61	1.53
3	A	401	LAB	C9-C10	2.83	1.61	1.53
3	C	401	LAB	O3-C15	2.44	1.47	1.43
3	A	401	LAB	O3-C15	2.44	1.47	1.43
4	C	402	ATP	C5-C4	2.43	1.47	1.40
4	A	402	ATP	C5-C4	2.36	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	LAB	C17-S1-C18	22.75	104.21	92.00
3	A	401	LAB	C17-S1-C18	22.26	103.94	92.00
4	A	402	ATP	N3-C2-N1	-3.59	123.07	128.68
4	C	402	ATP	N3-C2-N1	-3.52	123.18	128.68
4	C	402	ATP	C4-C5-N7	-3.04	106.23	109.40
3	C	401	LAB	C4-C5-C6	-2.91	106.32	112.59
4	A	402	ATP	C4-C5-N7	-2.90	106.38	109.40
3	A	401	LAB	C14-C15-C16	-2.76	108.36	113.75
3	A	401	LAB	C4-C5-C6	-2.58	107.02	112.59
4	C	402	ATP	PA-O3A-PB	-2.58	123.99	132.83
3	C	401	LAB	C14-C15-C16	-2.56	108.75	113.75
3	C	401	LAB	C19-C3-C4	2.56	119.57	115.27
4	A	402	ATP	PA-O3A-PB	-2.54	124.11	132.83
3	C	401	LAB	C9-C10-C11	-2.31	109.75	114.03
4	C	402	ATP	PB-O3B-PG	-2.30	124.92	132.83
3	C	401	LAB	O3-C15-C16	2.28	107.17	104.25
3	A	401	LAB	C19-C3-C4	2.27	119.09	115.27
3	A	401	LAB	O3-C15-C16	2.22	107.10	104.25
4	A	402	ATP	PB-O3B-PG	-2.17	125.37	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	LAB	O3-C15-C16-C17
3	C	401	LAB	O3-C15-C16-C17
4	A	402	ATP	PG-O3B-PB-O1B
3	A	401	LAB	O2-C1-C2-C3
3	C	401	LAB	O2-C1-C2-C3
4	C	402	ATP	PG-O3B-PB-O1B
3	A	401	LAB	O1-C1-C2-C3
3	C	401	LAB	O1-C1-C2-C3
4	C	402	ATP	PB-O3B-PG-O2G

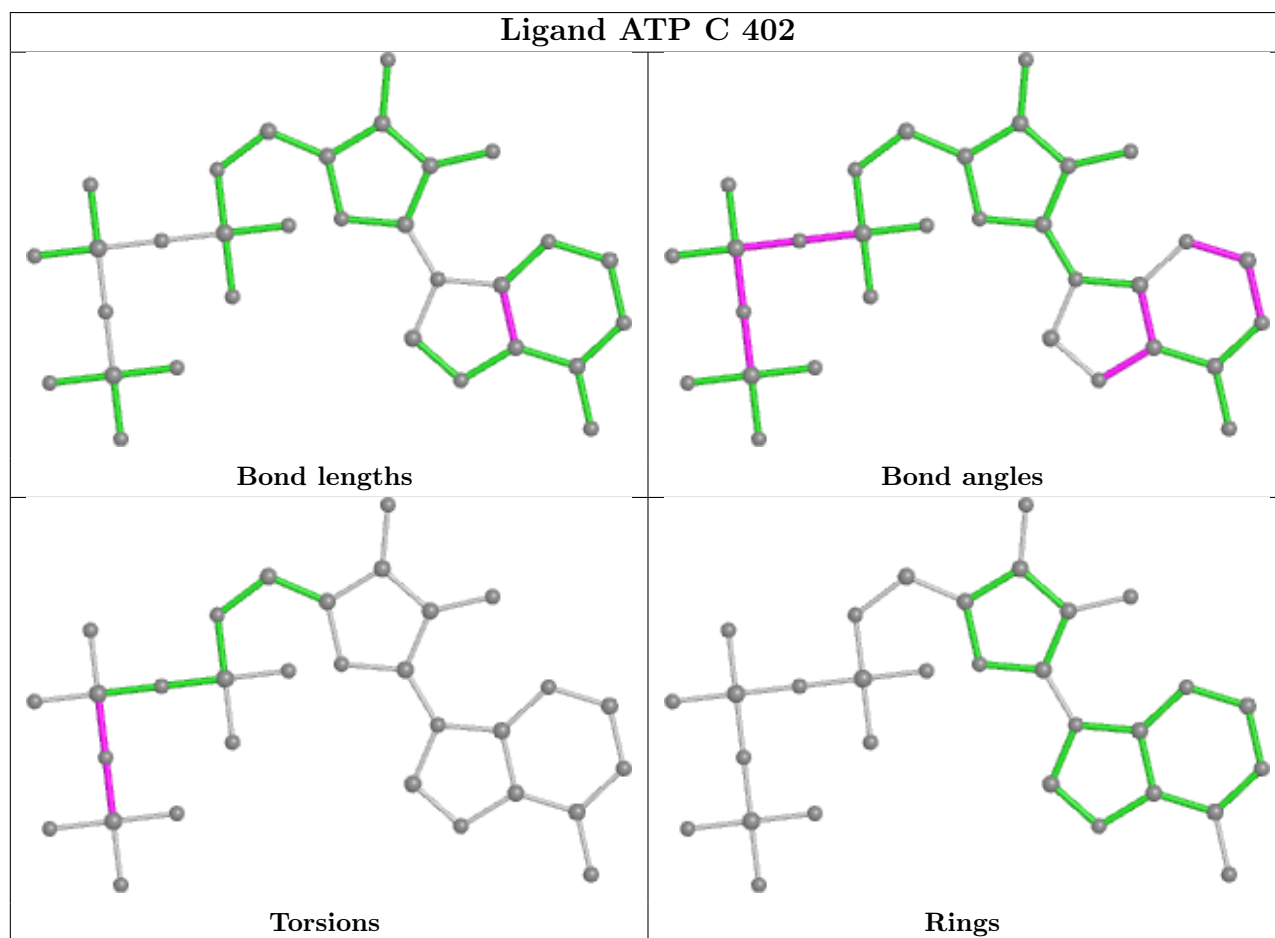
There are no ring outliers.

2 monomers are involved in 6 short contacts:

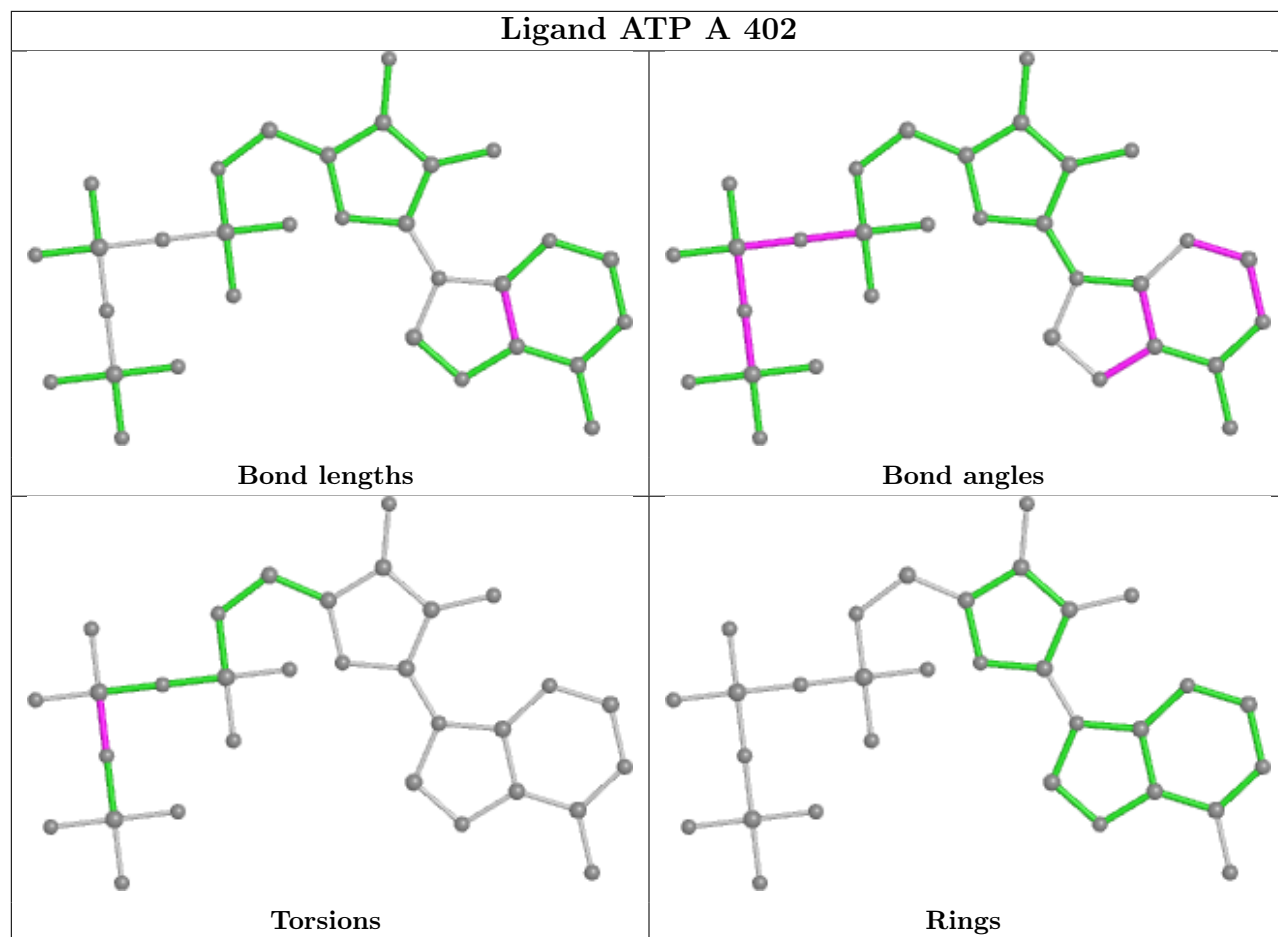
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	LAB	3	0
3	C	401	LAB	3	0

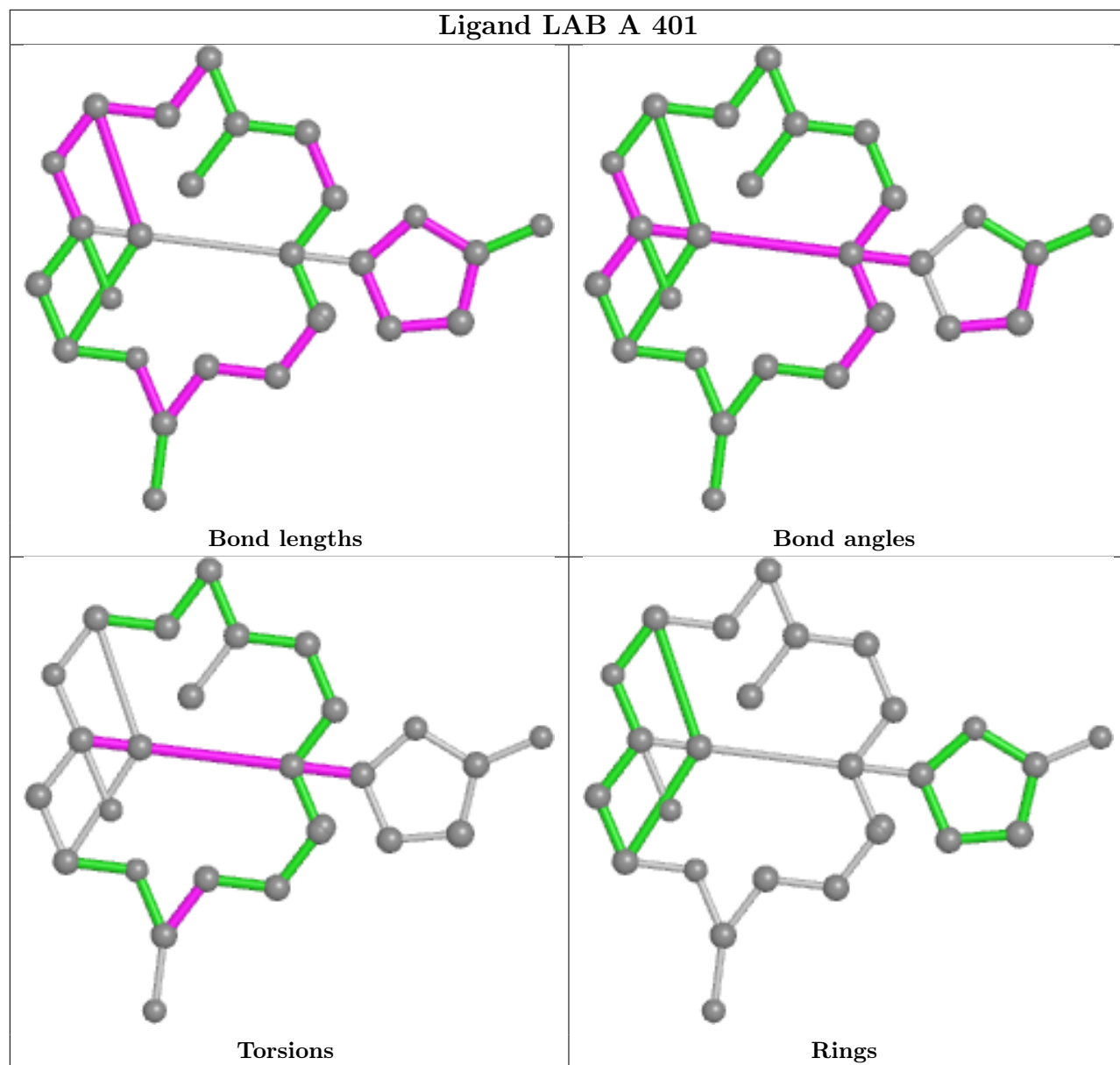
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

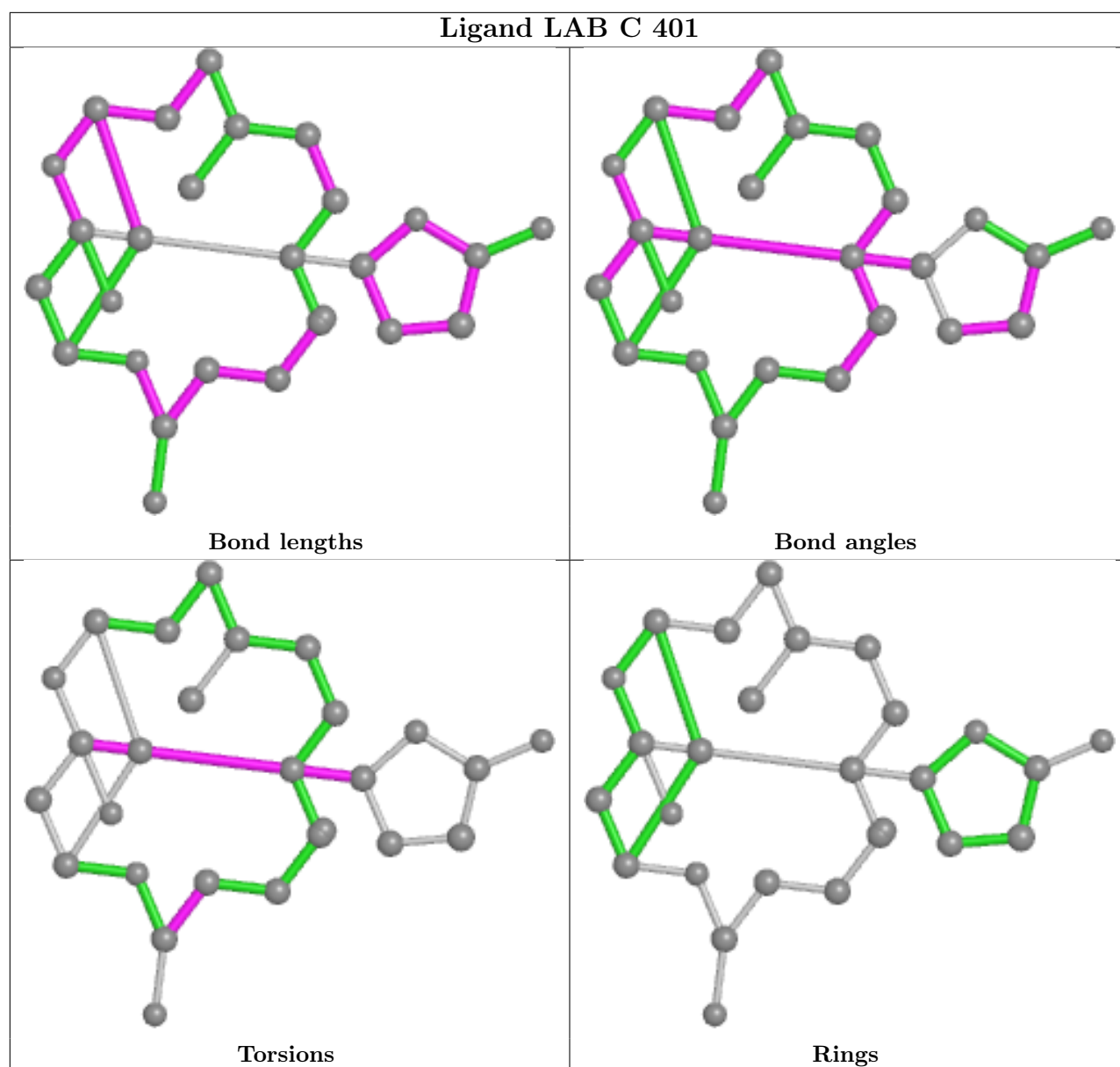
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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 [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	361/375 (96%)	0.30	15 (4%) 36 35	19, 30, 82, 193	0
1	C	360/375 (96%)	0.42	22 (6%) 21 20	22, 37, 86, 141	0
2	B	88/94 (93%)	1.12	17 (19%) 1 0	32, 67, 146, 157	0
2	D	88/94 (93%)	1.59	24 (27%) 0 0	41, 86, 144, 182	0
All	All	897/938 (95%)	0.56	78 (8%) 10 9	19, 38, 117, 193	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	ALA	10.7
2	B	18	ALA	10.1
2	B	19	ARG	8.6
2	D	21	SER	8.1
2	D	17	LYS	8.0
1	A	62	ARG	7.6
1	A	39	ARG	6.9
2	B	50[A]	PHE	6.6
2	D	1	MET	6.2
2	B	5	PHE	5.6
2	D	19	ARG	5.6
2	D	9	SER	5.5
1	C	100	GLU	5.4
2	B	17	LYS	5.2
1	C	62	ARG	4.8
2	B	15	GLU	4.2
2	D	87	LEU	4.1
2	D	5	PHE	3.9
2	B	10	ASP	3.8
1	C	86	TRP	3.7
2	D	22	THR	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	97	ALA	3.5
1	A	42	GLY	3.5
2	D	50	PHE	3.4
1	C	59	GLN	3.3
1	A	63	GLY	3.3
2	D	53	LEU	3.2
1	C	96	VAL	3.2
2	D	88	GLY	3.2
2	D	20	ALA	3.2
2	B	87	LEU	3.2
1	C	63	GLY	3.2
1	C	349	LEU	3.1
1	A	61	LYS	3.0
1	C	61	LYS	3.0
2	D	16	THR	3.0
2	D	11	ALA	3.0
1	A	372	ARG	2.9
2	B	84	LEU	2.9
2	D	31	PHE	2.9
2	D	7	ILE	2.9
1	C	354	GLN	2.8
1	C	60	SER	2.8
2	B	1	MET	2.7
2	D	23	ILE	2.7
1	A	356	TRP	2.7
1	C	41	GLN	2.6
1	A	64	ILE	2.6
1	C	234	SER	2.6
2	B	23	ILE	2.6
2	B	9	SER	2.5
1	C	373	LYS	2.5
2	B	8	ASP	2.5
2	D	35	ASP	2.5
1	A	57	GLU	2.5
1	C	57	GLU	2.5
1	A	366	GLY	2.5
2	B	22	THR	2.4
2	D	8	ASP	2.3
1	C	90	PHE	2.3
2	D	15	GLU	2.3
1	A	355	MET	2.3
1	C	370	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	10	ASP	2.2
2	D	54[A]	MET	2.2
1	A	270	GLU	2.2
1	C	40	HIS	2.2
1	C	83	GLU	2.2
1	C	53	TYR	2.2
1	C	355	MET	2.2
1	A	5	THR	2.2
2	B	86	LEU	2.1
2	D	2	VAL	2.1
1	C	367	PRO	2.1
2	B	11	ALA	2.1
2	B	14	THR	2.1
1	A	40	HIS	2.1
1	A	122	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	HIC	C	73	11/12	0.95	0.10	34,42,58,58	0
1	HIC	A	73	11/12	0.96	0.11	29,36,55,55	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, 95<sup>th</sup> 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.

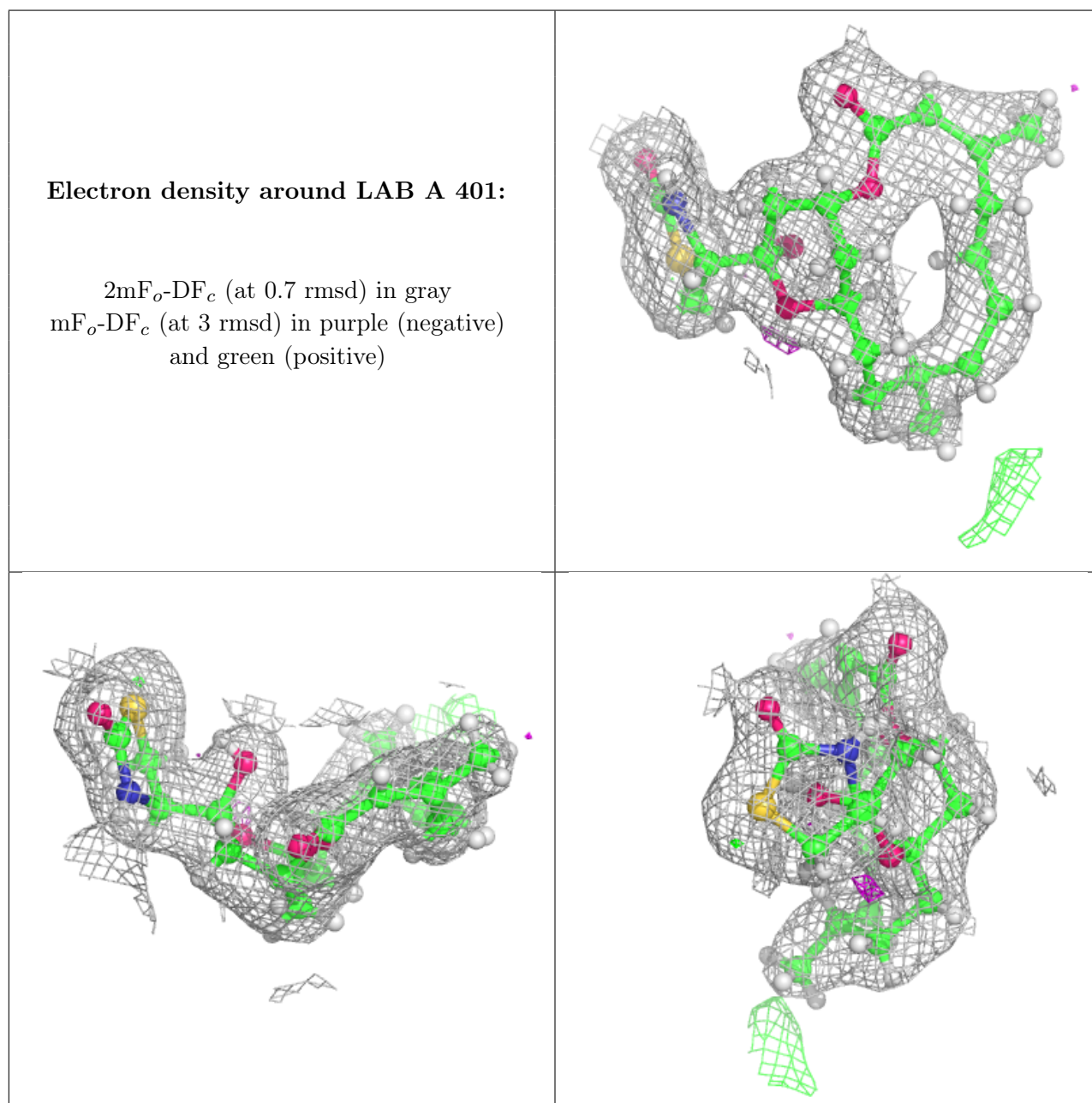
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	LAB	A	401	27/27	0.95	0.15	21,27,32,33	0

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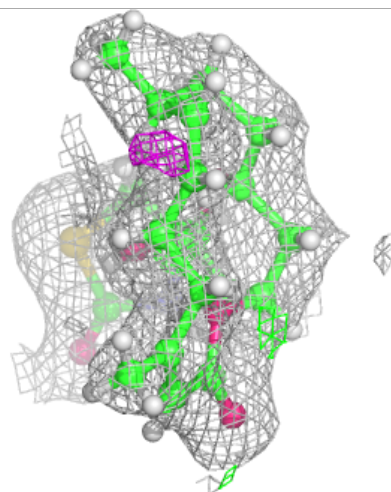
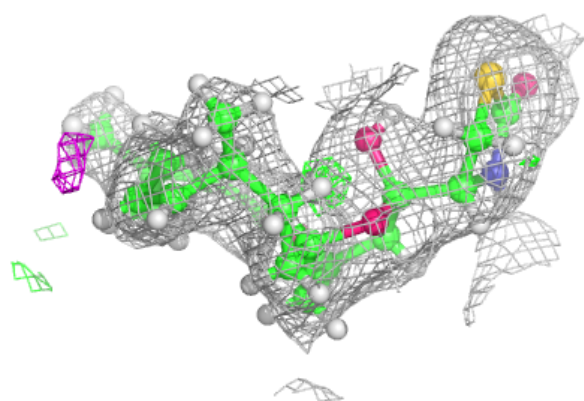
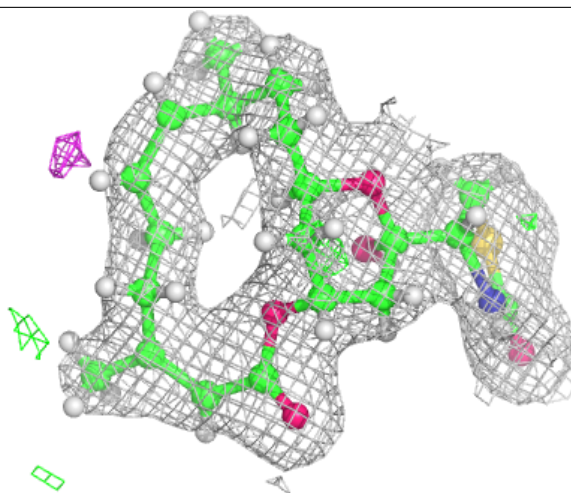
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LAB	C	401	27/27	0.95	0.12	24,33,38,39	0
4	ATP	A	402	31/31	0.97	0.15	14,22,27,30	0
4	ATP	C	402	31/31	0.97	0.13	21,26,31,32	0
5	MG	A	403	1/1	0.97	0.16	21,21,21,21	0
5	MG	C	403	1/1	0.98	0.06	21,21,21,21	0

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 C 401:**

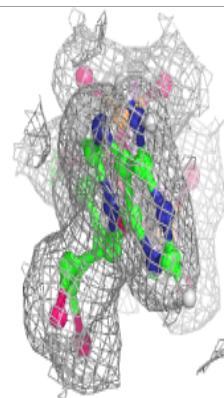
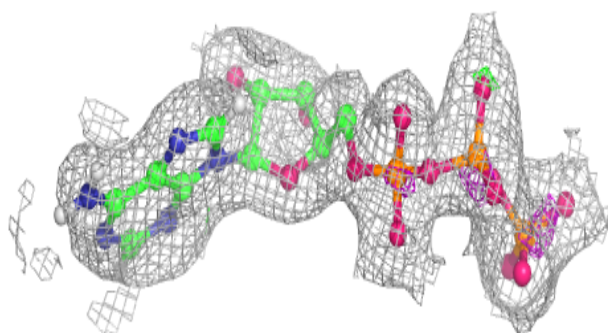
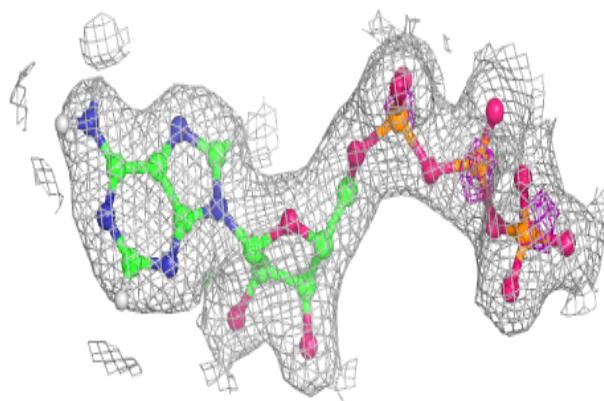
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



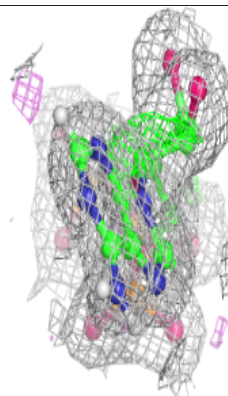
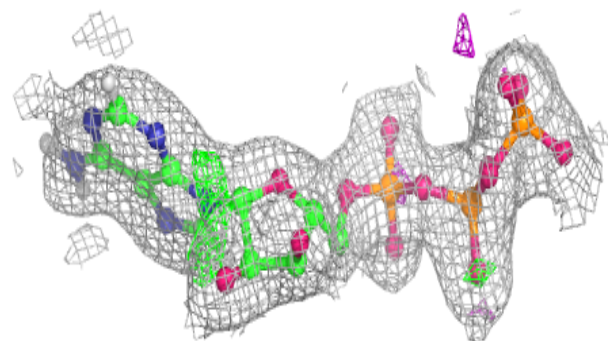
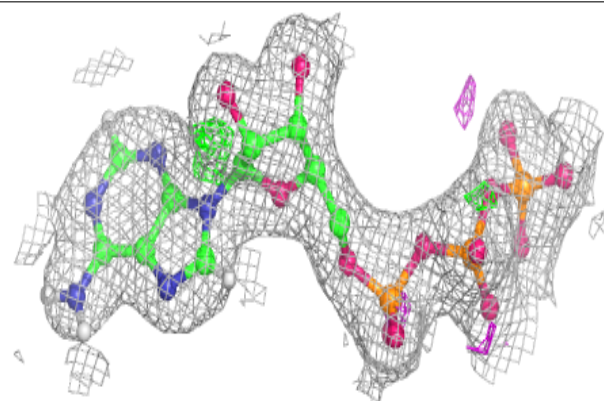


**Electron density around ATP A 402:**

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

**Electron density around ATP C 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 [i](#)

There are no such residues in this entry.