



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:21 am BST

PDB ID : 5NBN
Title : Crystal structure of the Arp4-N-actin-Arp8-Ino80HSA module of INO80
Authors : Knoll, K.R.; Eustermann, S.; Hopfner, K.P.
Deposited on : 2017-03-02
Resolution : 4.00 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 ⓘ 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 : 2.11
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) : 2.11

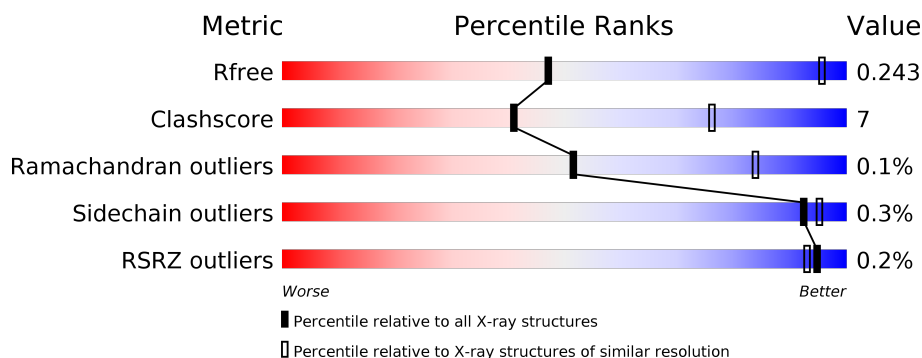
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	489	<div> <div>70%</div> <div>13%</div> <div>17%</div> </div>
1	B	489	<div> <div>71%</div> <div>12%</div> <div>17%</div> </div>
2	C	375	<div> <div>77%</div> <div>18%</div> <div>•</div> </div>
2	D	375	<div> <div>79%</div> <div>16%</div> <div>•</div> </div>
3	E	628	<div> <div>77%</div> <div>18%</div> <div>5%</div> </div>
3	F	628	<div> <div>77%</div> <div>18%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	147	 52% 7% 41%
4	H	147	 49% 10% 41%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23215 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	16	0	0
			3160	2016	522	611	11			
1	B	406	Total	C	N	O	S	16	0	0
			3156	2014	522	609	11			

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	359	Total	C	N	O	S	0	0	0
			2798	1776	470	535	17			
2	D	359	Total	C	N	O	S	0	0	0
			2798	1776	470	535	17			

- Molecule 3 is a protein called Actin-like protein ARP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	598	Total	C	N	O	S	0	0	0
			4818	3090	803	912	13			
3	F	598	Total	C	N	O	S	0	0	0
			4823	3094	804	912	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	254	MET	-	initiating methionine	UNP Q12386
F	254	MET	-	initiating methionine	UNP Q12386

- Molecule 4 is a protein called Putative DNA helicase INO80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	86	Total	C	N	O	S	0	0	0
			738	458	146	130	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	86	Total	C	N	O	S	0	0	0
			738	458	146	130	4			

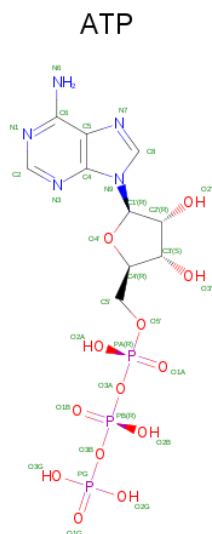
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	461	MET	-	initiating methionine	UNP P53115
G	599	ASN	-	expression tag	UNP P53115
G	600	TRP	-	expression tag	UNP P53115
G	601	SER	-	expression tag	UNP P53115
G	602	HIS	-	expression tag	UNP P53115
G	603	PRO	-	expression tag	UNP P53115
G	604	GLN	-	expression tag	UNP P53115
G	605	PHE	-	expression tag	UNP P53115
G	606	GLU	-	expression tag	UNP P53115
G	607	LYS	-	expression tag	UNP P53115
H	461	MET	-	initiating methionine	UNP P53115
H	599	ASN	-	expression tag	UNP P53115
H	600	TRP	-	expression tag	UNP P53115
H	601	SER	-	expression tag	UNP P53115
H	602	HIS	-	expression tag	UNP P53115
H	603	PRO	-	expression tag	UNP P53115
H	604	GLN	-	expression tag	UNP P53115
H	605	PHE	-	expression tag	UNP P53115
H	606	GLU	-	expression tag	UNP P53115
H	607	LYS	-	expression tag	UNP P53115

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

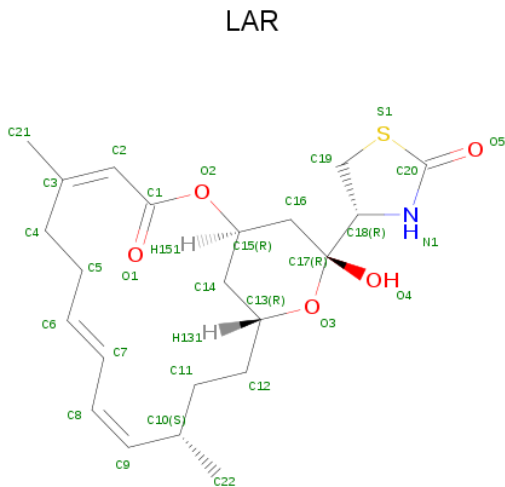
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Id	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is LATRUNCULIN A (three-letter code: LAR) (formula: $\text{C}_{22}\text{H}_{31}\text{NO}_5\text{S}$).



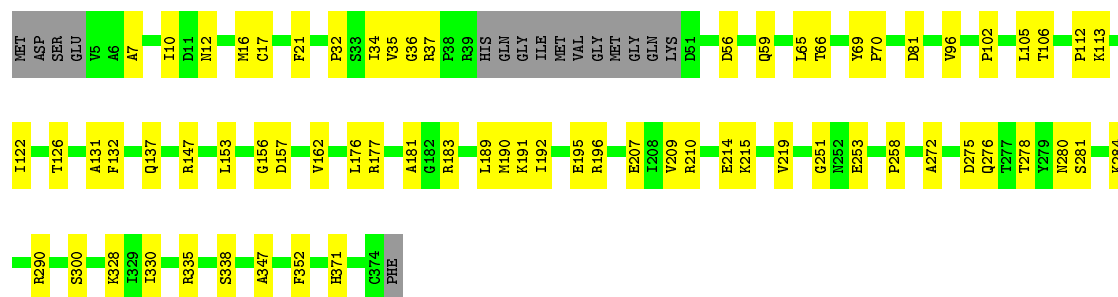
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
7	D	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 1: Actin-related protein 4

S461	L468	W469	K472	K473	E474	Y475	E476	E477	V478	G479	V480	L483	L484	W485	ASP	ARG	PHE																														
ALA	ASN	SER	ALA	ASP	THR	PRO	GLU	THR	GLY	LYS	ARG	PRO	GLU	GLY	LYS	ASN	E381	K394	D397	R401	A405	L410	T411	G412	G413	T414	S415	R423	E427	L428	T431	L432	L435	K436	F437	T441	G455	L458									
K201	F238	K243	C247	T254	E257	P273	G287	E280	W315	ASN	ARG	ASP	THR	VAL	PRO	LEU	LYS	ARG	THR	LYS	PRO	SER	GLY	VAL	ASN	LYS	ASP	LYS	VAL	THR	PRO	THR	GLU	GLY	LYS	GLU	GLN	GLU	ALA	VAL	SER	LYS	SER	THR	SER	PRO	ALA
MET	SER	ASN	ALA	LEU	GLN	VAL	TYR	GLY	GLY	ASP	GLU	VAL	A16	Y24	T25	S31	P41	Y44	G45	K46	K55	E59	E76	I81	T85	W90	L94	L98	P107	A108	E135	A136	C137	Y138	I160	G161	C165	N183	L192								

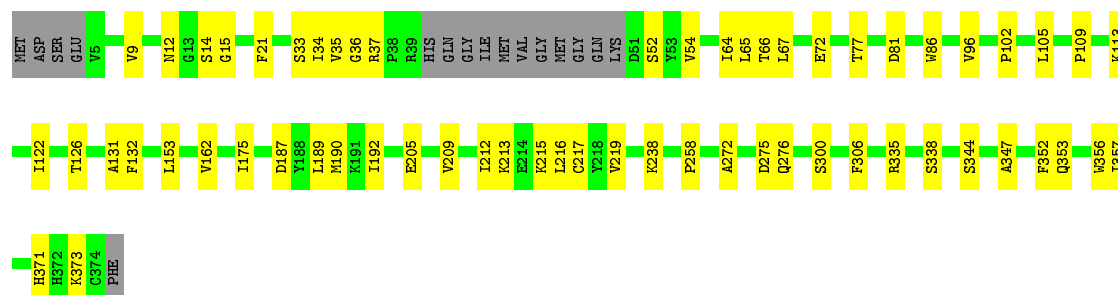
E477	SER	E257	MTT
V478	ALA	R268	SER
G479	ASP	S269	ASN
V480	PRO	V279	ALA
L483	ASN	R285	LEU
L484	GLU	V286	GLN
N485	THR	G287	VAL
ASP	GLY	E290	TYR
ARG	LYS	E291	GLY
PHE	ARG	L292	GLY
ARG	PRO	N308	ASP
	LEU	V315	GLU
	GLU	ARG	VAL
	GLU	ASN	S15
	GLU	ASP	A16
	GLY	THR	
	LYS	VAL	Y24
	PRO	PRO	T25
	PRO	LEU	Y44
	LYS	LYS	X55
	LYS	ARG	
	GLU	THR	K72
	GLU	LYS	E76
	GLU	THR	
	ASN	LYS	I81
	E381	PRO	T85
	Y390	LEU	Y99
	V398	THR	P107
	R401	LYS	A108
	A405	PRO	A136
		SER	C137
	G412	GLY	C145
	G413	VAL	R152
	T414	THR	I160
	S415	PRO	I185
	N429	THR	L198
	K430	GLU	R212
	I431	GLU	K213
	L432	LYS	F238
	L435	THR	
	K436	GLU	K243
	F437	LYS	E244
	G455	GLU	T254
	I458	GLN	
	L459	ALA	
	T460	VAL	
	S461	SER	
	L462	LYS	
	W469	SER	
	E474	THR	
	Y475	SER	
	E476	ALA	
		ASN	





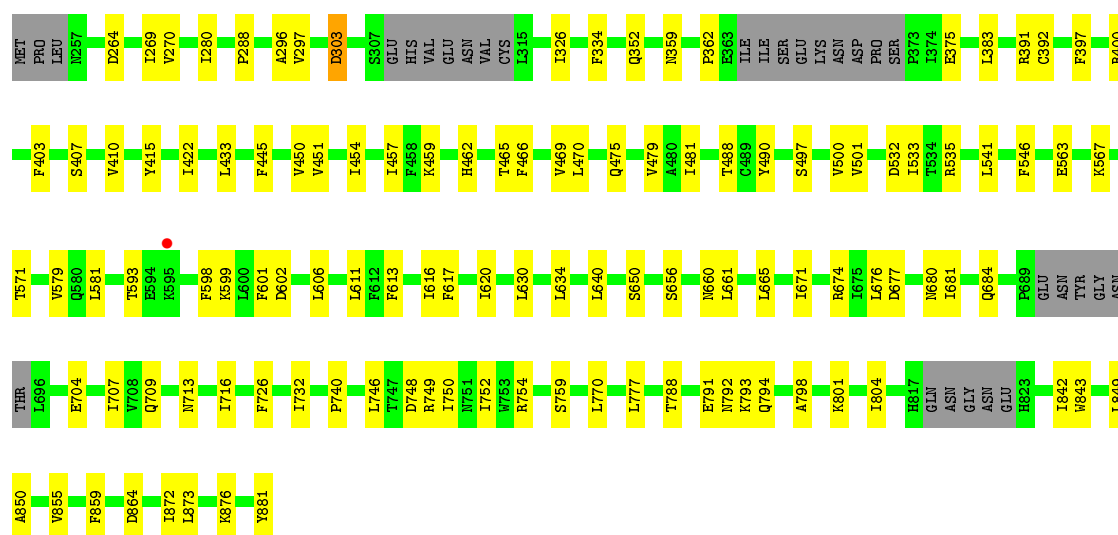
• Molecule 2: Actin

Chain D: 79% 16%



• Molecule 3: Actin-like protein ARP8

Chain E: 77% 18% 5%



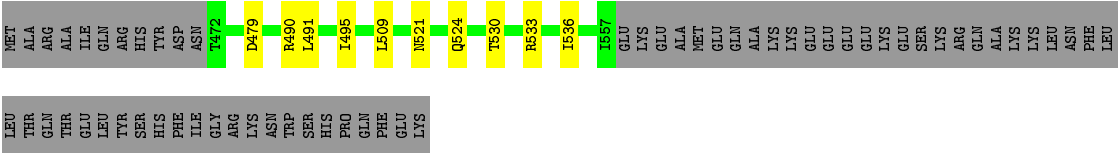
• Molecule 3: Actin-like protein ARP8

Chain F: 77% 18% 5%

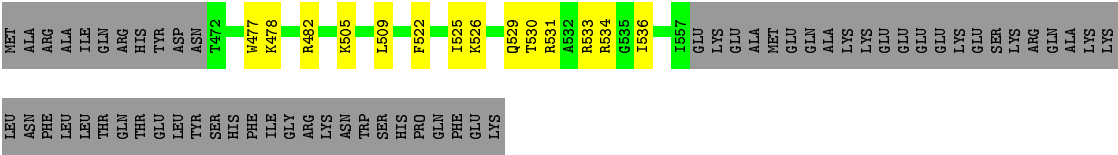




● Molecule 4: Putative DNA helicase INO80



● Molecule 4: Putative DNA helicase INO80



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	172.29 Å 263.91 Å 241.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 4.00 49.40 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.40-4.00) 100.0 (49.40-4.00)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 4.00 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.193 , 0.242 0.193 , 0.243	Depositor DCC
R_{free} test set	2380 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23215	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: CA, HIC, ATP, LAR

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	0.25	0/3229	0.42	0/4389
1	B	0.24	0/3225	0.43	0/4384
2	C	0.25	0/2846	0.42	0/3855
2	D	0.25	0/2846	0.42	0/3855
3	E	0.26	0/4924	0.45	0/6674
3	F	0.25	0/4929	0.45	0/6679
4	G	0.26	0/748	0.38	0/990
4	H	0.25	0/748	0.38	0/990
All	All	0.25	0/23495	0.43	0/31816

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	3160	0	3084	49	0
1	B	3156	0	3080	38	0
2	C	2798	0	2765	50	0
2	D	2798	0	2765	35	0
3	E	4818	0	4767	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4823	0	4780	75	0
4	G	738	0	769	6	0
4	H	738	0	769	9	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	0	12	2	0
6	B	31	0	12	0	0
6	C	31	0	12	2	0
6	D	31	0	12	1	0
7	C	29	0	31	7	0
7	D	29	0	31	0	0
All	All	23215	0	22889	326	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 7.

The worst 5 of 326 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:C:16:MET:HA	2:C:32:PRO:HA	1.62	0.82
3:F:488:THR:HB	3:F:842:ILE:HD13	1.63	0.80
3:F:733:VAL:HG23	3:F:841:ILE:HD12	1.65	0.78
3:E:872:ILE:HD11	3:E:876:LYS:HD2	1.70	0.73
1:A:473:LYS:O	1:A:477:GLU:HB3	1.88	0.73

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	402/489 (82%)	387 (96%)	15 (4%)	0	100	100
1	B	402/489 (82%)	387 (96%)	15 (4%)	0	100	100
2	C	354/375 (94%)	349 (99%)	5 (1%)	0	100	100
2	D	354/375 (94%)	348 (98%)	6 (2%)	0	100	100
3	E	588/628 (94%)	558 (95%)	29 (5%)	1 (0%)	47	79
3	F	588/628 (94%)	557 (95%)	30 (5%)	1 (0%)	47	79
4	G	84/147 (57%)	82 (98%)	2 (2%)	0	100	100
4	H	84/147 (57%)	83 (99%)	1 (1%)	0	100	100
All	All	2856/3278 (87%)	2751 (96%)	103 (4%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	362	PRO
3	F	362	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	345/434 (80%)	345 (100%)	0	100	100
1	B	344/434 (79%)	344 (100%)	0	100	100
2	C	305/319 (96%)	304 (100%)	1 (0%)	92	95
2	D	305/319 (96%)	304 (100%)	1 (0%)	92	95
3	E	540/574 (94%)	538 (100%)	2 (0%)	91	94
3	F	541/574 (94%)	539 (100%)	2 (0%)	91	94
4	G	81/136 (60%)	79 (98%)	2 (2%)	47	68
4	H	81/136 (60%)	81 (100%)	0	100	100
All	All	2542/2926 (87%)	2534 (100%)	8 (0%)	92	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	303	ASP
4	G	509	LEU
3	F	749	ARG
3	E	264	ASP
3	F	342	LYS

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

Mol	Chain	Res	Type
3	E	462	HIS

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
2	HIC	D	73	2	8,11,12	1.71	2 (25%)	6,14,16	1.21	1 (16%)
2	HIC	C	73	2	8,11,12	1.66	1 (12%)	6,14,16	1.30	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
2	HIC	D	73	2	-	2/5/6/8	0/1/1/1
2	HIC	C	73	2	-	4/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	73	HIC	CD2-CG	3.75	1.41	1.36
2	C	73	HIC	CD2-CG	3.65	1.41	1.36
2	D	73	HIC	CZ-NE2	-2.06	1.42	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	73	HIC	CB-CA-C	-2.46	106.86	111.47
2	D	73	HIC	CB-CA-C	-2.39	106.98	111.47

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	73	HIC	C-CA-CB-CG
2	C	73	HIC	N-CA-CB-CG
2	D	73	HIC	CA-CB-CG-ND1
2	C	73	HIC	CA-CB-CG-ND1
2	D	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	D	502	5	26,33,33	0.93	1 (3%)	31,52,52	1.43	5 (16%)
6	ATP	B	502	5	26,33,33	0.91	1 (3%)	31,52,52	1.50	4 (12%)
7	LAR	D	503	-	30,31,31	5.39	16 (53%)	32,43,43	5.82	13 (40%)
6	ATP	C	502	5	26,33,33	0.96	1 (3%)	31,52,52	1.38	5 (16%)
6	ATP	A	502	5	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
7	LAR	C	503	-	30,31,31	5.42	15 (50%)	32,43,43	5.44	12 (37%)

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	ATP	D	502	5	-	5/18/38/38	0/3/3/3
6	ATP	B	502	5	-	5/18/38/38	0/3/3/3
7	LAR	D	503	-	-	10/23/51/51	0/2/3/3
6	ATP	C	502	5	-	7/18/38/38	0/3/3/3
6	ATP	A	502	5	-	4/18/38/38	0/3/3/3
7	LAR	C	503	-	-	3/23/51/51	0/2/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	LAR	C20-N1	15.02	1.54	1.34
7	D	503	LAR	C20-N1	14.92	1.54	1.34
7	D	503	LAR	C2-C3	13.89	1.60	1.33
7	C	503	LAR	C2-C3	13.86	1.59	1.33
7	C	503	LAR	C20-S1	-9.46	1.56	1.77

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	LAR	C19-S1-C20	25.15	105.49	92.00
7	C	503	LAR	C19-S1-C20	22.24	103.93	92.00
7	D	503	LAR	O4-C17-O3	-13.67	85.46	110.06
7	C	503	LAR	O4-C17-O3	-13.53	85.71	110.06
7	D	503	LAR	O3-C17-C18	11.10	118.49	104.25

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

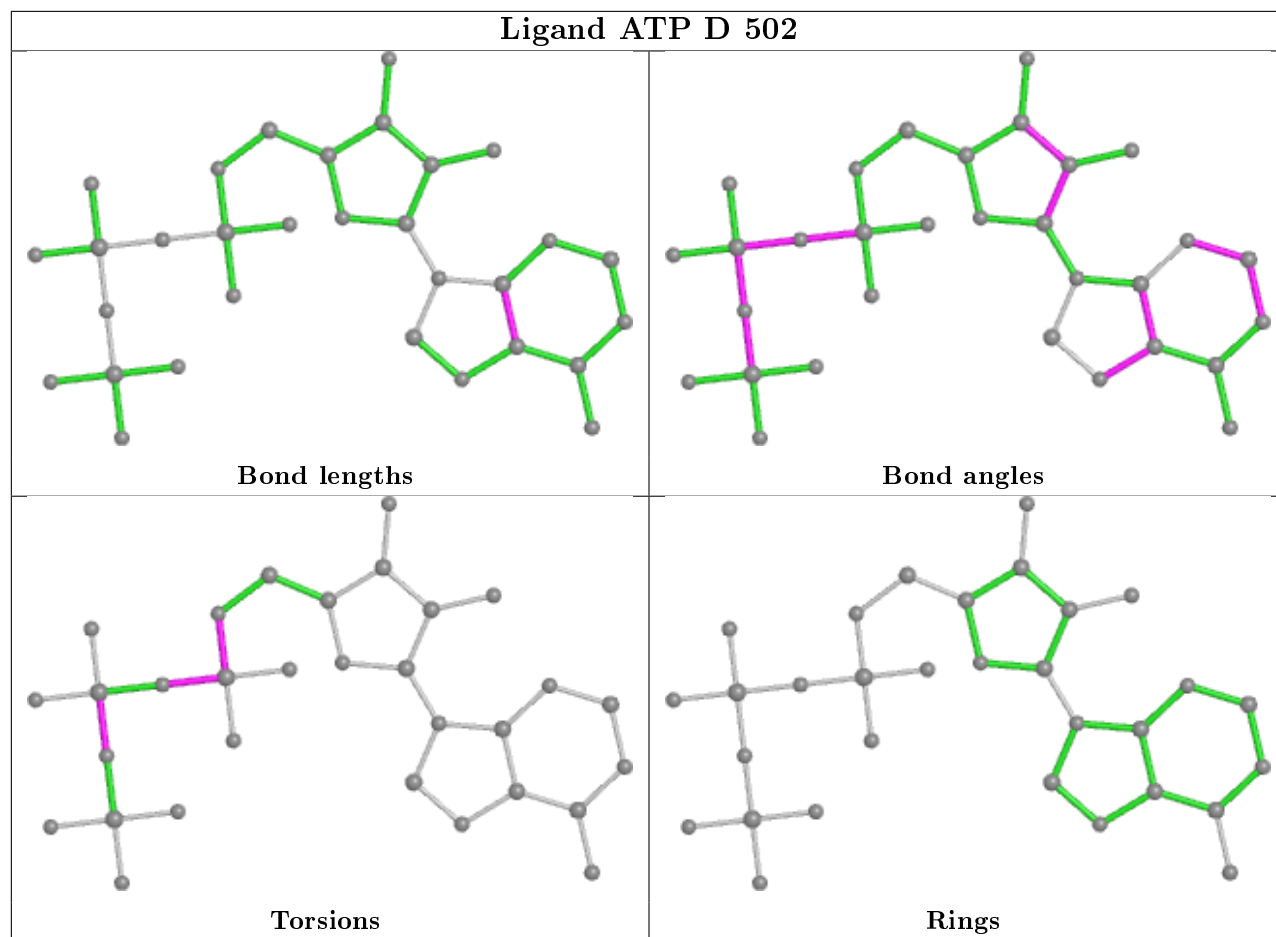
Mol	Chain	Res	Type	Atoms
6	C	502	ATP	C5'-O5'-PA-O1A
6	D	502	ATP	C5'-O5'-PA-O1A
6	B	502	ATP	C5'-O5'-PA-O3A
6	B	502	ATP	O4'-C4'-C5'-O5'
6	A	502	ATP	C5'-O5'-PA-O2A

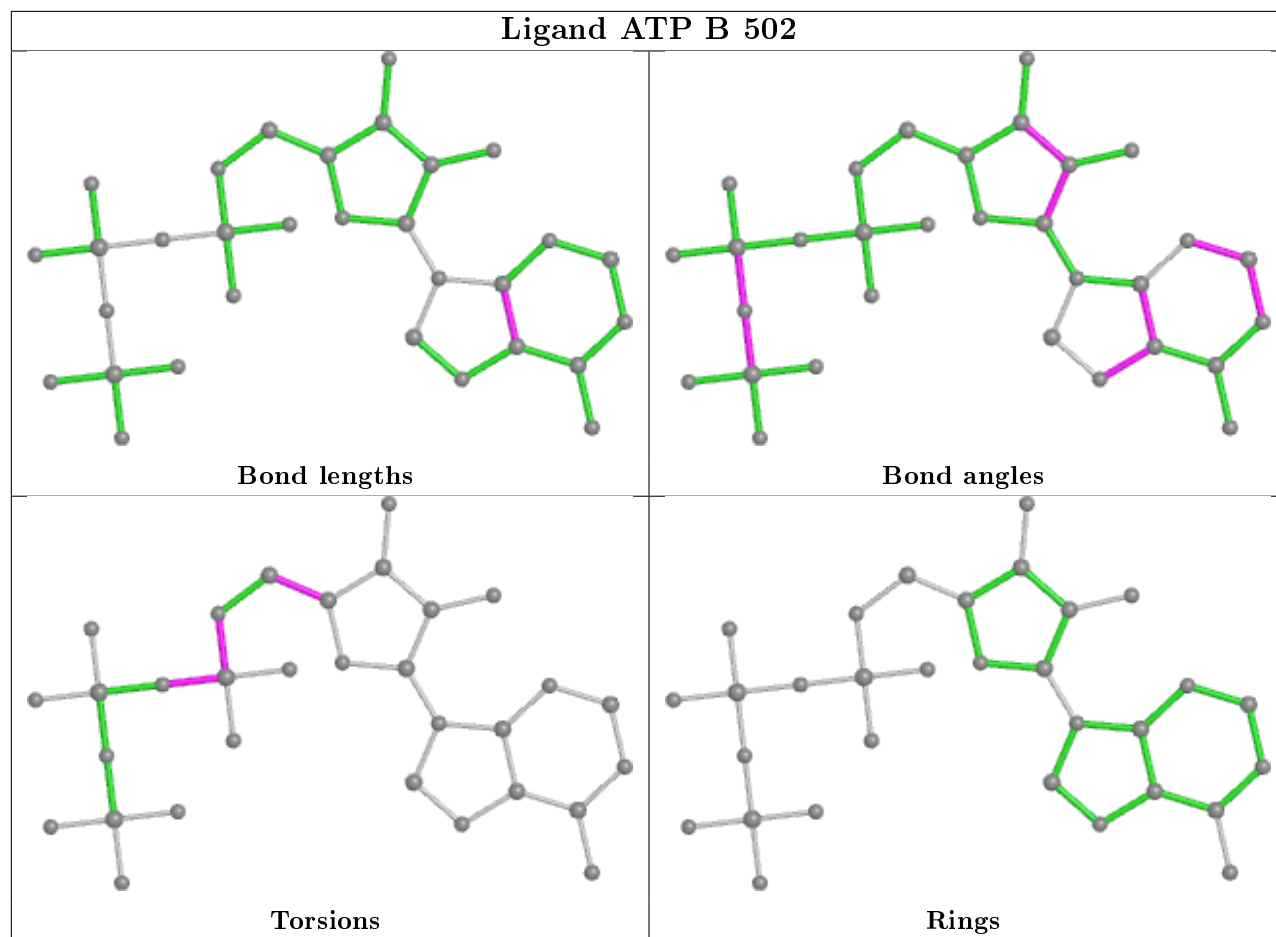
There are no ring outliers.

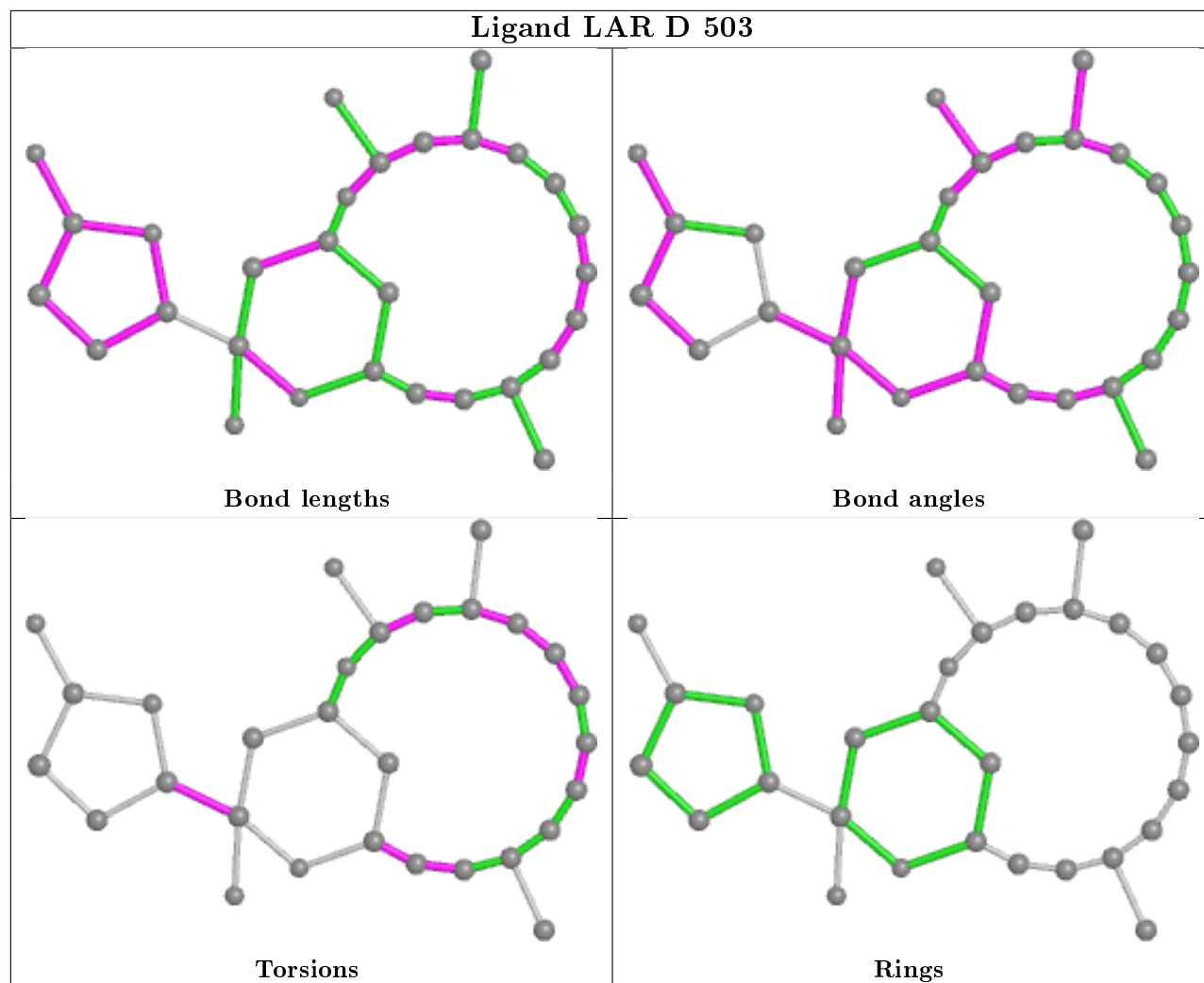
4 monomers are involved in 12 short contacts:

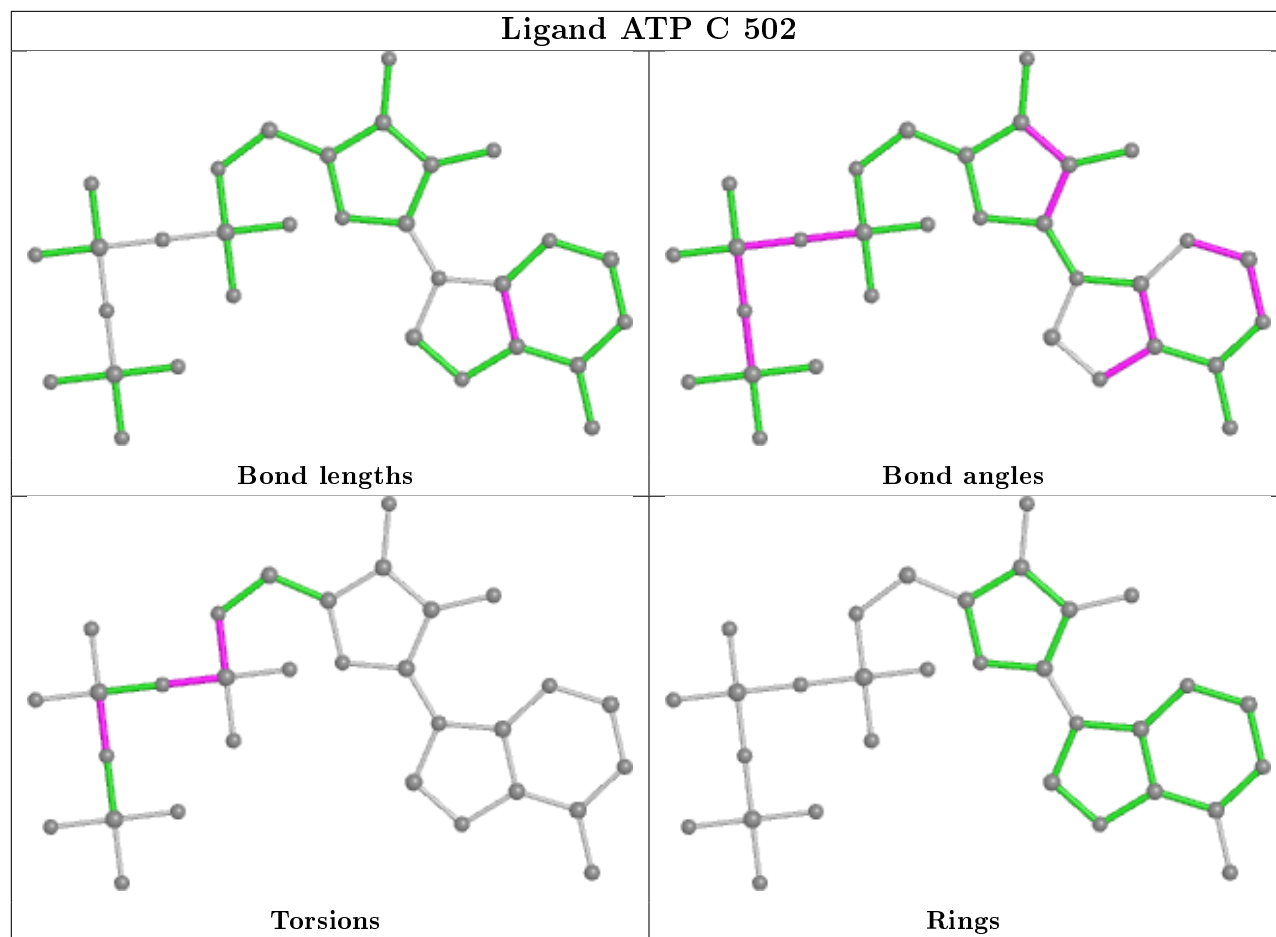
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	502	ATP	1	0
6	C	502	ATP	2	0
6	A	502	ATP	2	0
7	C	503	LAR	7	0

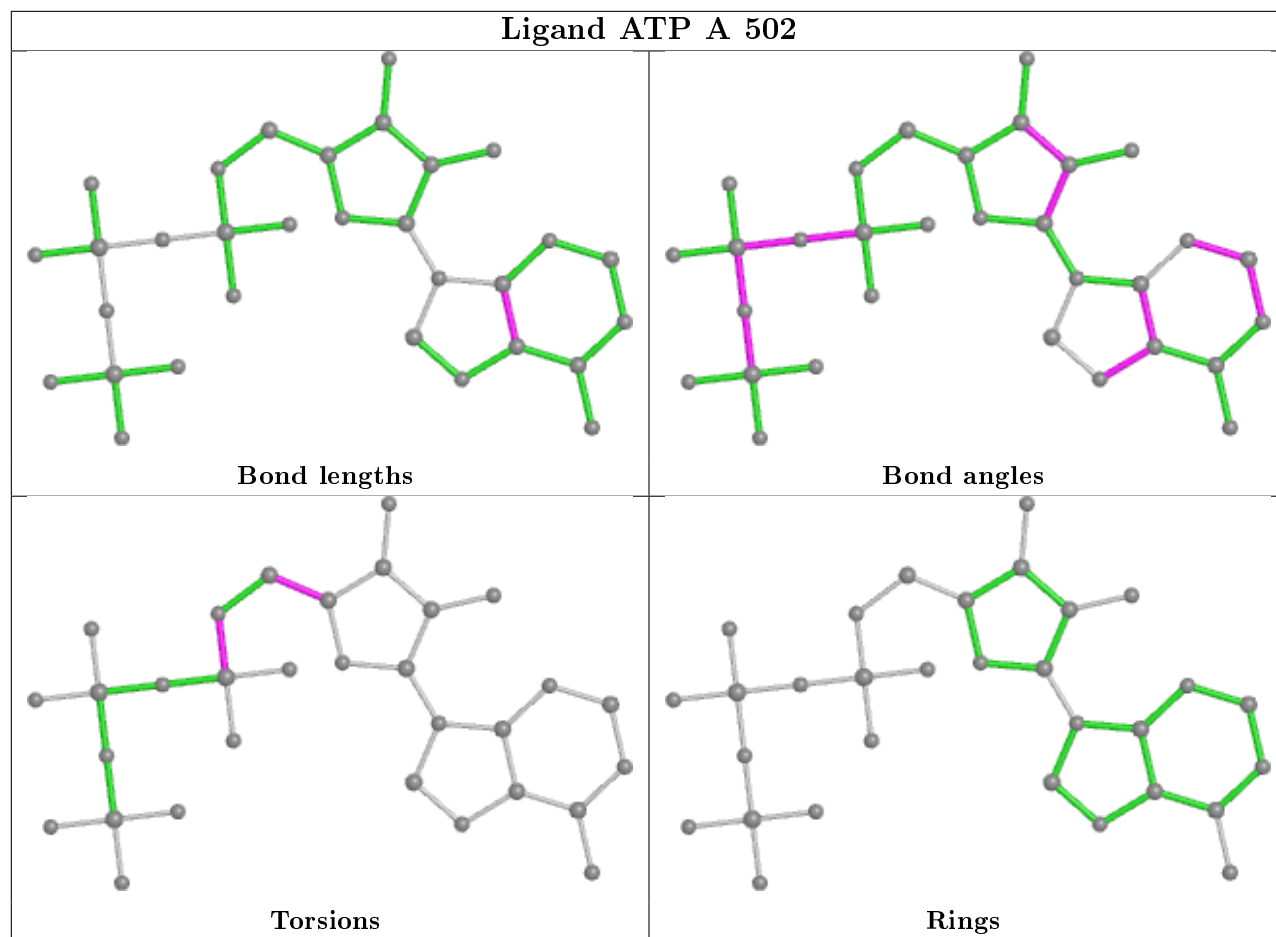
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

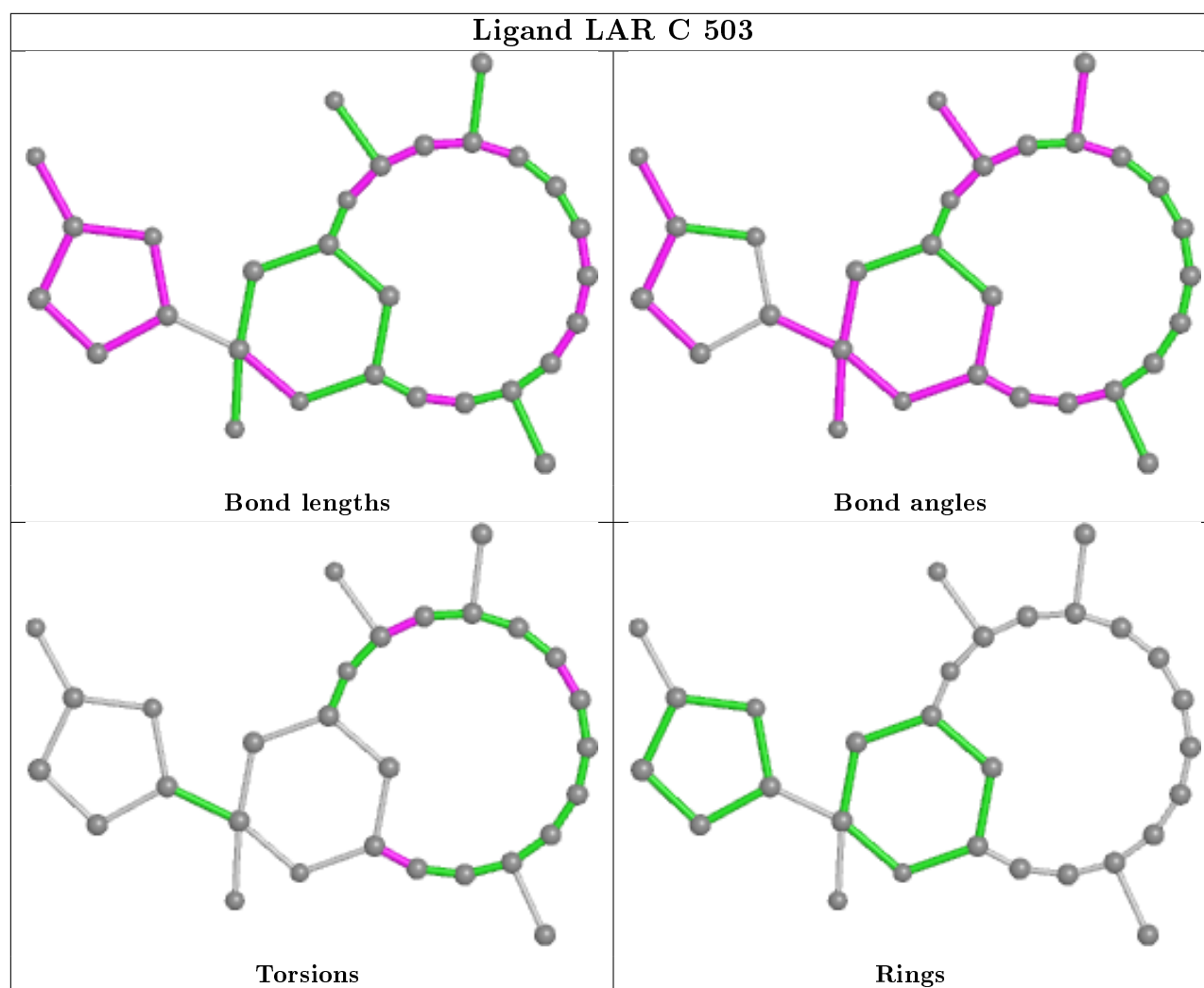












5.7 Other polymers [i](#)

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, 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	406/489 (83%)	-0.31	1 (0%) 95 93	79, 122, 174, 224	4 (0%)
1	B	406/489 (83%)	-0.24	2 (0%) 91 85	86, 137, 182, 219	4 (0%)
2	C	358/375 (95%)	-0.45	0 100 100	66, 101, 145, 187	0
2	D	358/375 (95%)	-0.54	0 100 100	53, 88, 128, 163	0
3	E	598/628 (95%)	-0.33	1 (0%) 95 93	63, 125, 189, 232	0
3	F	598/628 (95%)	-0.34	2 (0%) 94 90	54, 120, 189, 231	0
4	G	86/147 (58%)	-0.52	0 100 100	81, 126, 165, 199	0
4	H	86/147 (58%)	-0.60	0 100 100	68, 117, 163, 179	0
All	All	2896/3278 (88%)	-0.37	6 (0%) 95 93	53, 118, 179, 232	8 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	GLU	3.3
3	F	586	ASN	2.2
1	A	55	LYS	2.1
3	E	595	LYS	2.1
1	B	55	LYS	2.0

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

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
2	HIC	C	73	11/12	0.92	0.21	89,119,130,131	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HIC	D	73	11/12	0.93	0.19	84,96,122,142	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

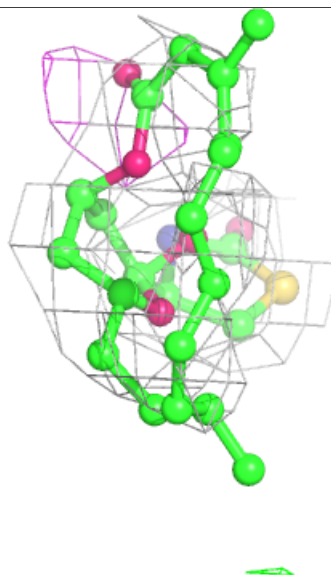
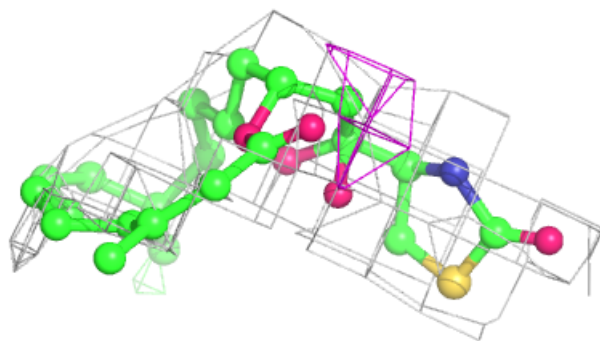
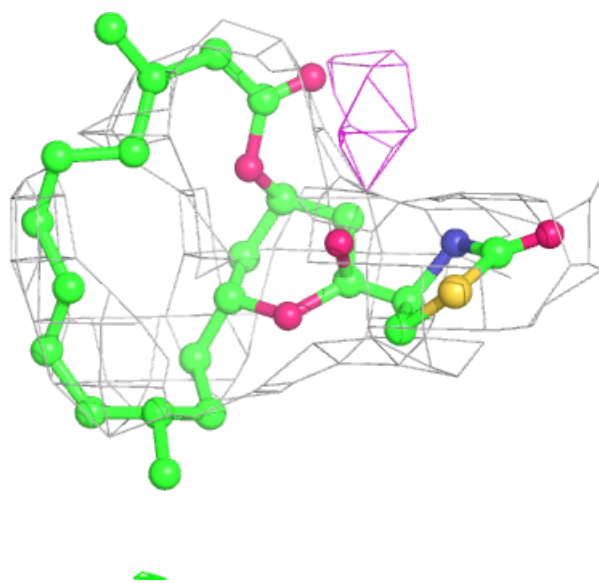
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	LAR	D	503	29/29	0.92	0.36	70,99,116,126	0
7	LAR	C	503	29/29	0.93	0.46	105,114,133,145	0
6	ATP	B	502	31/31	0.94	0.25	90,107,165,177	0
5	CA	A	501	1/1	0.94	0.41	117,117,117,117	0
6	ATP	A	502	31/31	0.95	0.35	70,96,130,153	0
5	CA	D	501	1/1	0.95	0.29	62,62,62,62	0
6	ATP	C	502	31/31	0.95	0.22	60,96,116,129	0
5	CA	B	501	1/1	0.96	0.46	143,143,143,143	0
5	CA	C	501	1/1	0.96	0.17	74,74,74,74	0
6	ATP	D	502	31/31	0.96	0.21	56,73,89,99	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.

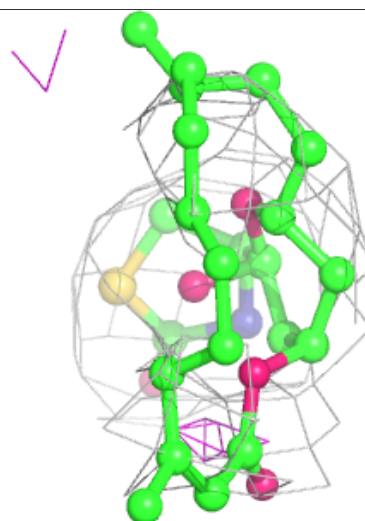
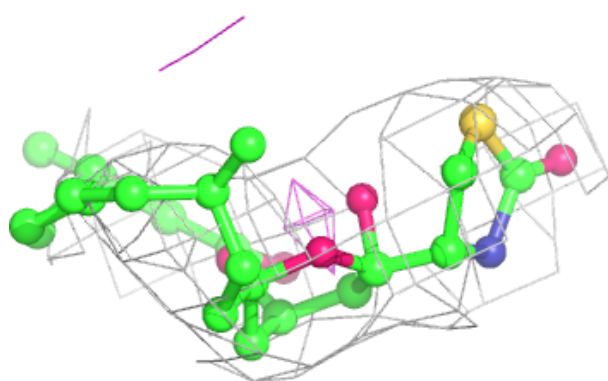
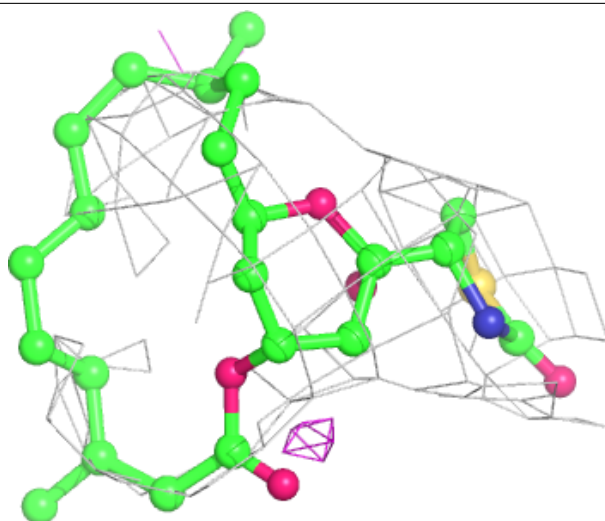
Electron density around LAR D 503:

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



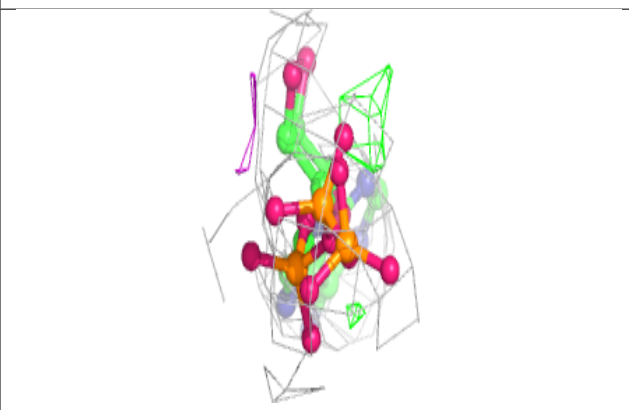
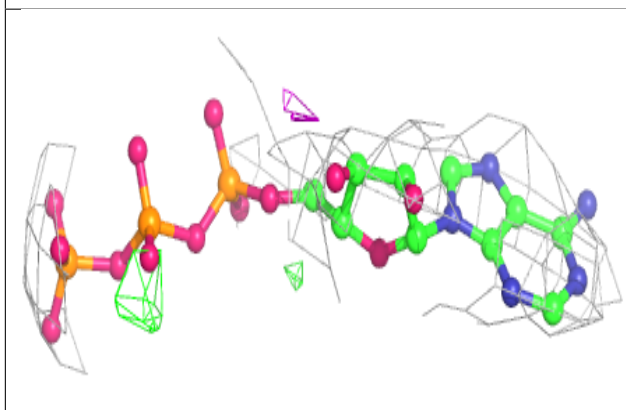
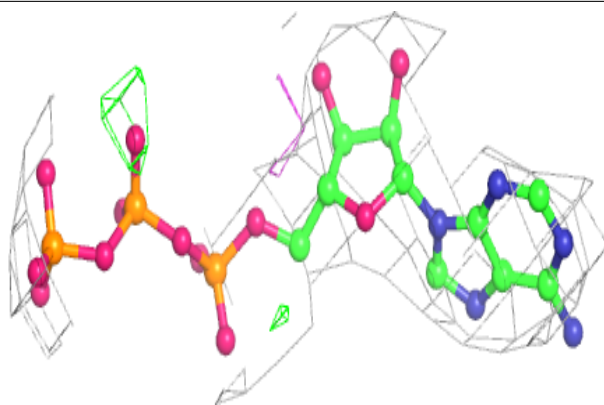
Electron density around LAR C 503:

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

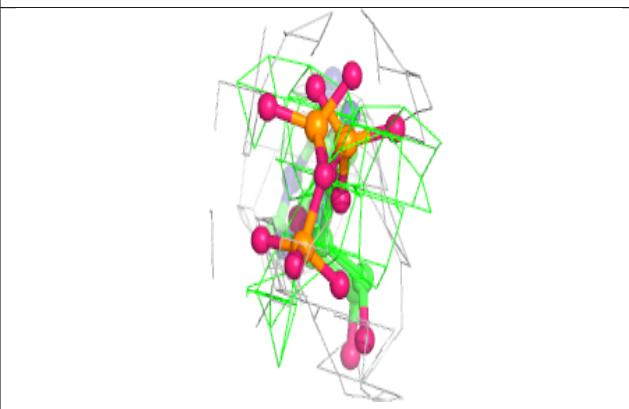
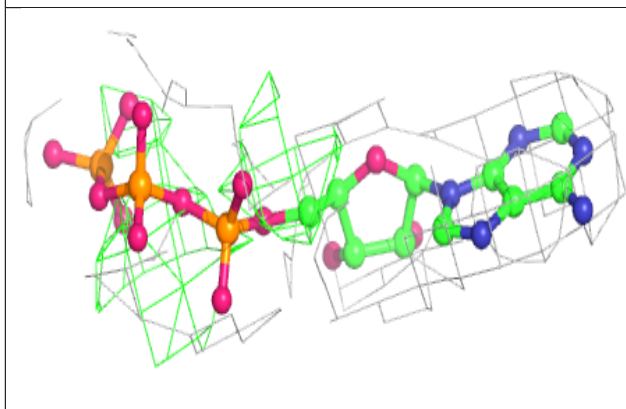
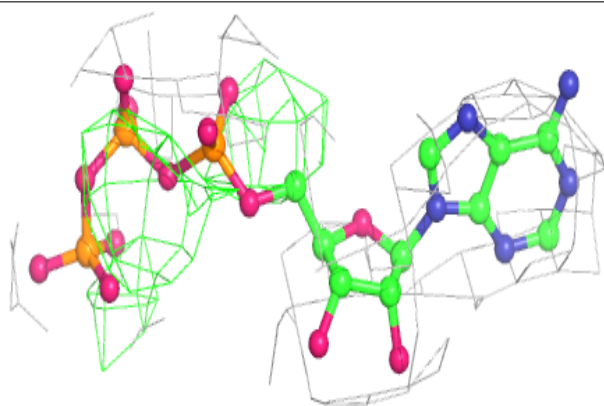


Electron density around ATP B 502:

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

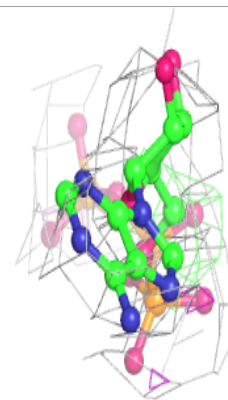
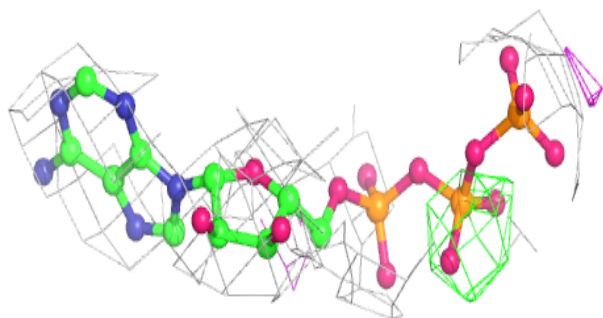
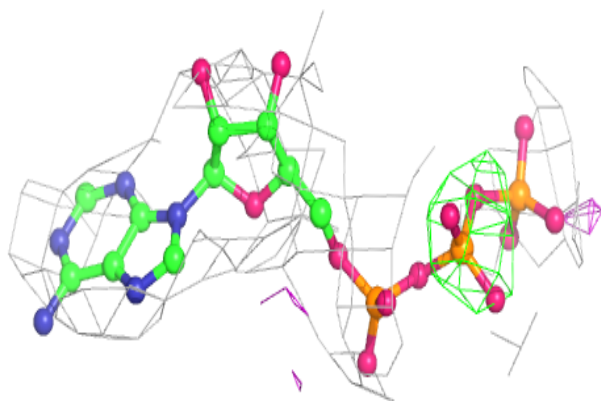
**Electron density around ATP A 502:**

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

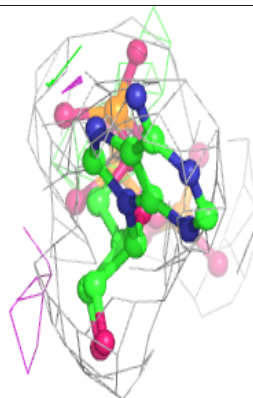
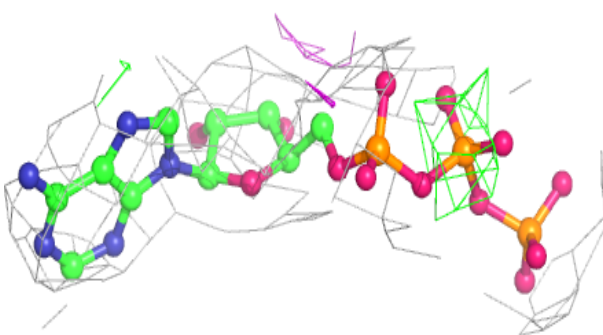
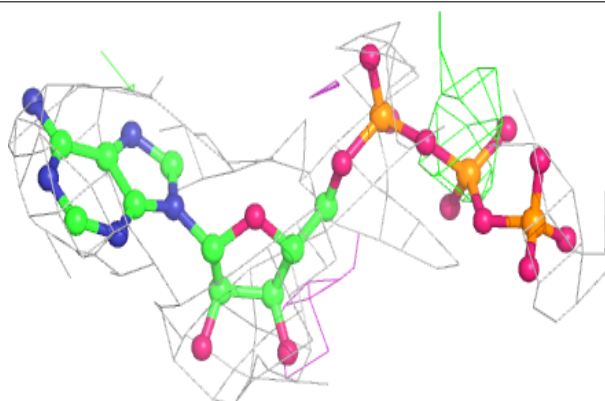


Electron density around ATP C 502:

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

**Electron density around ATP D 502:**

$2mF_o-DF_c$ (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.