



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 08:42 PM UTC

PDB ID : 6DEC / pdb\_00006dec  
Title : Crystal structure of Bos taurus Arp2/3 complex binding with C-terminus of Homo sapiens SPIN90  
Authors : Nolen, B.J.; Luan, Q.  
Deposited on : 2018-05-11  
Resolution : 4.60 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](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

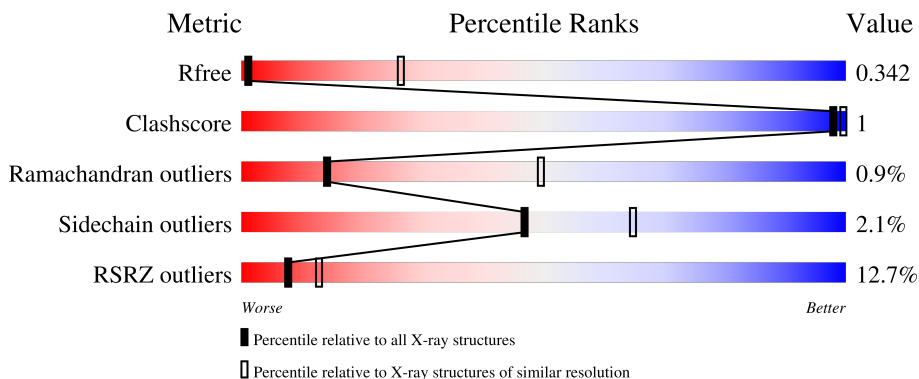
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	418	 8% 88% 6% • 5%
1	H	418	 14% 85% 6% • 8%
2	B	394	 9% 87% 7% 6%
2	I	394	 10% 50% • • 47%
3	C	372	 12% 86% • • 9%

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Mol	Chain	Length	Quality of chain
3	J	372	
4	D	300	
4	K	300	
5	E	178	
5	L	178	
6	F	168	
6	N	168	
7	G	151	
7	O	151	
8	M	455	
8	P	455	
9	Q	6	
10	R	9	

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 20563 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 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	398	2010	1202	404	404	0	0	0
1	H	386	1948	1169	389	390	0	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	369	1850	1103	372	375	0	0	0
2	I	209	1030	612	209	209	0	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	339	1757	1070	347	340	0	0	0
3	J	258	1274	758	258	258	0	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	279	1389	830	279	280	0	0	0
4	K	283	1429	855	288	286	0	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	163	Total	C	N	O	0	0	0
			815	488	163	164			
5	L	138	Total	C	N	O	0	0	0
			685	409	138	138			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	165	Total	C	N	O	0	0	0
			829	496	168	165			
6	N	163	Total	C	N	O	0	0	0
			825	496	166	163			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	116	Total	C	N	O	0	0	0
			577	345	116	116			
7	O	132	Total	C	N	O	0	0	0
			648	384	132	132			

- Molecule 8 is a protein called NCK-interacting protein with SH3 domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	329	Total	C	N	O	S	0	0	0
			1638	979	329	329	1			
8	P	328	Total	C	N	O		0	0	0
			1656	995	332	329				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	268	SER	-	expression tag	UNP Q9NZQ3
P	268	SER	-	expression tag	UNP Q9NZQ3

- Molecule 9 is a protein called unidentified.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Q	6	Total	C	N	O	0	0	0
			30	18	6	6			

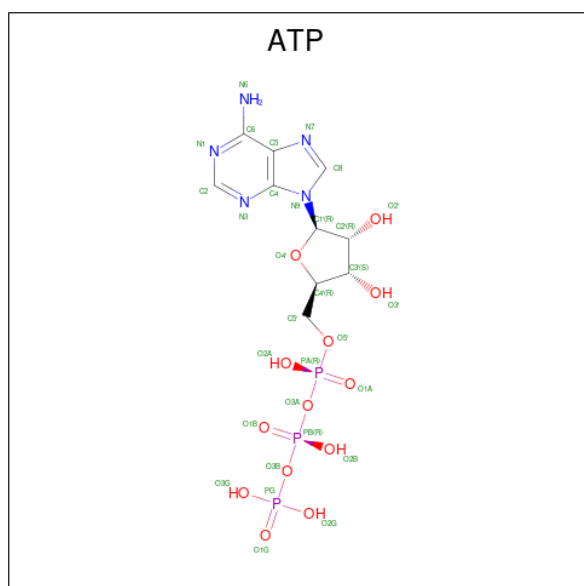
- Molecule 10 is a protein called unidentified.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	R	9	45	27	9	9	0	0	0

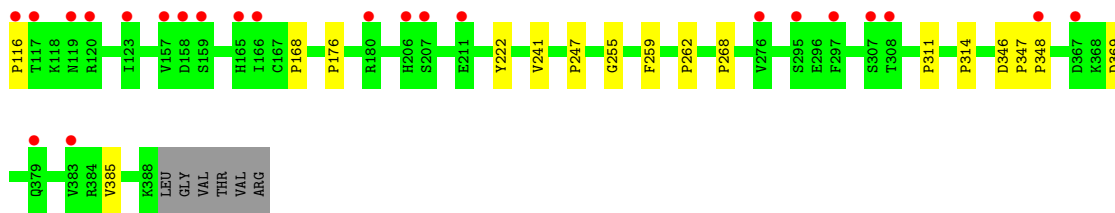
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
11	A	1	1	1	0	0
11	B	1	1	1	0	0
11	H	1	1	1	0	0
11	I	1	1	1	0	0

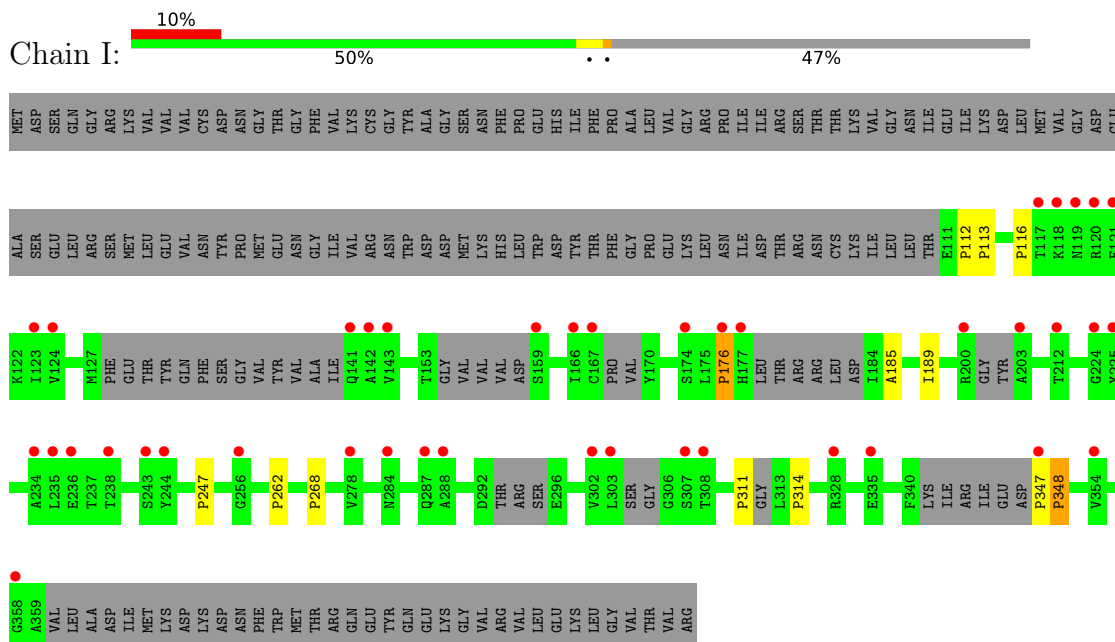
- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



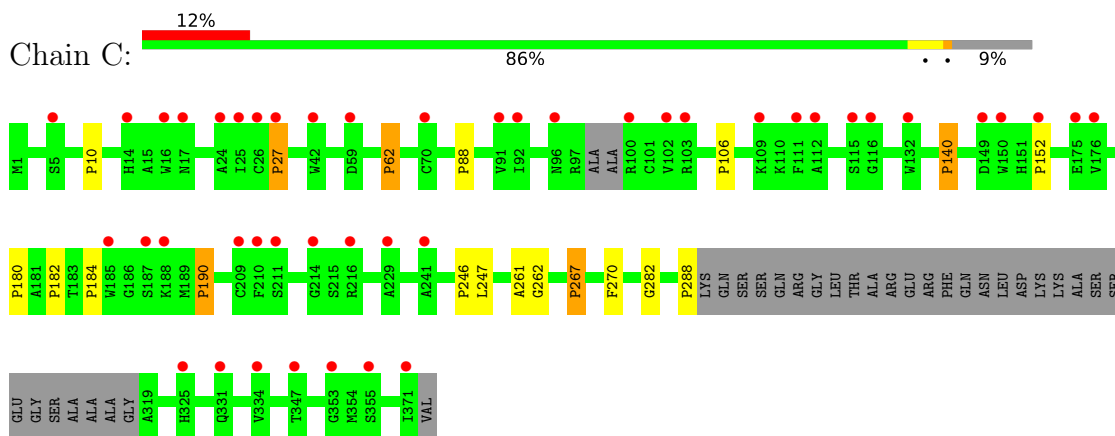




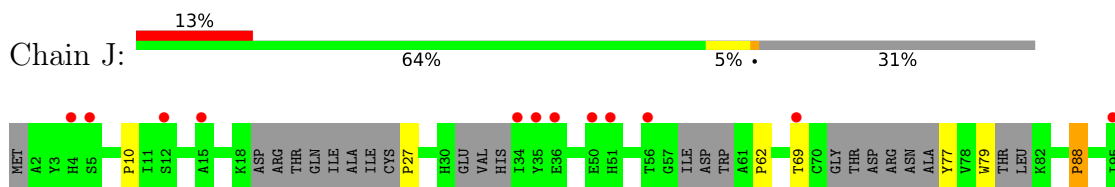
• Molecule 2: Actin-related protein 2

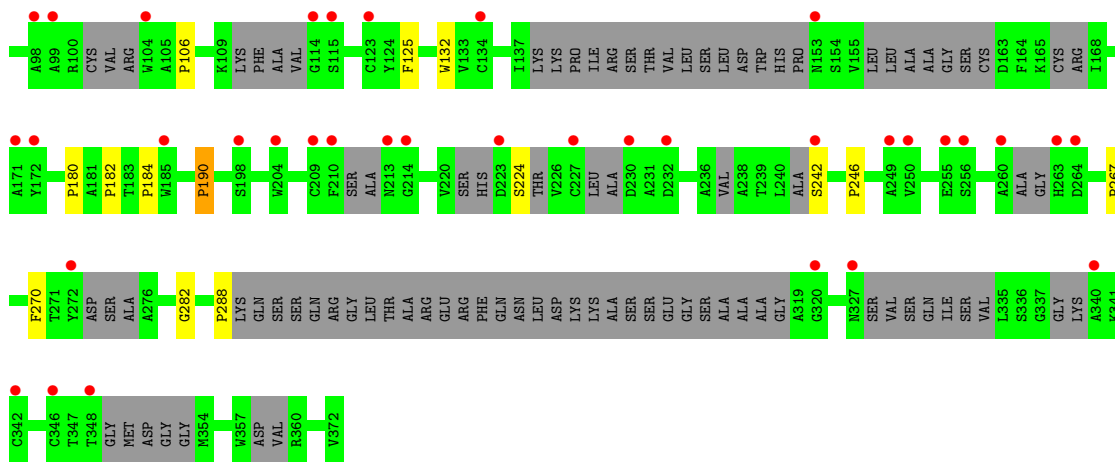


• Molecule 3: Actin-related protein 2/3 complex subunit 1B

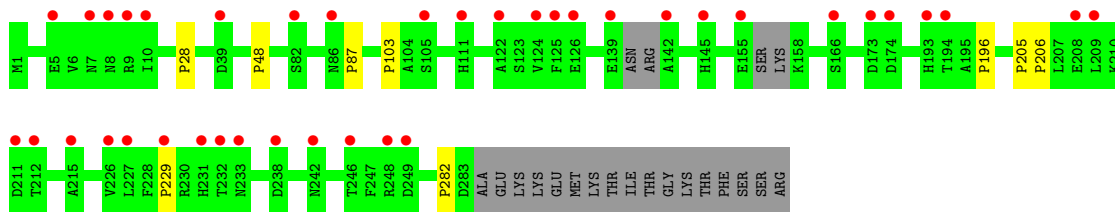
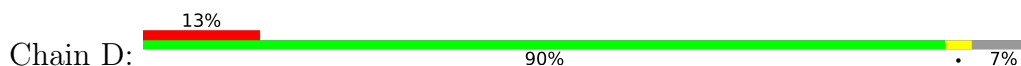


• Molecule 3: Actin-related protein 2/3 complex subunit 1B

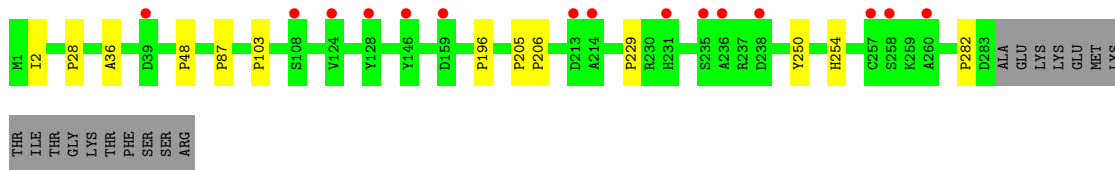
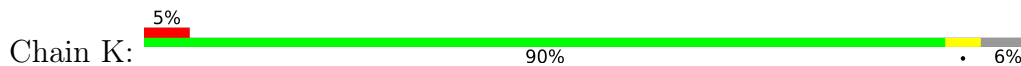




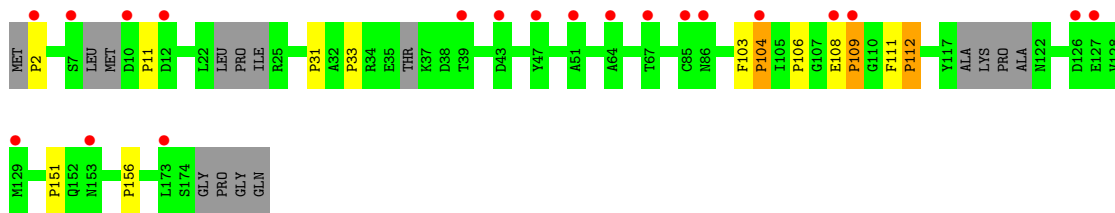
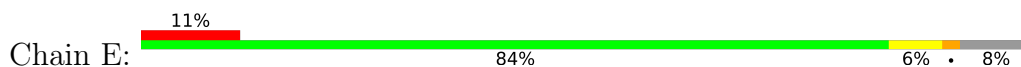
• Molecule 4: Actin-related protein 2/3 complex subunit 2



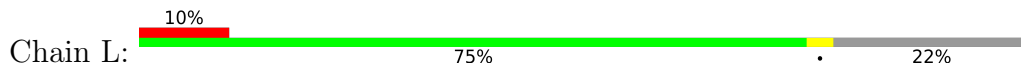
• Molecule 4: Actin-related protein 2/3 complex subunit 2



• Molecule 5: Actin-related protein 2/3 complex subunit 3



• Molecule 5: Actin-related protein 2/3 complex subunit 3







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.84Å 197.38Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 4.60 48.94 – 4.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.94-4.60) 94.1 (48.94-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 4.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.275 , 0.314 0.317 , 0.342	Depositor DCC
$R_{free}$ test set	1975 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	196.7	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.025 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	20563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ATP, CA

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	0.48	0/2015	1.09	26/2799 (0.9%)
1	H	0.47	0/1947	1.06	26/2699 (1.0%)
2	B	0.46	0/1851	1.00	18/2567 (0.7%)
2	I	0.46	0/1020	0.99	11/1403 (0.8%)
3	C	0.43	0/1772	0.91	14/2466 (0.6%)
3	J	0.41	0/1250	0.94	12/1702 (0.7%)
4	D	0.44	0/1387	0.91	9/1929 (0.5%)
4	K	0.45	0/1432	0.89	9/1994 (0.5%)
5	E	0.41	0/810	0.97	10/1120 (0.9%)
5	L	0.41	0/682	0.89	5/947 (0.5%)
6	F	0.49	0/828	0.94	4/1155 (0.3%)
6	N	0.47	0/824	0.89	4/1147 (0.3%)
7	G	0.46	0/577	0.98	4/800 (0.5%)
7	O	0.43	0/645	0.92	4/891 (0.4%)
8	M	0.44	0/1635	0.98	16/2279 (0.7%)
8	P	0.45	0/1656	0.98	16/2305 (0.7%)
All	All	0.45	0/20331	0.97	188/28203 (0.7%)

There are no bond length outliers.

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PRO	N-CA-CB	12.44	110.16	103.19
7	G	63	PRO	N-CA-CB	11.49	110.47	102.65
7	O	63	PRO	N-CA-CB	11.13	110.25	102.35
1	A	362	PRO	N-CA-CB	8.97	110.47	103.30
1	A	179	PRO	N-CA-CB	8.68	110.56	103.36

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	2010	0	906	2	0
1	H	1948	0	873	3	0
2	B	1850	0	839	4	0
2	I	1030	0	449	1	0
3	C	1757	0	843	3	0
3	J	1274	0	551	5	0
4	D	1389	0	632	0	0
4	K	1429	0	663	3	0
5	E	815	0	349	0	0
5	L	685	0	291	0	0
6	F	829	0	371	0	0
6	N	825	0	370	1	0
7	G	577	0	282	0	0
7	O	648	0	311	0	0
8	M	1638	0	737	0	0
8	P	1656	0	760	1	0
9	Q	30	0	8	0	0
10	R	45	0	11	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
12	A	31	0	12	1	0
12	B	31	0	12	0	0
12	H	31	0	12	0	0
12	I	31	0	12	0	0
All	All	20563	0	9294	21	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 1.

The worst 5 of 21 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:J:224:SER:O	3:J:242:SER:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:2:ILE:O	4:K:254:HIS:NE2	2.26	0.60
2:B:222:TYR:CZ	2:B:259:PHE:HB3	2.42	0.54
2:B:241:VAL:HA	2:B:255:GLY:HA2	1.90	0.53
4:K:250:TYR:OH	6:N:160:VAL:O	2.24	0.52

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	392/418 (94%)	374 (95%)	13 (3%)	5 (1%)	9	41
1	H	372/418 (89%)	355 (95%)	13 (4%)	4 (1%)	11	45
2	B	365/394 (93%)	337 (92%)	25 (7%)	3 (1%)	16	53
2	I	189/394 (48%)	180 (95%)	7 (4%)	2 (1%)	11	45
3	C	333/372 (90%)	305 (92%)	24 (7%)	4 (1%)	10	42
3	J	210/372 (56%)	202 (96%)	7 (3%)	1 (0%)	24	63
4	D	273/300 (91%)	268 (98%)	5 (2%)	0	100	100
4	K	281/300 (94%)	275 (98%)	6 (2%)	0	100	100
5	E	151/178 (85%)	141 (93%)	4 (3%)	6 (4%)	2	18
5	L	132/178 (74%)	131 (99%)	1 (1%)	0	100	100
6	F	163/168 (97%)	160 (98%)	3 (2%)	0	100	100
6	N	159/168 (95%)	154 (97%)	4 (2%)	1 (1%)	21	58
7	G	114/151 (76%)	112 (98%)	1 (1%)	1 (1%)	14	49
7	O	126/151 (83%)	123 (98%)	2 (2%)	1 (1%)	16	53
8	M	323/455 (71%)	311 (96%)	10 (3%)	2 (1%)	21	58
8	P	320/455 (70%)	307 (96%)	8 (2%)	5 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3903/4872 (80%)	3735 (96%)	133 (3%)	35 (1%)	14 49

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	PRO
1	A	157	GLN
3	C	140	PRO
5	E	108	GLU
5	E	112	PRO

### 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	8/363 (2%)	8 (100%)	0	100 100
1	H	7/363 (2%)	6 (86%)	1 (14%)	3 14
2	B	6/345 (2%)	6 (100%)	0	100 100
3	C	10/313 (3%)	10 (100%)	0	100 100
4	D	1/264 (0%)	1 (100%)	0	100 100
4	K	5/264 (2%)	5 (100%)	0	100 100
5	E	1/159 (1%)	1 (100%)	0	100 100
6	F	1/155 (1%)	1 (100%)	0	100 100
6	N	2/155 (1%)	2 (100%)	0	100 100
7	G	1/123 (1%)	1 (100%)	0	100 100
8	M	1/392 (0%)	1 (100%)	0	100 100
8	P	5/392 (1%)	5 (100%)	0	100 100
All	All	48/3288 (2%)	47 (98%)	1 (2%)	47 65

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

Mol	Chain	Res	Type
1	H	192	HIS

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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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$
12	ATP	B	502	11	32,33,33	1.44	5 (15%)	48,52,52	1.74	9 (18%)
12	ATP	I	502	11	32,33,33	1.43	5 (15%)	48,52,52	1.74	9 (18%)
12	ATP	H	502	11	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)
12	ATP	A	502	11	32,33,33	1.41	4 (12%)	48,52,52	1.76	9 (18%)

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
12	ATP	B	502	11	-	6/22/38/38	0/3/3/3
12	ATP	I	502	11	-	2/22/38/38	0/3/3/3
12	ATP	H	502	11	-	3/22/38/38	0/3/3/3
12	ATP	A	502	11	-	1/22/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	502	ATP	C5-C4	4.82	1.47	1.39
12	H	502	ATP	C5-C4	4.80	1.47	1.39
12	A	502	ATP	C5-C4	4.79	1.47	1.39
12	I	502	ATP	C5-C4	4.71	1.47	1.39
12	A	502	ATP	C5-C6	2.83	1.48	1.41

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	502	ATP	C5-C4-N3	-6.02	118.43	126.72
12	A	502	ATP	C5-C4-N3	-5.89	118.60	126.72
12	I	502	ATP	C5-C4-N3	-5.81	118.72	126.72
12	B	502	ATP	C5-C4-N3	-5.69	118.88	126.72
12	H	502	ATP	N3-C4-N9	4.74	135.23	127.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	502	ATP	O4'-C4'-C5'-O5'
12	B	502	ATP	C3'-C4'-C5'-O5'
12	B	502	ATP	PG-O3B-PB-O1B
12	B	502	ATP	PG-O3B-PB-O2B
12	B	502	ATP	PB-O3A-PA-O1A

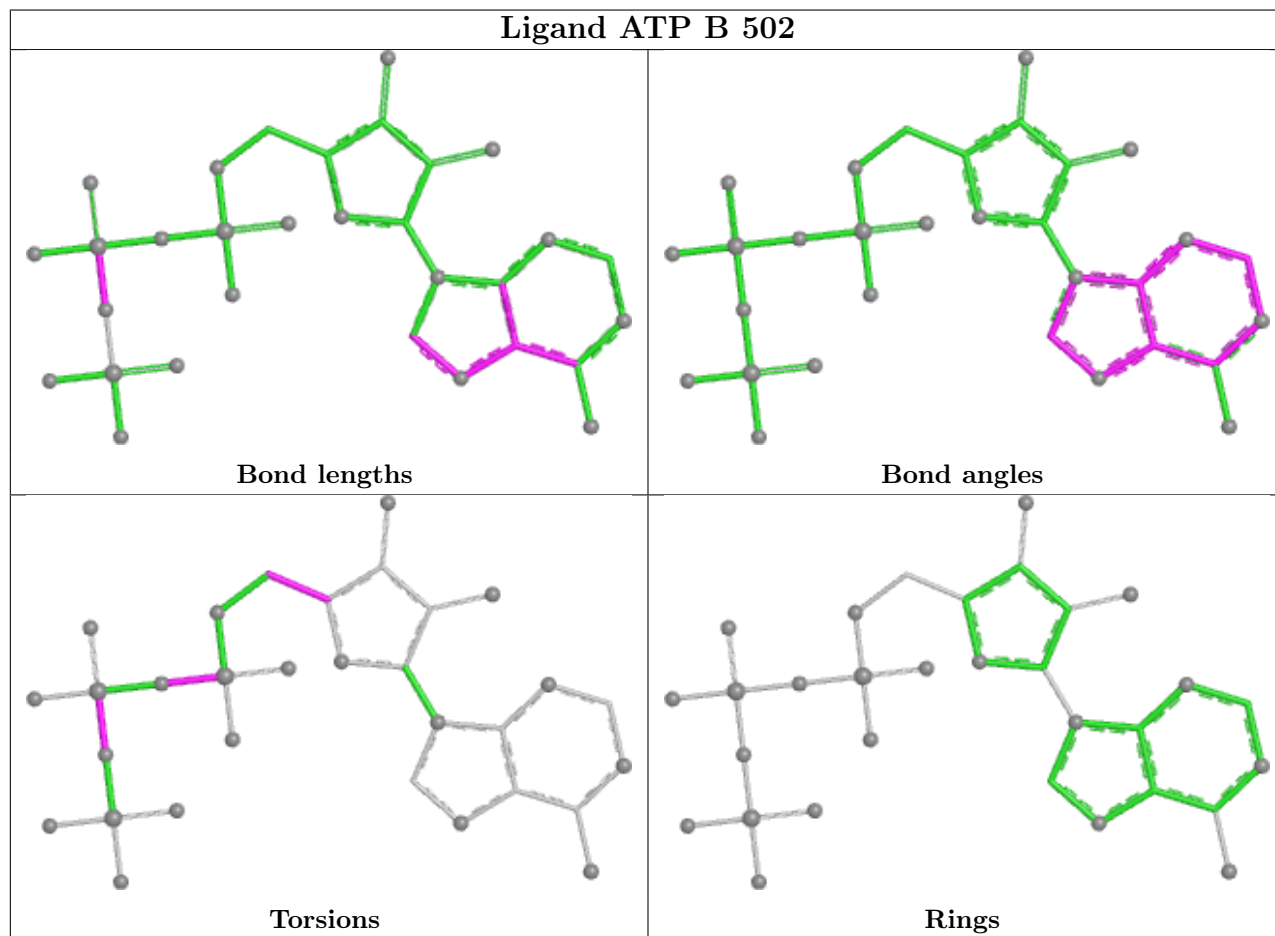
There are no ring outliers.

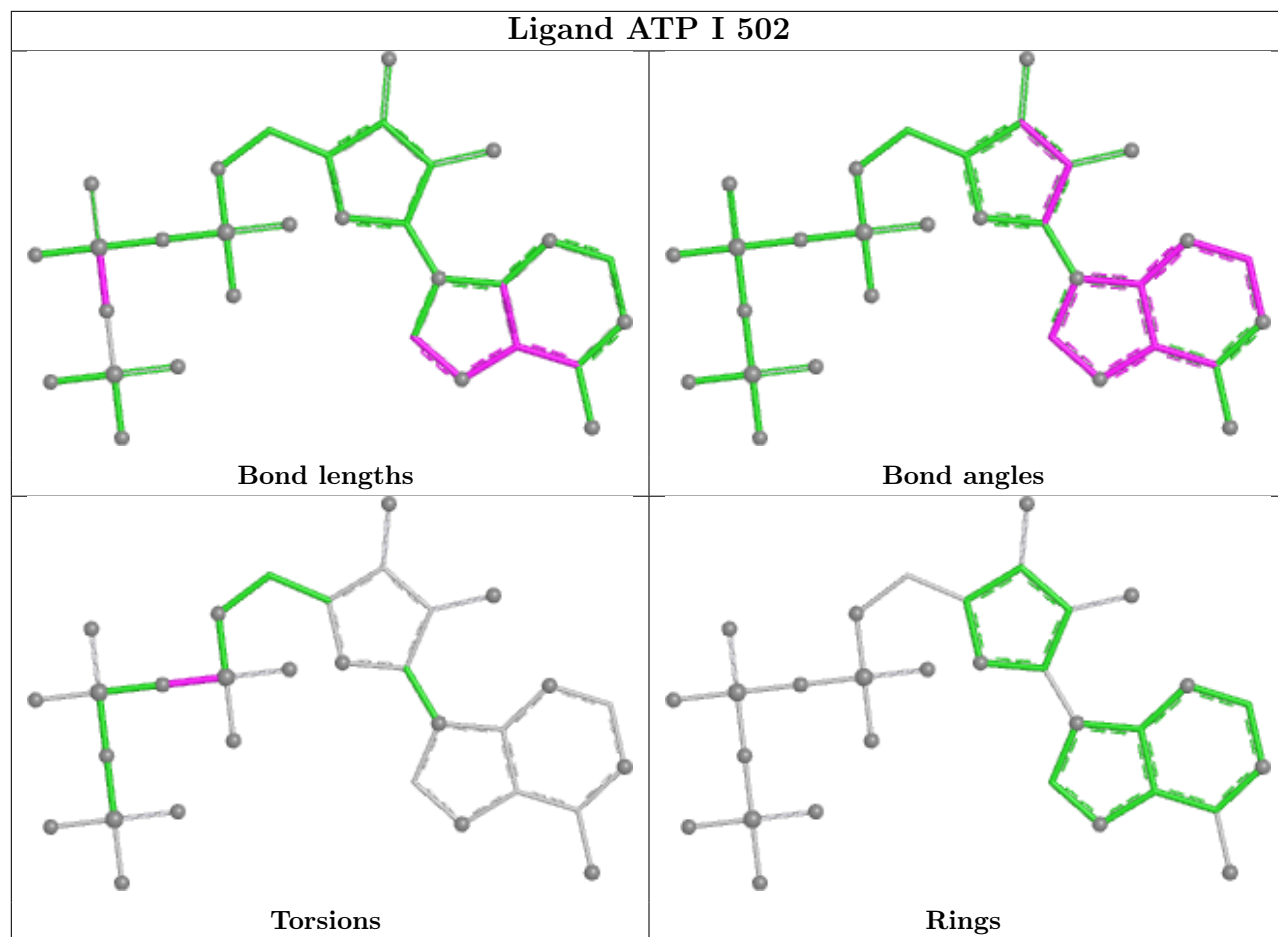
1 monomer is involved in 1 short contact:

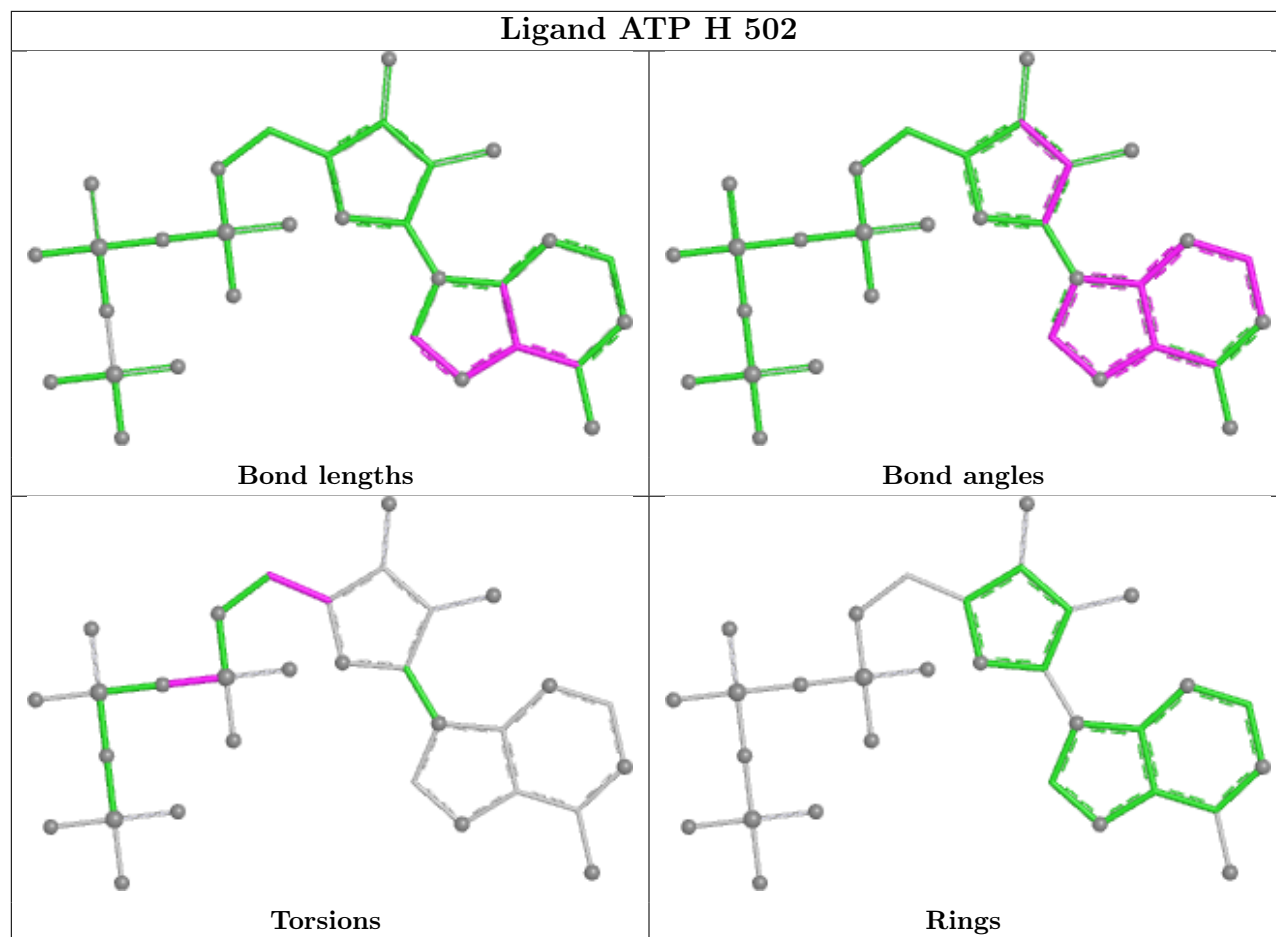
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	502	ATP	1	0

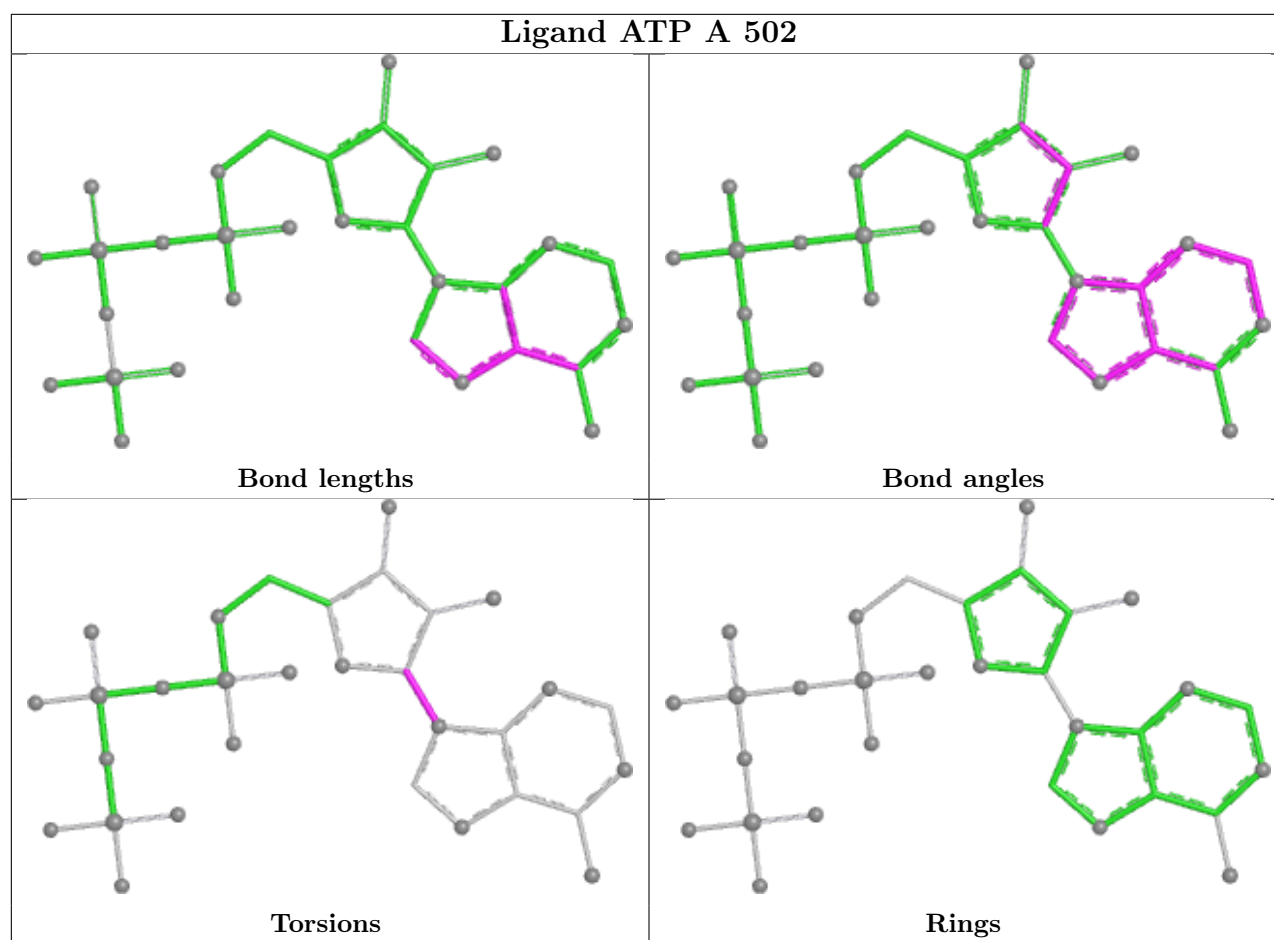
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	19:MET	C	21:ALA	N	4.49

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	398/418 (95%)	0.63	35 (8%) 15 19	76, 138, 200, 295	0
1	H	386/418 (92%)	0.82	57 (14%) 5 11	82, 157, 246, 311	0
2	B	369/394 (93%)	0.51	37 (10%) 12 17	66, 155, 253, 296	0
2	I	209/394 (53%)	1.03	41 (19%) 3 7	121, 215, 330, 447	0
3	C	339/372 (91%)	0.68	45 (13%) 7 12	78, 140, 193, 229	0
3	J	258/372 (69%)	1.14	48 (18%) 3 8	140, 245, 321, 379	0
4	D	279/300 (93%)	0.77	39 (13%) 6 12	71, 219, 342, 423	0
4	K	283/300 (94%)	0.43	15 (5%) 32 31	76, 146, 213, 256	0
5	E	163/178 (91%)	0.80	20 (12%) 8 13	117, 178, 251, 281	0
5	L	138/178 (77%)	0.90	17 (12%) 8 13	145, 242, 330, 351	0
6	F	165/168 (98%)	0.53	9 (5%) 30 30	58, 118, 203, 233	0
6	N	163/168 (97%)	0.78	25 (15%) 5 11	78, 156, 224, 288	0
7	G	116/151 (76%)	0.73	17 (14%) 6 11	90, 179, 281, 305	0
7	O	132/151 (87%)	0.95	17 (12%) 7 12	142, 248, 305, 333	0
8	M	329/455 (72%)	1.01	58 (17%) 4 9	102, 202, 289, 315	0
8	P	328/455 (72%)	0.58	33 (10%) 12 17	71, 156, 277, 312	0
9	Q	0/6	-	-	-	-
10	R	0/9	-	-	-	-
All	All	4055/4887 (82%)	0.75	513 (12%) 8 13	58, 172, 284, 447	0

The worst 5 of 513 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	85	CYS	8.7
3	J	327	ASN	8.4
8	M	380	GLN	7.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	167	CYS	7.5
1	H	54	GLY	7.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

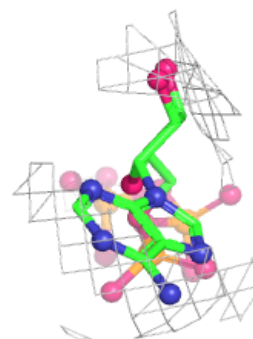
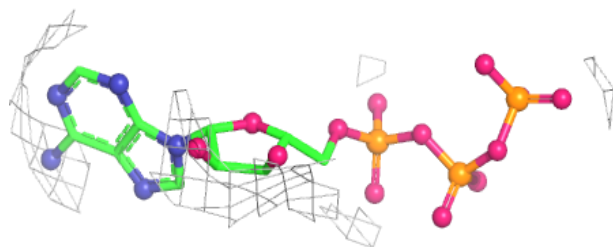
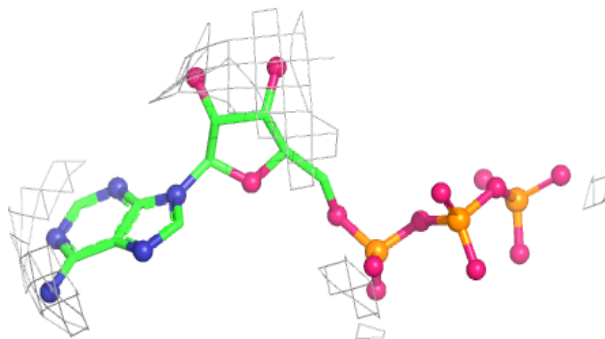
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
12	ATP	I	502	31/31	0.78	0.11	177,240,301,313	0
12	ATP	H	502	31/31	0.80	0.20	129,147,198,226	0
11	CA	I	501	1/1	0.87	0.10	301,301,301,301	0
12	ATP	B	502	31/31	0.89	0.14	100,117,145,151	0
12	ATP	A	502	31/31	0.90	0.14	106,119,162,181	0
11	CA	H	501	1/1	0.93	0.31	144,144,144,144	0
11	CA	A	501	1/1	0.96	0.26	87,87,87,87	0
11	CA	B	501	1/1	0.97	0.17	116,116,116,116	0

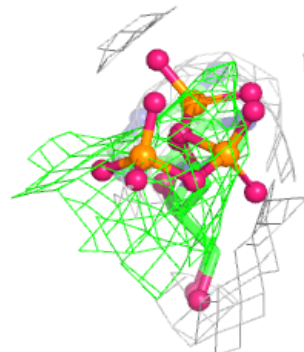
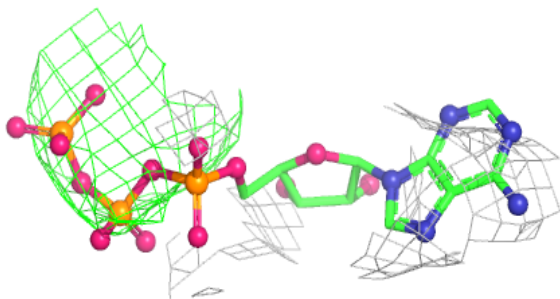
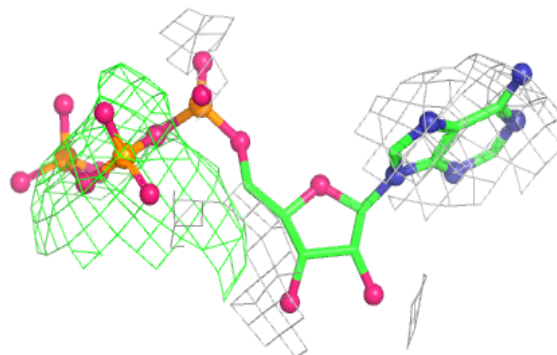
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP I 502:**

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

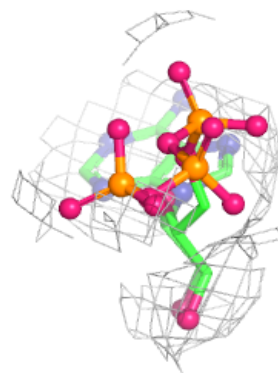
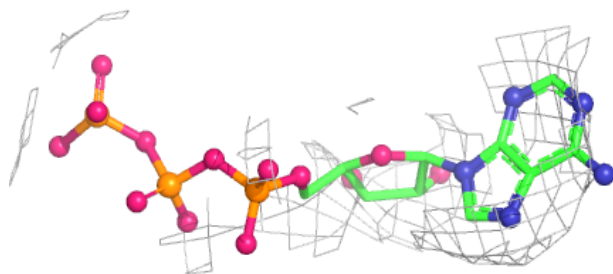
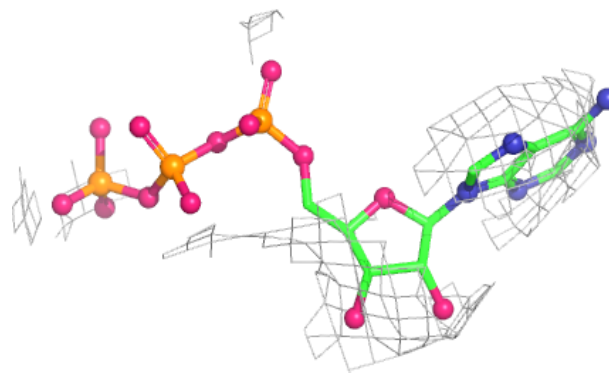
**Electron density around ATP H 502:**

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

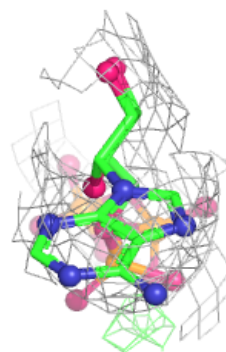
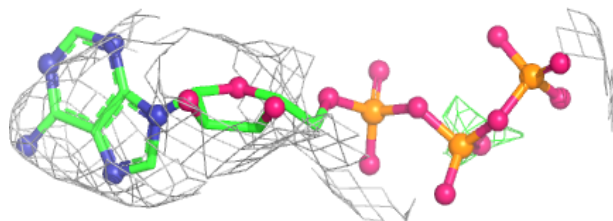
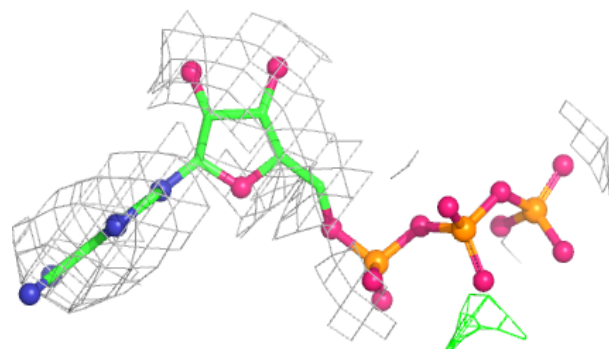


**Electron density around ATP B 502:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.