wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 05:23 PM EDT

PDB ID	:	6DEC
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

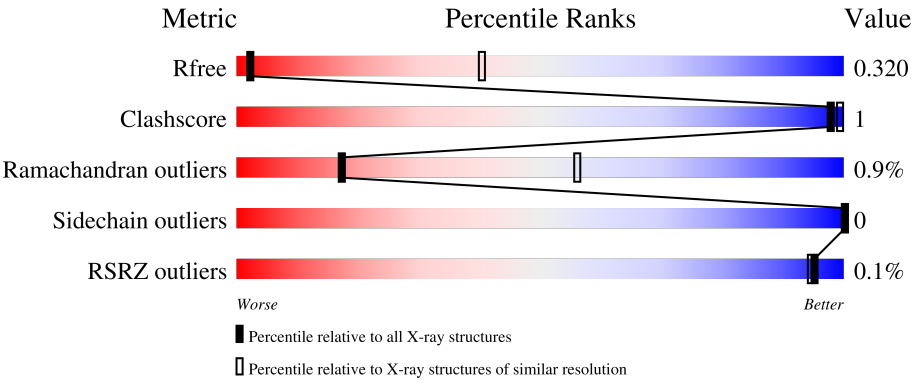
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	88% 6% • 5%
1	H	418	86% 6% • 8%
2	B	394	87% 7% 6%
2	I	394	50% • • 47%
3	C	372	86% • • 9%

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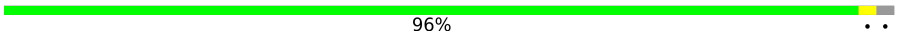
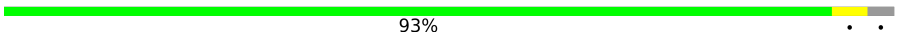
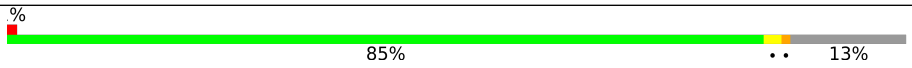
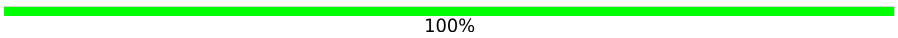
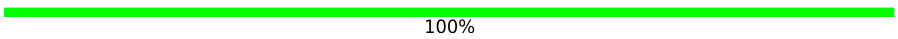
Mol	Chain	Length	Quality of chain
3	J	372	
4	D	300	
4	K	300	
5	E	178	
5	L	178	
6	F	168	
6	N	168	
7	G	151	
7	O	151	
8	M	455	
8	P	455	
9	Q	6	
10	R	9	

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
1	A	398	Total 2010	C 1202	N 404	O 404	0	0	0
1	H	386	Total 1948	C 1169	N 389	O 390	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	369	Total 1850	C 1103	N 372	O 375	0	0	0
2	I	209	Total 1030	C 612	N 209	O 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
3	C	339	Total 1757	C 1070	N 347	O 340	0	0	0
3	J	258	Total 1274	C 758	N 258	O 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
4	D	279	Total 1389	C 830	N 279	O 280	0	0	0
4	K	283	Total 1429	C 855	N 288	O 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 815	C 488	N 163	O 164	0	0	0
5	L	138	Total 685	C 409	N 138	O 138	0	0	0

- 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 829	C 496	N 168	O 165	0	0	0
6	N	163	Total 825	C 496	N 166	O 163	0	0	0

- 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 577	C 345	N 116	O 116	0	0	0
7	O	132	Total 648	C 384	N 132	O 132	0	0	0

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

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

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 30	C 18	N 6	O 6	0	0	0

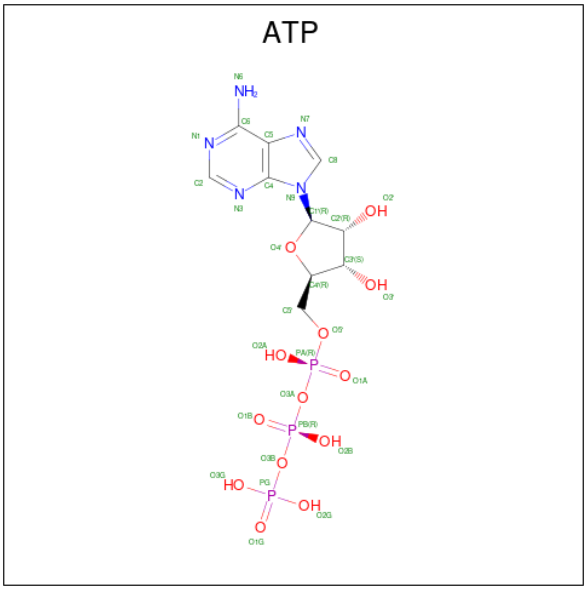
- Molecule 10 is a protein called unidentified.

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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



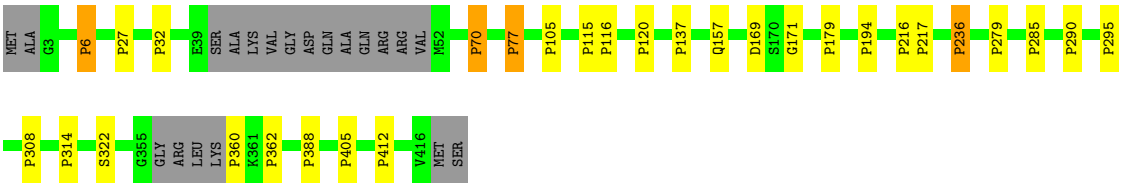
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C N O P 31 10 5 13 3	0	0
12	B	1	Total C N O P 31 10 5 13 3	0	0
12	H	1	Total C N O P 31 10 5 13 3	0	0
12	I	1	Total C N O P 31 10 5 13 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

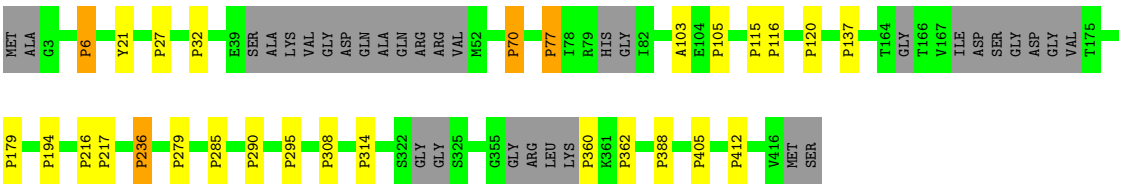
• Molecule 1: Actin-related protein 3

Chain A:



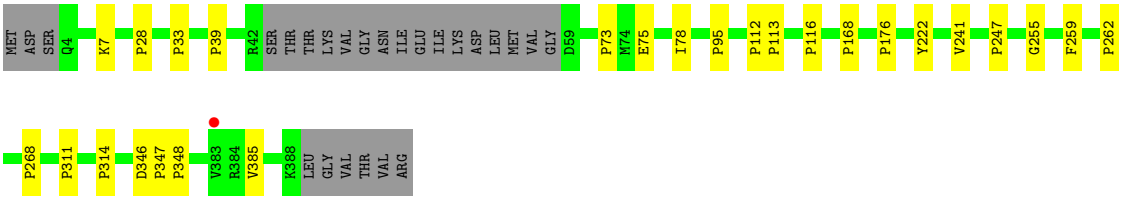
• Molecule 1: Actin-related protein 3

Chain H:



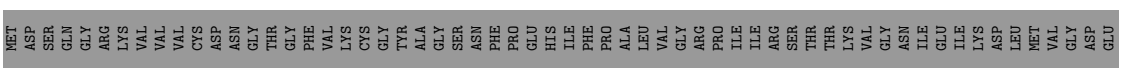
• Molecule 2: Actin-related protein 2

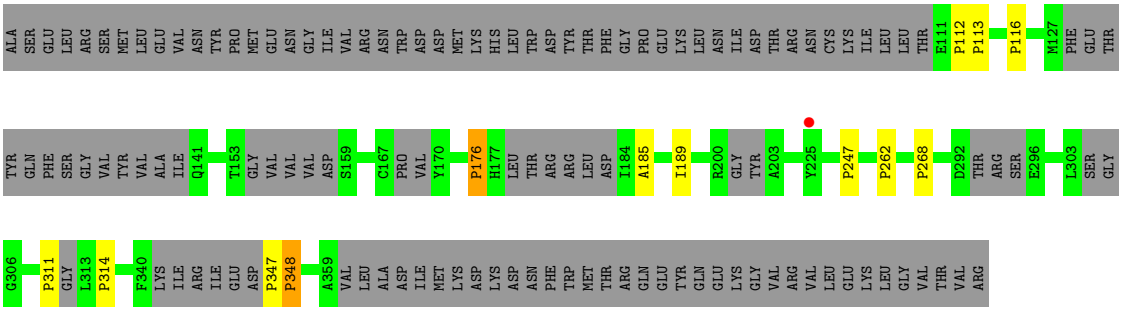
Chain B:



• Molecule 2: Actin-related protein 2

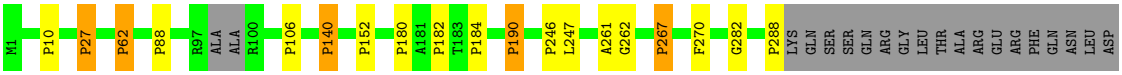
Chain I:





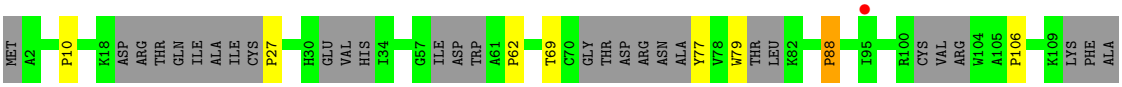
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

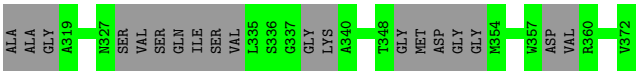
Chain C:



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

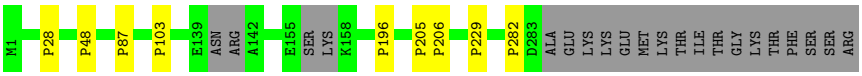
Chain J:





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

Chain D:

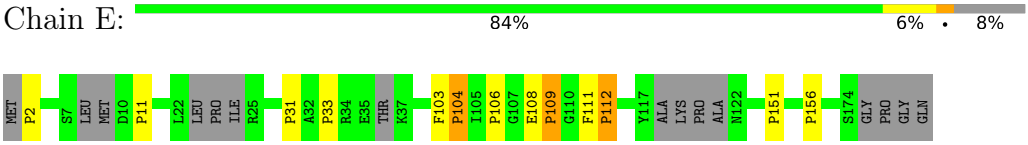


• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain K:

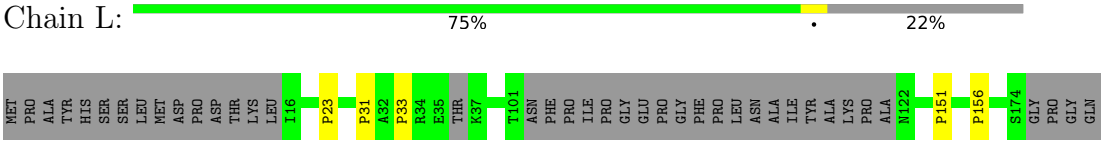
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



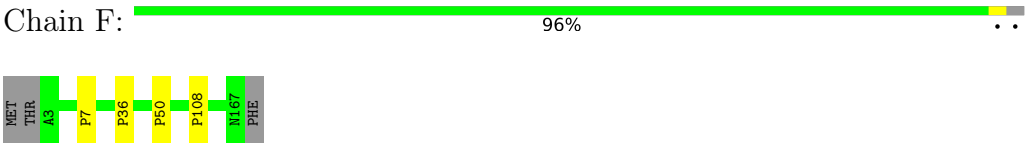
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain L:



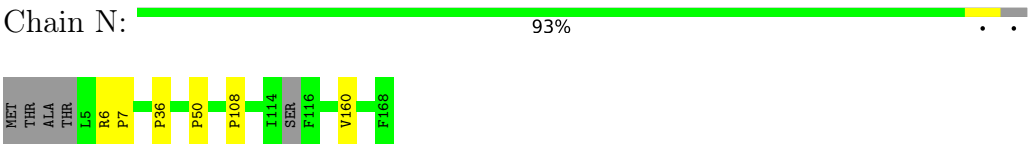
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



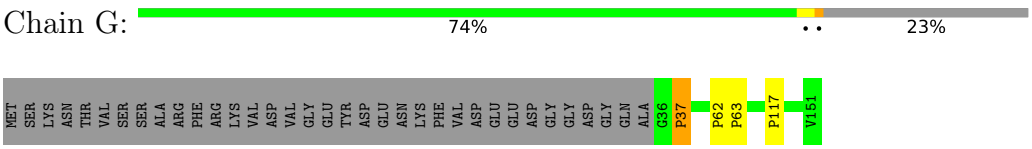
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain N:



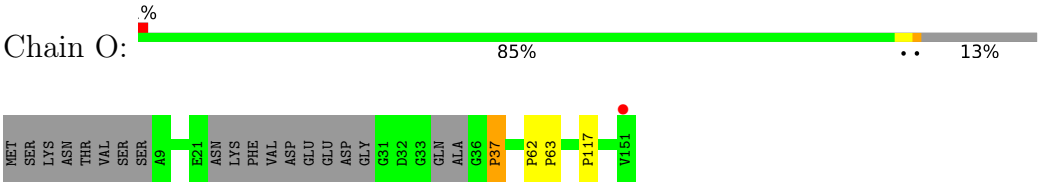
• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



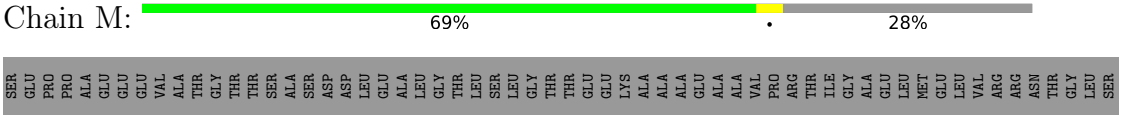
• Molecule 7: Actin-related protein 2/3 complex subunit 5

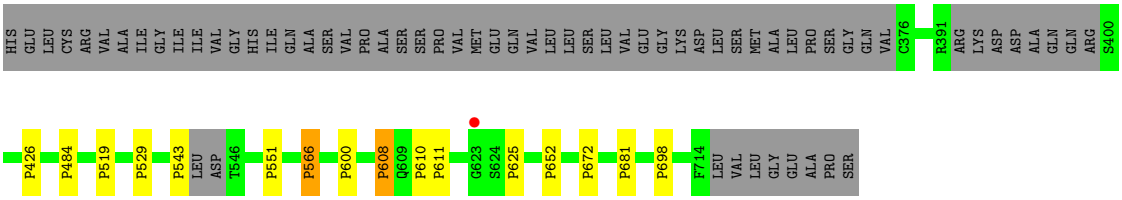
Chain O:



• Molecule 8: NCK-interacting protein with SH3 domain

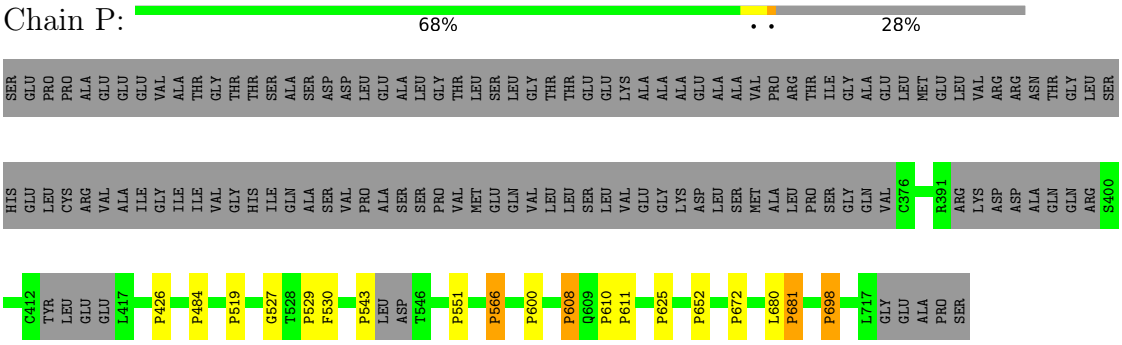
Chain M:





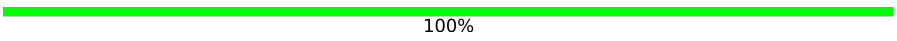
• Molecule 8: NCK-interacting protein with SH3 domain

Chain P:



• Molecule 9: unidentified

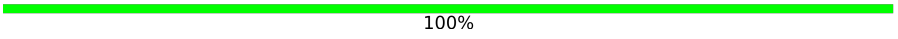
Chain Q:



There are no outlier residues recorded for this chain.

• Molecule 10: unidentified

Chain R:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	179.84Å 197.38Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 4.60 48.94 – 4.47	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.94-4.60) 89.4 (48.94-4.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.275 , 0.314 0.295 , 0.320	Depositor DCC
R_{free} test set	1975 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	196.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 311.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	20563	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/2015	0.66	26/2799 (0.9%)
1	H	0.34	0/1947	0.66	26/2699 (1.0%)
2	B	0.33	0/1851	0.57	17/2567 (0.7%)
2	I	0.33	0/1020	0.59	11/1403 (0.8%)
3	C	0.32	0/1772	0.54	14/2466 (0.6%)
3	J	0.32	0/1250	0.58	12/1702 (0.7%)
4	D	0.33	0/1387	0.50	9/1929 (0.5%)
4	K	0.34	0/1432	0.50	9/1994 (0.5%)
5	E	0.32	0/810	0.64	10/1120 (0.9%)
5	L	0.32	0/682	0.53	5/947 (0.5%)
6	F	0.36	0/828	0.49	4/1155 (0.3%)
6	N	0.35	0/824	0.48	4/1147 (0.3%)
7	G	0.33	0/577	0.53	4/800 (0.5%)
7	O	0.32	0/645	0.50	4/891 (0.4%)
8	M	0.32	0/1635	0.58	16/2279 (0.7%)
8	P	0.33	0/1656	0.60	16/2305 (0.7%)
All	All	0.33	0/20331	0.57	187/28203 (0.7%)

There are no bond length outliers.

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	566	PRO	N-CA-CB	6.33	110.89	103.30
8	P	608	PRO	N-CA-CB	6.31	110.87	103.30
8	P	566	PRO	N-CA-CB	6.26	110.81	103.30
8	P	551	PRO	N-CA-CB	6.24	110.79	103.30
8	P	681	PRO	N-CA-CB	6.20	110.74	103.30

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	2	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	20	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 20 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%)	12 48
1	H	372/418 (89%)	355 (95%)	13 (4%)	4 (1%)	14 52
2	B	365/394 (93%)	337 (92%)	25 (7%)	3 (1%)	19 60
2	I	189/394 (48%)	180 (95%)	7 (4%)	2 (1%)	14 52
3	C	333/372 (90%)	305 (92%)	24 (7%)	4 (1%)	13 50
3	J	210/372 (56%)	202 (96%)	7 (3%)	1 (0%)	29 68
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%)	3 26
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%)	25 65
7	G	114/151 (76%)	112 (98%)	1 (1%)	1 (1%)	17 56
7	O	126/151 (83%)	123 (98%)	2 (2%)	1 (1%)	19 60
8	M	323/455 (71%)	311 (96%)	10 (3%)	2 (1%)	25 65
8	P	320/455 (70%)	307 (96%)	8 (2%)	5 (2%)	9 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3903/4872 (80%)	3735 (96%)	133 (3%)	35 (1%)	17 56

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%)	7 (100%)	0	100 100
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%)	48 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	H	502	11	26,33,33	0.94	1 (3%)	31,52,52	1.55	5 (16%)
12	ATP	A	502	11	26,33,33	0.96	1 (3%)	31,52,52	1.55	5 (16%)
12	ATP	I	502	11	26,33,33	0.93	1 (3%)	31,52,52	1.52	5 (16%)
12	ATP	B	502	11	26,33,33	0.96	1 (3%)	31,52,52	1.43	5 (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
12	ATP	H	502	11	-	3/18/38/38	0/3/3/3
12	ATP	A	502	11	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ATP	I	502	11	-	1/18/38/38	0/3/3/3
12	ATP	B	502	11	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	502	ATP	C5-C4	2.56	1.47	1.40
12	H	502	ATP	C5-C4	2.54	1.47	1.40
12	A	502	ATP	C5-C4	2.53	1.47	1.40
12	I	502	ATP	C5-C4	2.48	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	502	ATP	PB-O3B-PG	-3.63	120.36	132.83
12	A	502	ATP	PB-O3B-PG	-3.52	120.74	132.83
12	I	502	ATP	PA-O3A-PB	-3.44	121.03	132.83
12	A	502	ATP	PA-O3A-PB	-3.40	121.17	132.83
12	H	502	ATP	PA-O3A-PB	-3.39	121.21	132.83

There are no chirality outliers.

5 of 10 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.

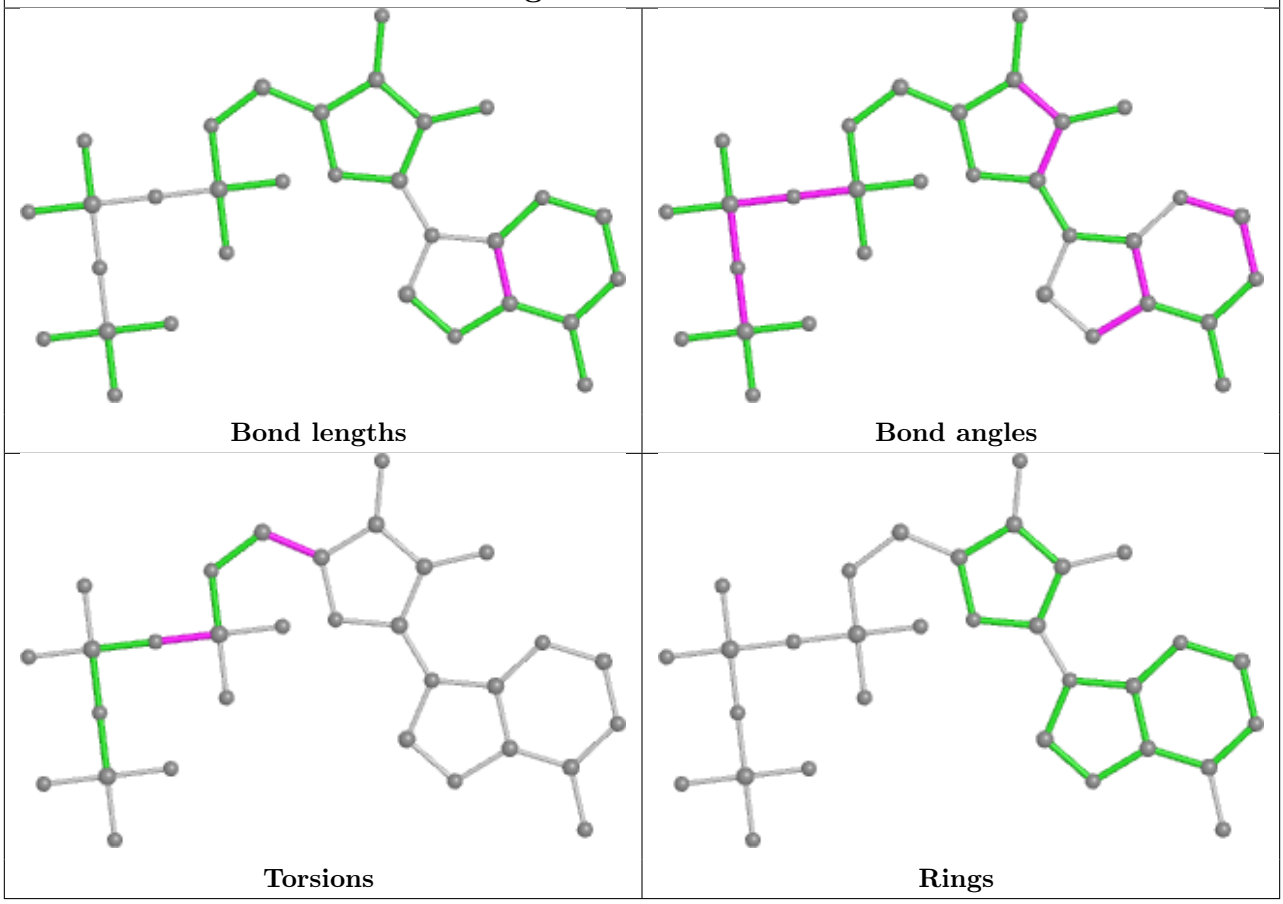
1 monomer is involved in 1 short contact:

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

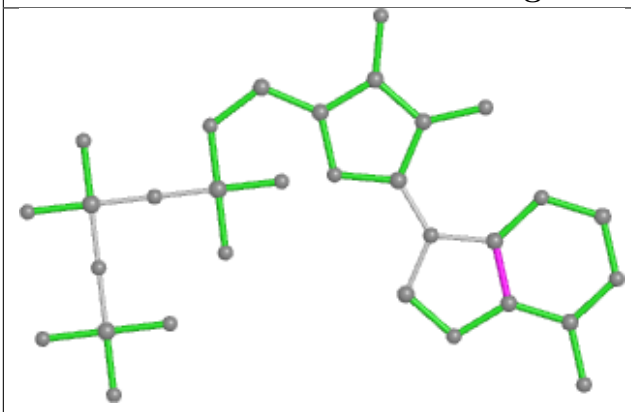
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

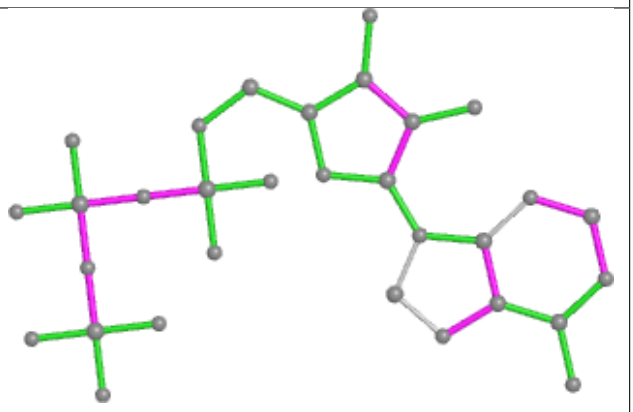
Ligand ATP H 502



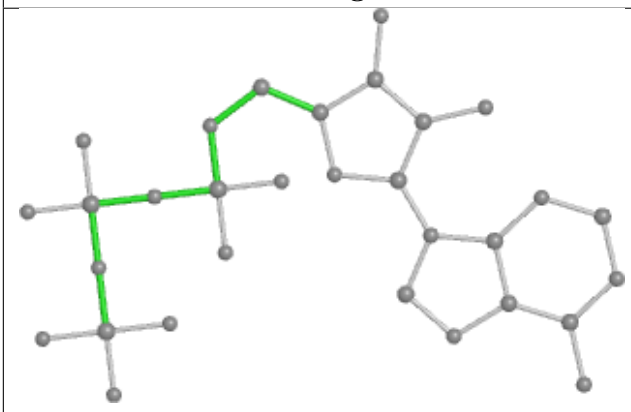
Ligand ATP A 502



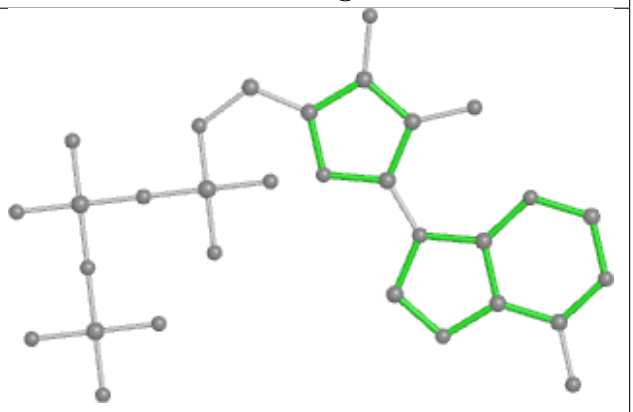
Bond lengths



Bond angles

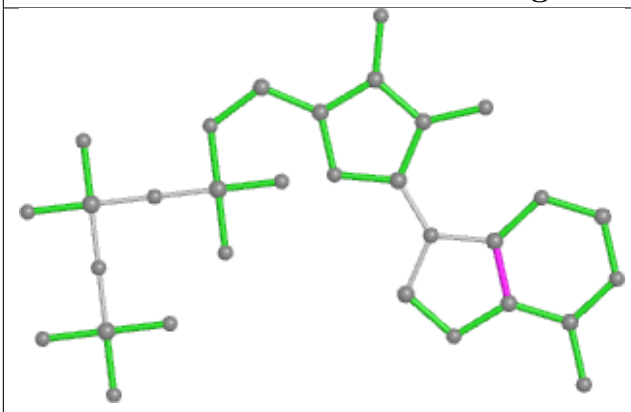


Torsions

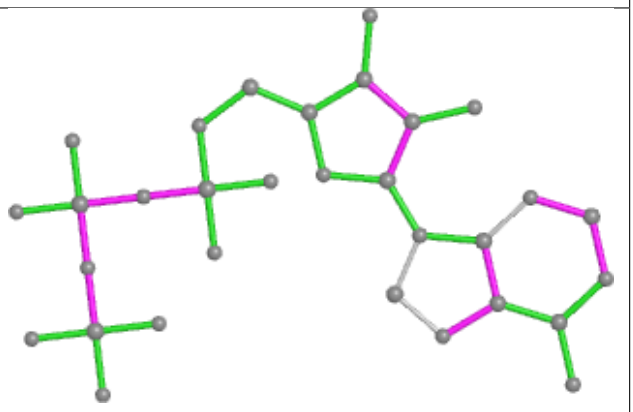


Rings

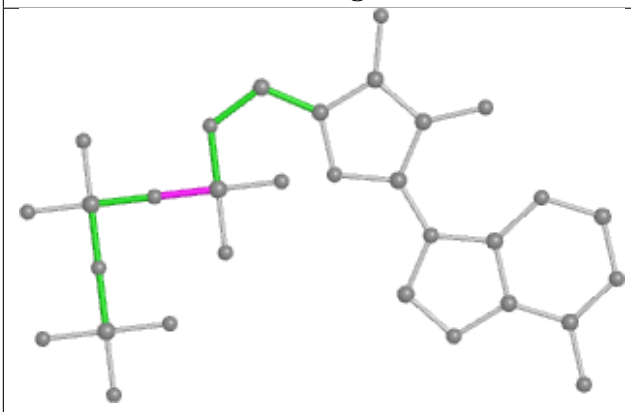
Ligand ATP I 502



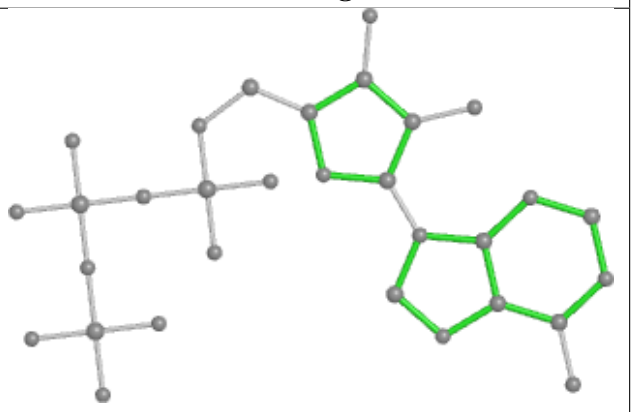
Bond lengths



Bond angles

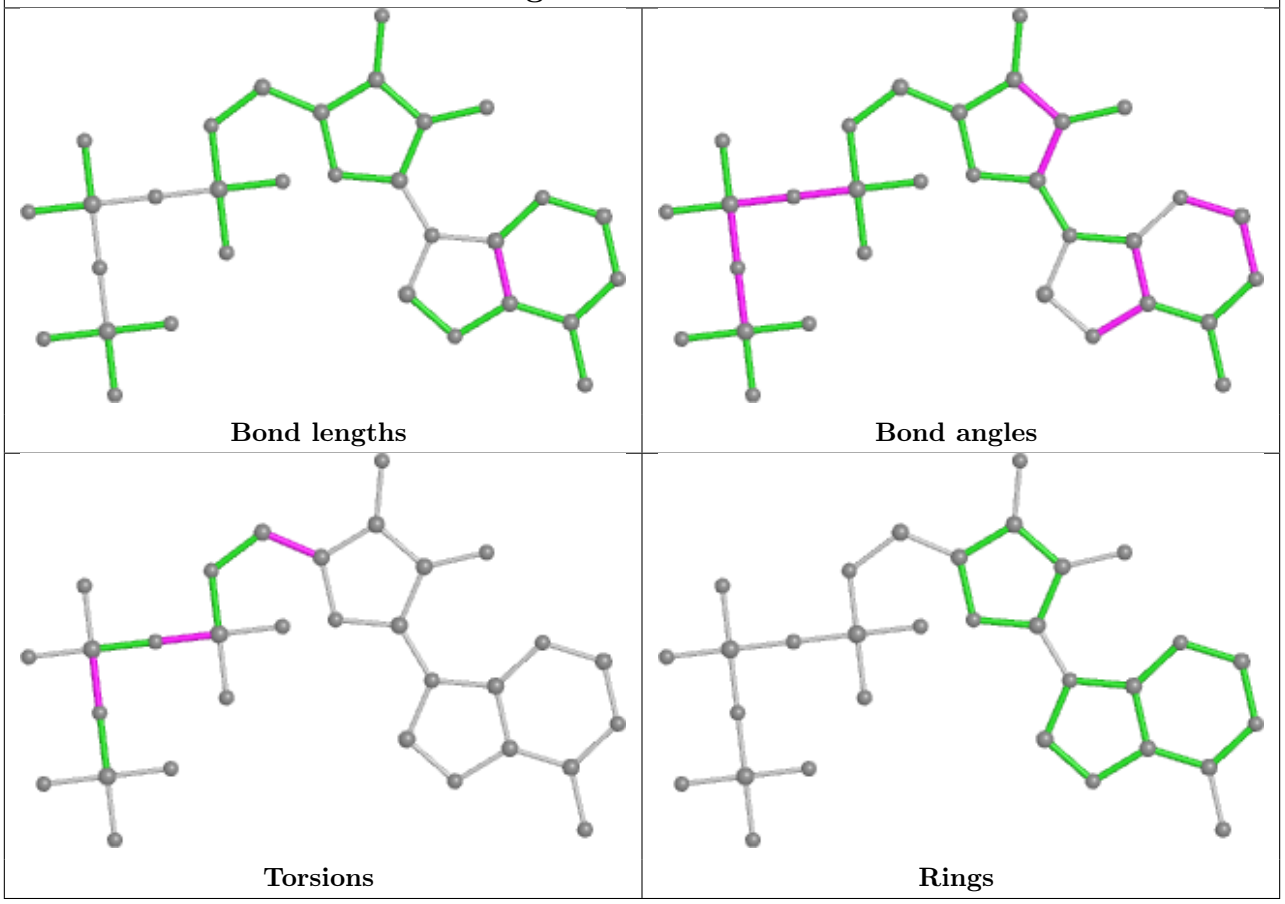


Torsions



Rings

Ligand ATP B 502



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

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^{th} 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	398/418 (95%)	-0.82	0 100 100	76, 138, 200, 295	0
1	H	386/418 (92%)	-0.81	0 100 100	82, 157, 246, 311	0
2	B	369/394 (93%)	-0.78	1 (0%) 94 90	66, 155, 253, 296	0
2	I	209/394 (53%)	-0.65	1 (0%) 91 85	121, 215, 330, 447	0
3	C	339/372 (91%)	-0.67	0 100 100	78, 140, 193, 229	0
3	J	258/372 (69%)	-0.46	1 (0%) 92 87	140, 245, 321, 379	0
4	D	279/300 (93%)	-0.73	0 100 100	71, 219, 342, 423	0
4	K	283/300 (94%)	-0.86	0 100 100	76, 146, 213, 256	0
5	E	163/178 (91%)	-0.73	0 100 100	117, 178, 251, 281	0
5	L	138/178 (77%)	-0.52	0 100 100	145, 242, 330, 351	0
6	F	165/168 (98%)	-0.84	0 100 100	58, 118, 203, 233	0
6	N	163/168 (97%)	-0.81	0 100 100	78, 156, 224, 288	0
7	G	116/151 (76%)	-0.88	0 100 100	90, 179, 281, 305	0
7	O	132/151 (87%)	-0.55	1 (0%) 86 79	142, 248, 305, 333	0
8	M	329/455 (72%)	-0.70	1 (0%) 94 90	102, 202, 289, 315	0
8	P	328/455 (72%)	-0.88	0 100 100	71, 156, 277, 312	0
9	Q	0/6	-	-	-	-
10	R	0/9	-	-	-	-
All	All	4055/4887 (82%)	-0.74	5 (0%) 95 94	58, 172, 284, 447	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	M	623	GLY	2.7
3	J	95	ILE	2.7
2	I	225	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
7	O	151	VAL	2.4
2	B	383	VAL	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

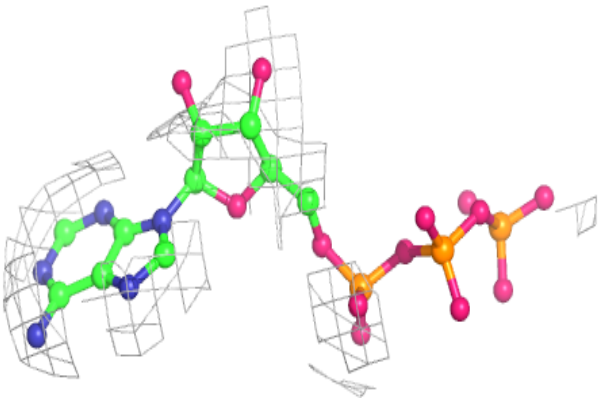
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

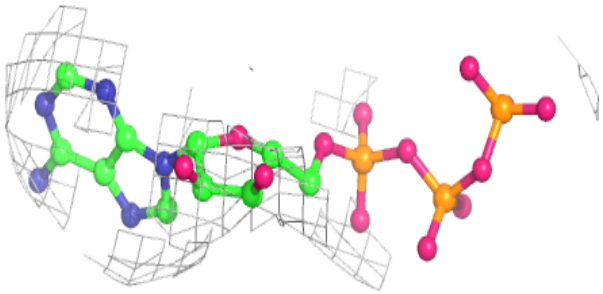
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CA	I	501	1/1	0.82	0.32	301,301,301,301	0
12	ATP	I	502	31/31	0.85	0.18	177,240,301,313	0
12	ATP	H	502	31/31	0.93	0.25	129,147,198,226	0
12	ATP	B	502	31/31	0.93	0.22	100,117,145,151	0
12	ATP	A	502	31/31	0.95	0.16	106,119,162,181	0
11	CA	H	501	1/1	0.98	0.25	144,144,144,144	0
11	CA	A	501	1/1	0.98	0.23	87,87,87,87	0
11	CA	B	501	1/1	0.99	0.27	116,116,116,116	0

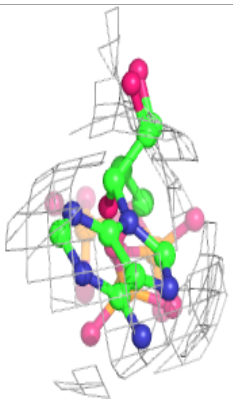
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

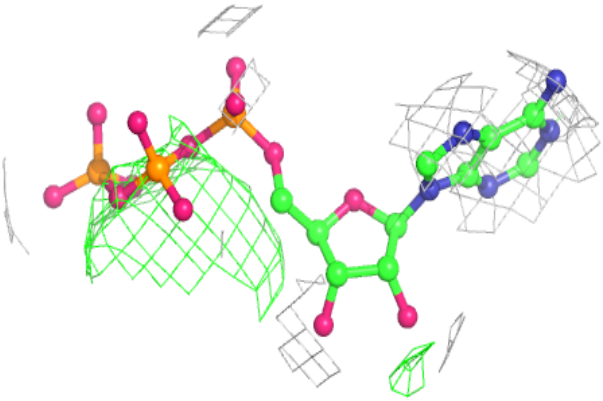


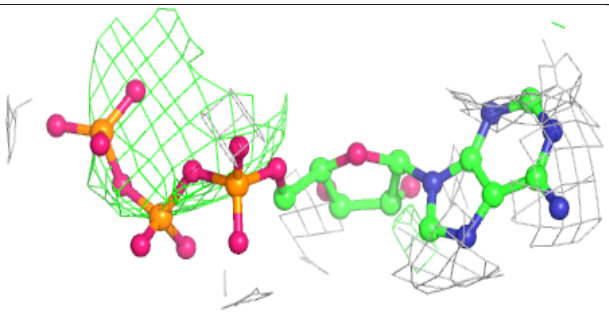


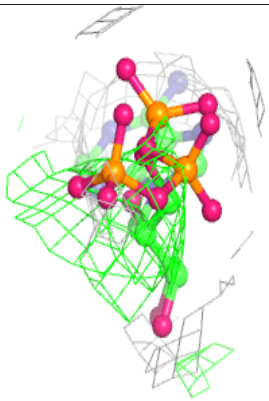


Electron density around ATP H 502:

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

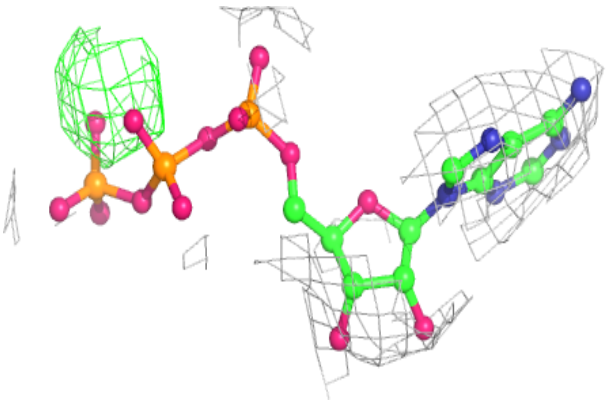


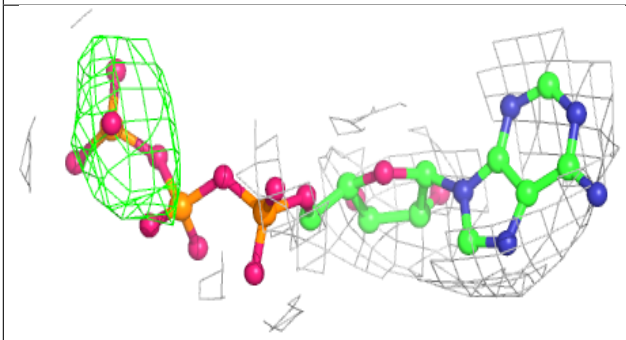


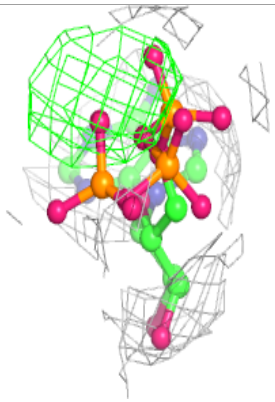


Electron density around ATP B 502:

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

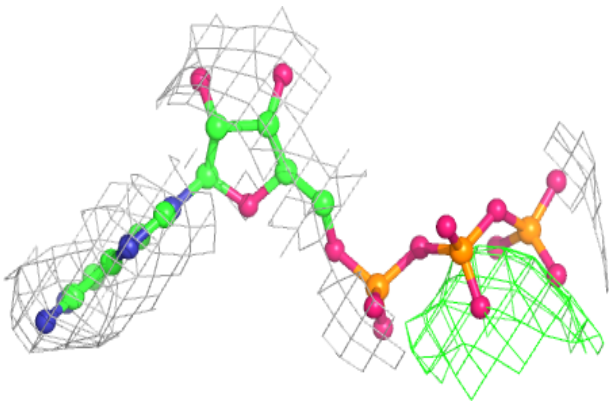


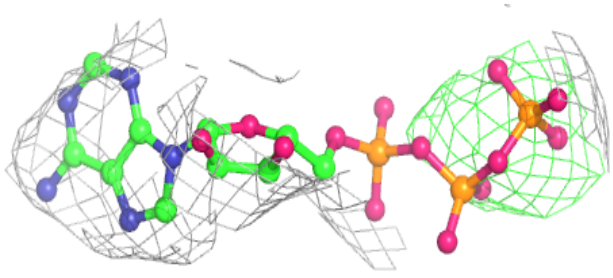


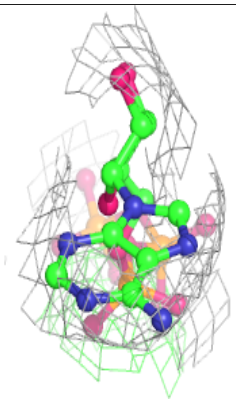


Electron density around ATP A 502:

$2mF_o$-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.