wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 09:57 PM JST

PDB ID	:	6JWS
Title	:	Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with Pteroate
Authors	:	Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on	:	2019-04-21
Resolution	:	2.30 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:

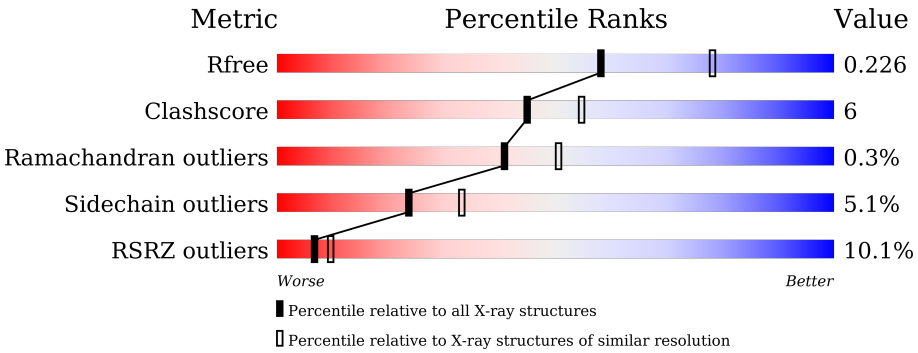
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	728	9% 65% 10% · 24%
1	B	728	7% 67% 12% · 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10011 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihyd ropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4545	2927	749	846	23			
1	B	589	Total	C	N	O	S	0	0	0
			4857	3128	800	903	26			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	UNP Q25704
A	714	VAL	-	expression tag	UNP Q25704
A	715	ASP	-	expression tag	UNP Q25704
A	716	LYS	-	expression tag	UNP Q25704
A	717	LEU	-	expression tag	UNP Q25704
A	718	ALA	-	expression tag	UNP Q25704
A	719	ALA	-	expression tag	UNP Q25704
A	720	ALA	-	expression tag	UNP Q25704
A	721	LEU	-	expression tag	UNP Q25704
A	722	GLU	-	expression tag	UNP Q25704
A	723	HIS	-	expression tag	UNP Q25704
A	724	HIS	-	expression tag	UNP Q25704
A	725	HIS	-	expression tag	UNP Q25704
A	726	HIS	-	expression tag	UNP Q25704
A	727	HIS	-	expression tag	UNP Q25704
A	728	HIS	-	expression tag	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704

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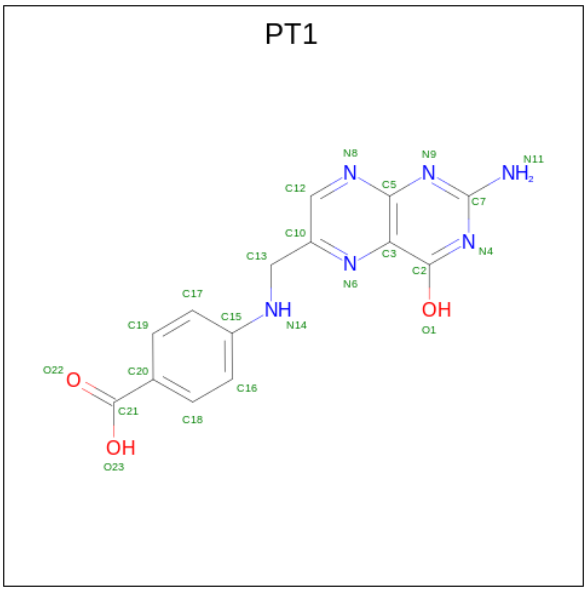
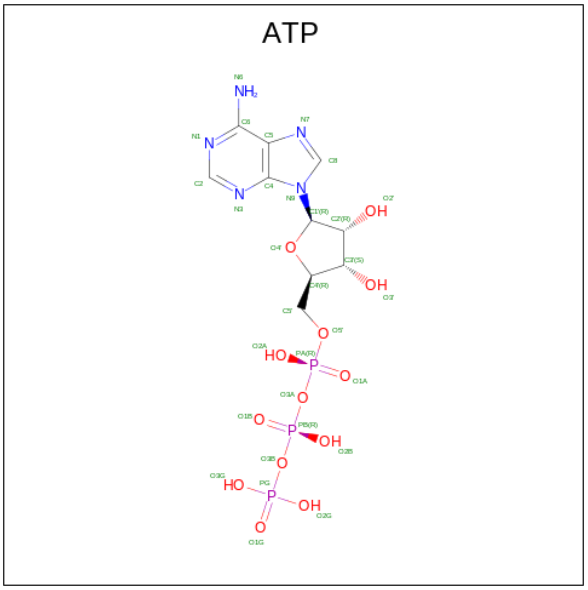
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	UNP Q25704
B	716	LYS	-	expression tag	UNP Q25704
B	717	LEU	-	expression tag	UNP Q25704
B	718	ALA	-	expression tag	UNP Q25704
B	719	ALA	-	expression tag	UNP Q25704
B	720	ALA	-	expression tag	UNP Q25704
B	721	LEU	-	expression tag	UNP Q25704
B	722	GLU	-	expression tag	UNP Q25704
B	723	HIS	-	expression tag	UNP Q25704
B	724	HIS	-	expression tag	UNP Q25704
B	725	HIS	-	expression tag	UNP Q25704
B	726	HIS	-	expression tag	UNP Q25704
B	727	HIS	-	expression tag	UNP Q25704
B	728	HIS	-	expression tag	UNP Q25704

- Molecule 2 is PTEROIC ACID (three-letter code: PT1) (formula: $C_{14}H_{12}N_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	14	6	3		
2	B	1	Total	C	N	O	0	0
			23	14	6	3		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		

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

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

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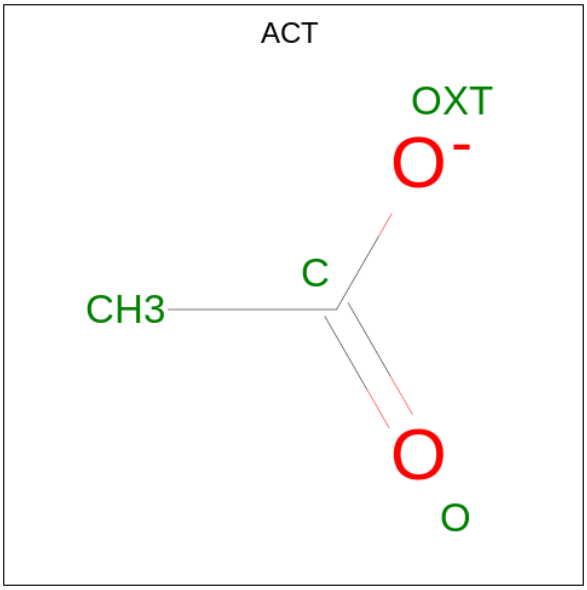
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

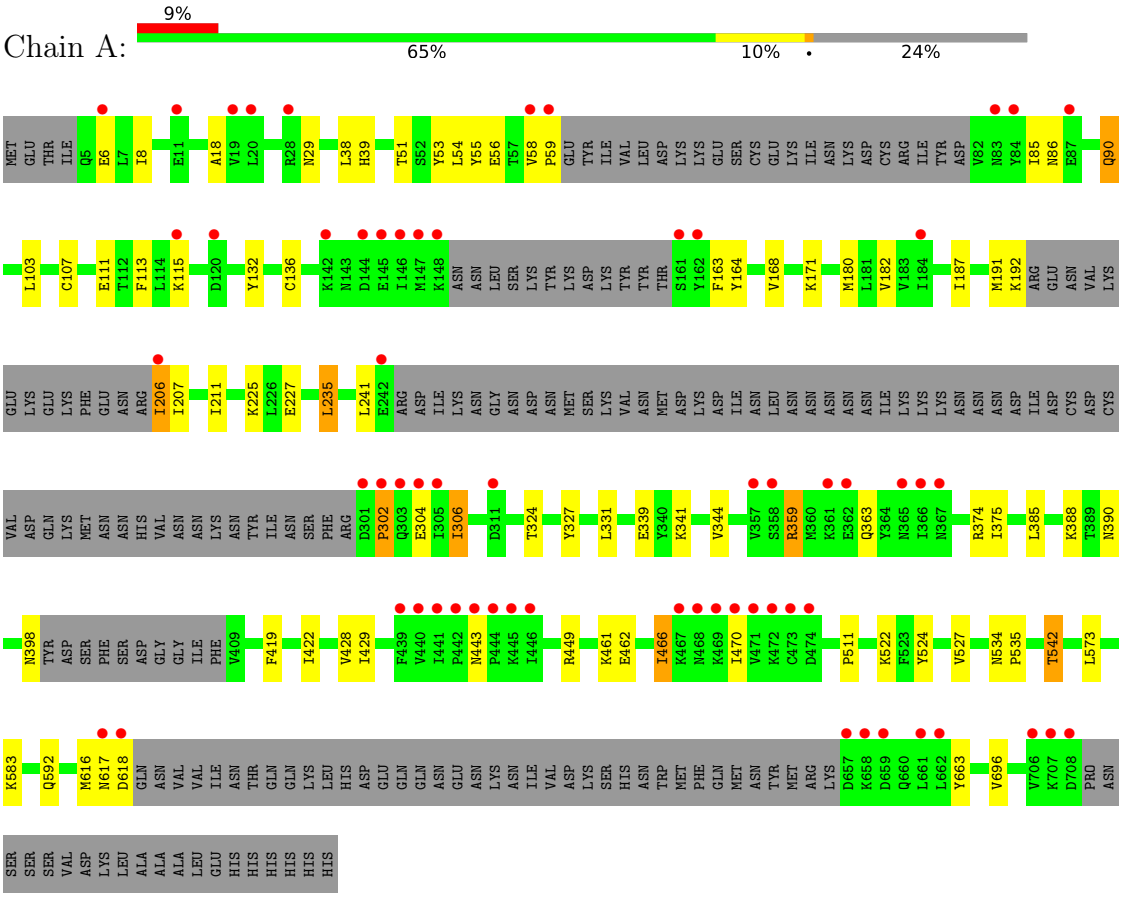
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	230	Total O 230 230	0	0
7	B	250	Total O 250 250	0	0

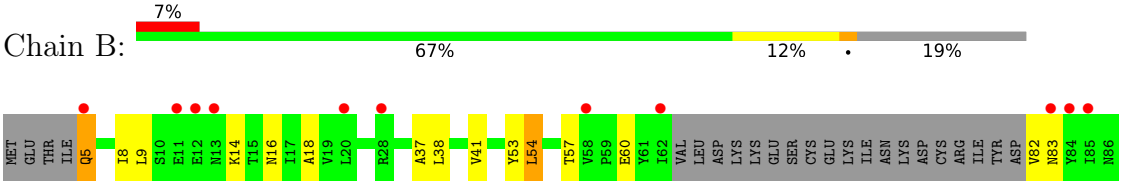
3 Residue-property plots (i)

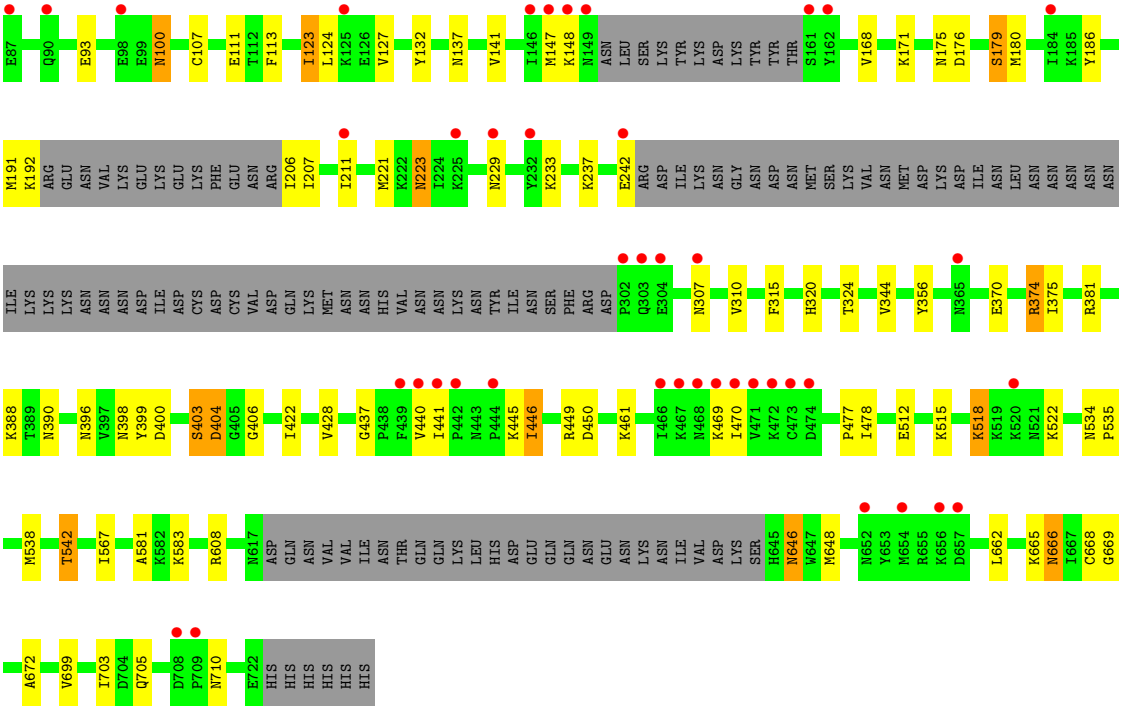
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase



• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase




E87 Q90 E93 E98 E99 N100 C107 E111 T112 F113 I123 L124 K125 E126 V127 Y132 N137 V141 I146 M147 K148 N149 ASN LEU SER LYS TYR LYS ASP LYS TYR TYR THR S161 Y162 V168 K171 N175 D176 S179 M180 I184 K185 Y186
M191 K192 ARG GLU ASN VAL LYS GLU LYS GLU LYS PHE GLU ASN ARG I206 I207 I211 M221 K222 N223 I224 K226 N229 Y232 K233 K237 E242 ARG ASP ILE LYS ASN GLY ASN ASP ASN MET SER LYS VAL ASN MET ASP LYS ASP ILE ASN LEU ASN ASN ASN ASN
ILE LYS LYS LYS ASN ASN ASN ASP ILE ASP CYS ASP CYS VAL ASP GLN LYS MET ASN ASN HIS VAL ASN ASN LYS ASN TYR ILE ASN SER PHE ARG ASP P302 Q303 E304 N307 V310 F315 H320 T324 V344 Y356 N365 E370 R374 I375 R381
K388 T389 N390 N396 V397 N398 Y399 D400 S403 D404 G405 G406 I422 V428 G437 P438 F439 V440 I441 P442 N443 P444 K445 I446 R449 D450 K461 I466 K467 N468 K469 I470 V471 K472 C473 D474 P477 I478 E512 K515 K518 K519 K520 N521 K522 N534 P535
M538 T542 I567 A581 K582 K583 R608 N617 ASP GLN ASN VAL VAL ILE ASN THR GLN GLN LYS LEU HIS ASP GLU GLN GLN ASN GLU ASN LYS ASN ILE VAL ASP LYS SER H645 N646 W647 M648 N652 Y653 M654 R655 K656 D657 L662 K665 N666 T667 C668 G669
A672 V699 I703 D704 Q705 D708 P709 M710 E722 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.91Å 136.76Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.30 29.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.58-2.30) 94.0 (29.56-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.05 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.233 0.183 , 0.226	Depositor DCC
R_{free} test set	8123 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10011	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: MG, CA, ATP, ACT, PT1

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	0.34	0/4617	0.67	0/6229
1	B	0.33	0/4940	0.67	0/6665
All	All	0.33	0/9557	0.67	0/12894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4545	0	4650	54	0
1	B	4857	0	4943	76	0
2	A	23	0	10	0	0
2	B	23	0	10	0	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	6	0	0
7	A	230	0	0	5	0
7	B	250	0	0	6	0
All	All	10011	0	9649	124	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 6.

The worst 5 of 124 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)
1:B:107:CYS:SG	1:B:171:LYS:HE3	1.91	1.08
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.50	0.91
1:B:107:CYS:SG	1:B:171:LYS:CE	2.65	0.84
1:B:107:CYS:HG	1:B:171:LYS:HE3	1.45	0.78
1:B:648:MET:CE	1:B:668:CYS:SG	2.72	0.78

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	537/728 (74%)	517 (96%)	19 (4%)	1 (0%)	47 58
1	B	577/728 (79%)	559 (97%)	16 (3%)	2 (0%)	41 50
All	All	1114/1456 (76%)	1076 (97%)	35 (3%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	470	ILE

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Mol	Chain	Res	Type
1	B	404	ASP
1	A	466	ILE

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	525/696 (75%)	501 (95%)	24 (5%)	27	38
1	B	558/696 (80%)	527 (94%)	31 (6%)	21	29
All	All	1083/1392 (78%)	1028 (95%)	55 (5%)	24	33

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	GLU
1	B	223	ASN
1	B	710	ASN
1	B	522	LYS
1	B	123	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	B	229	ASN
1	B	223	ASN
1	B	240	HIS
1	A	308	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	ACT	A	805	-	3,3,3	1.11	0	3,3,3	0.65	0
2	PT1	A	801	-	24,25,25	1.46	3 (12%)	31,35,35	1.98	9 (29%)
6	ACT	A	806	-	3,3,3	1.02	0	3,3,3	0.82	0
3	ATP	A	802	4	26,33,33	0.66	0	31,52,52	0.79	0
3	ATP	B	802	4	26,33,33	0.65	0	31,52,52	0.80	0
6	ACT	B	805	-	3,3,3	1.10	0	3,3,3	0.68	0
6	ACT	B	806	-	3,3,3	1.15	0	3,3,3	0.75	0
2	PT1	B	801	-	24,25,25	1.66	5 (20%)	31,35,35	2.39	7 (22%)

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	PT1	B	801	-	-	1/9/9/9	0/3/3/3
3	ATP	A	802	4	-	8/18/38/38	0/3/3/3
3	ATP	B	802	4	-	7/18/38/38	0/3/3/3
2	PT1	A	801	-	-	3/9/9/9	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PT1	C3-C5	3.76	1.47	1.40
2	B	801	PT1	C3-C5	3.73	1.47	1.40
2	A	801	PT1	C10-N6	3.49	1.38	1.32
2	B	801	PT1	C17-C15	2.68	1.43	1.39
2	B	801	PT1	C7-N11	2.39	1.38	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	PT1	N8-C5-N9	6.99	123.80	115.82
2	B	801	PT1	C7-N9-C5	6.03	122.24	115.36
2	B	801	PT1	N9-C7-N4	-4.94	120.64	127.22
2	B	801	PT1	C12-N8-C5	4.76	121.47	116.69
2	A	801	PT1	C7-N9-C5	4.67	120.69	115.36

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	ATP	C5'-O5'-PA-O1A
3	A	802	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	C3'-C4'-C5'-O5'
3	B	802	ATP	PB-O3B-PG-O2G
3	B	802	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

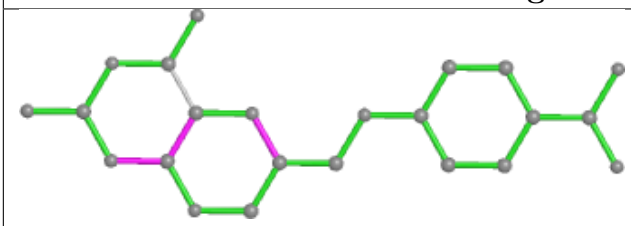
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ATP	1	0
3	B	802	ATP	1	0

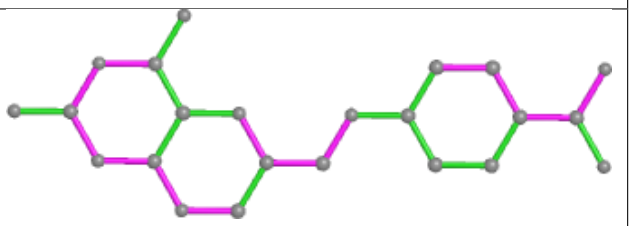
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

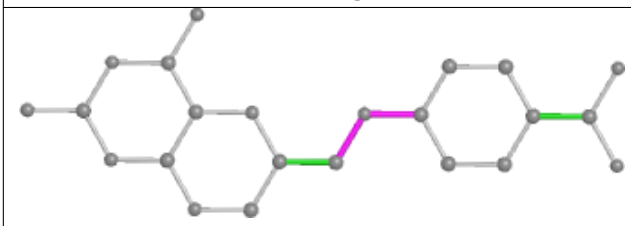
Ligand PT1 A 801



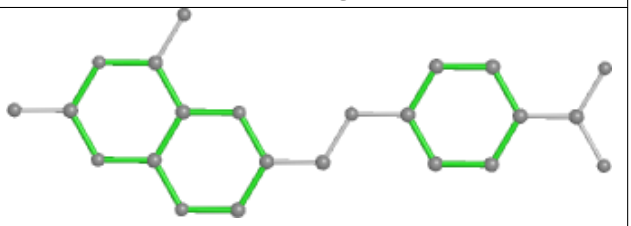
Bond lengths



Bond angles

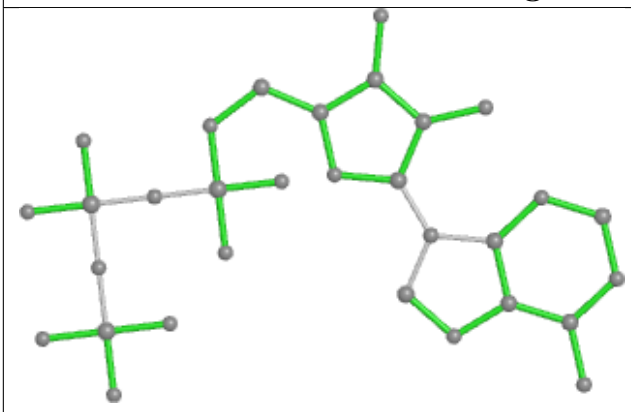


Torsions

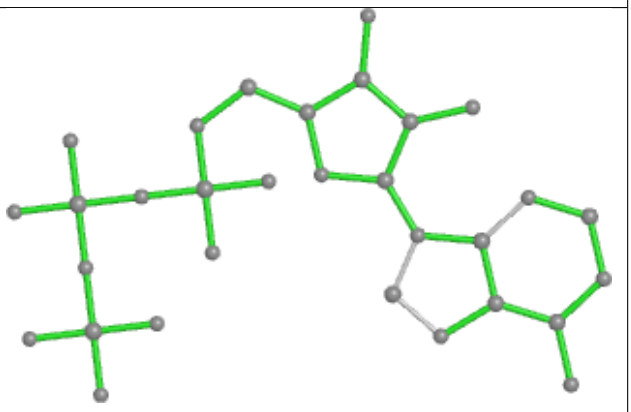


Rings

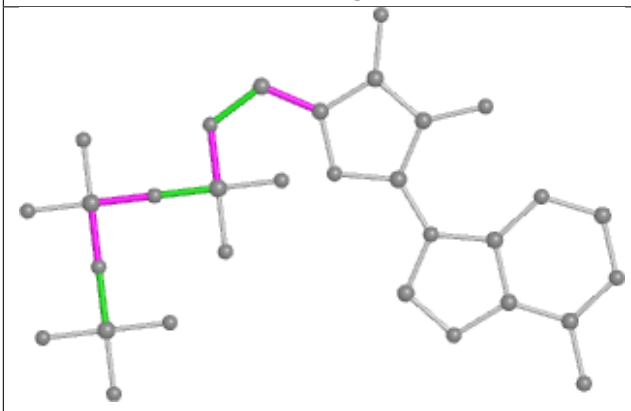
Ligand ATP A 802



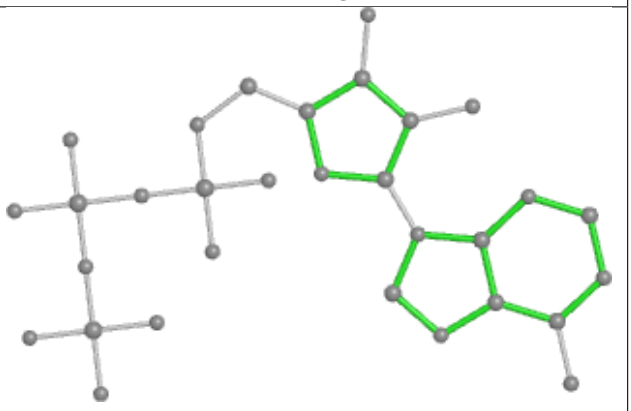
Bond lengths



Bond angles

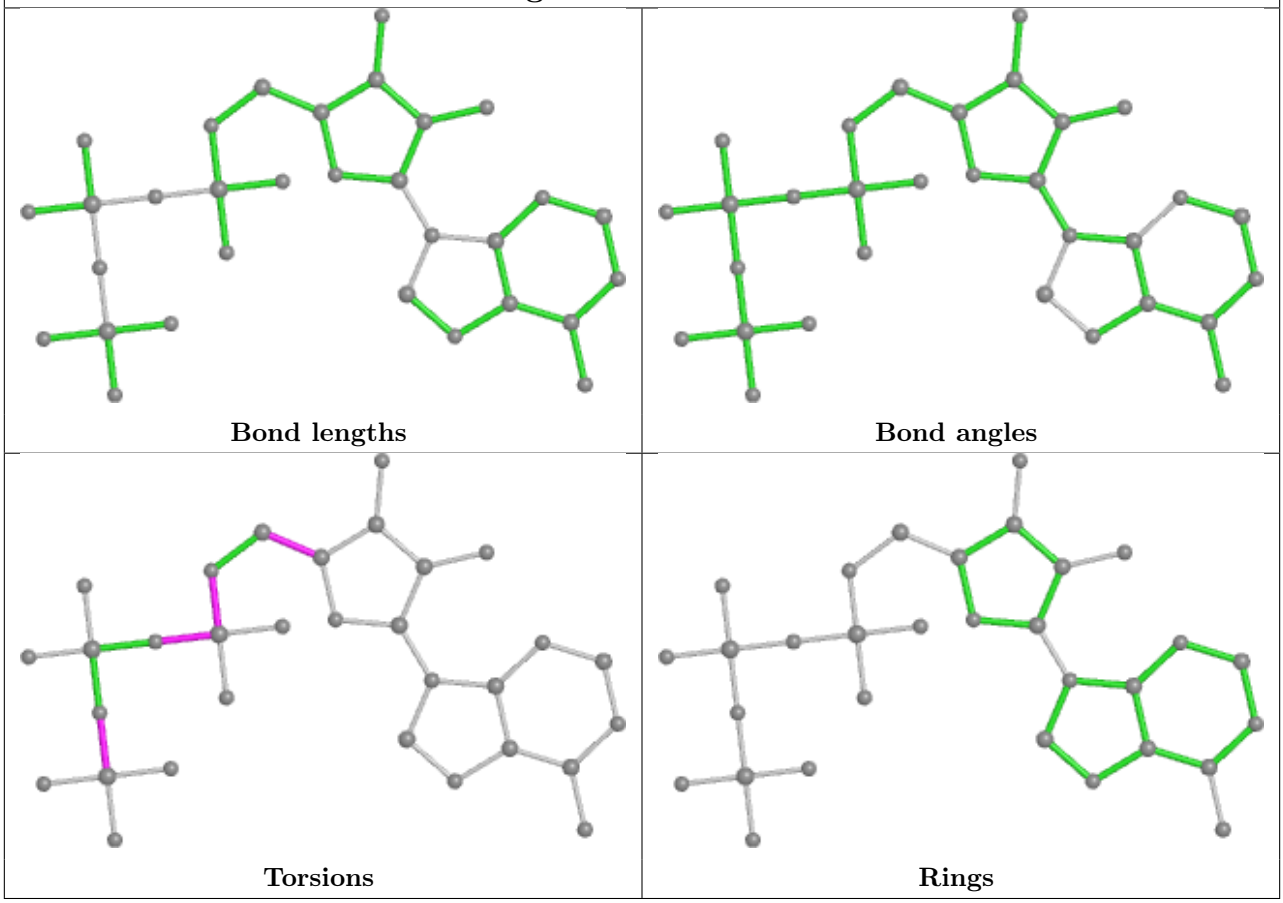


Torsions

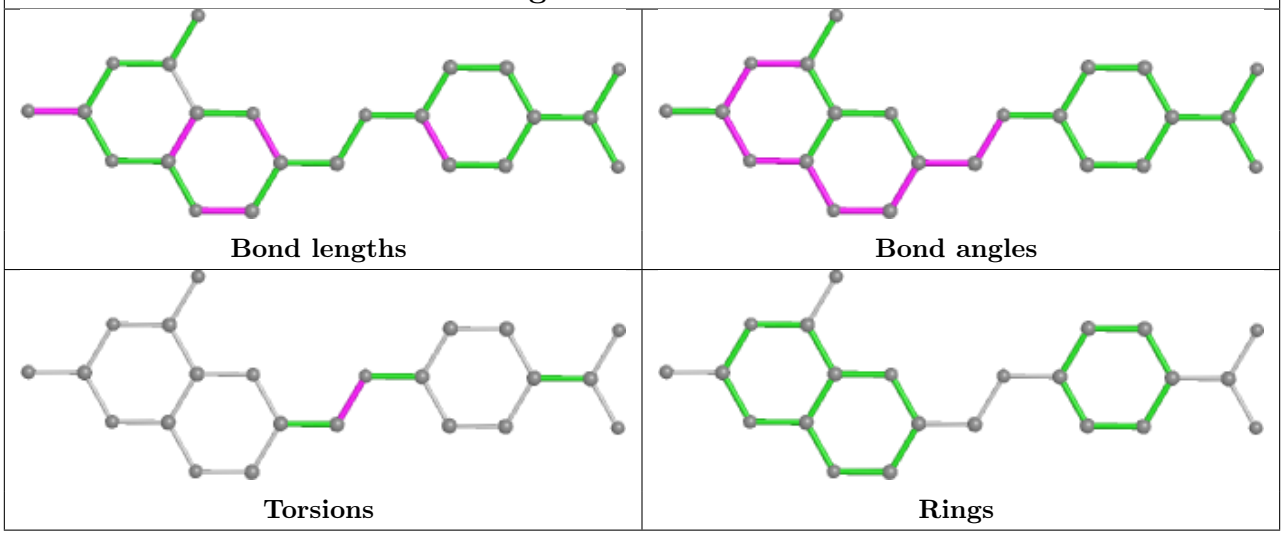


Rings

Ligand ATP B 802



Ligand PT1 B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	551/728 (75%)	0.28	62 (11%) 5 7	8, 26, 99, 120	0
1	B	589/728 (80%)	0.25	53 (8%) 9 12	7, 30, 97, 120	0
All	All	1140/1456 (78%)	0.27	115 (10%) 7 9	7, 28, 99, 120	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	ILE	14.8
1	A	471	VAL	11.3
1	B	473	CYS	10.8
1	A	147	MET	9.3
1	A	441	ILE	8.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

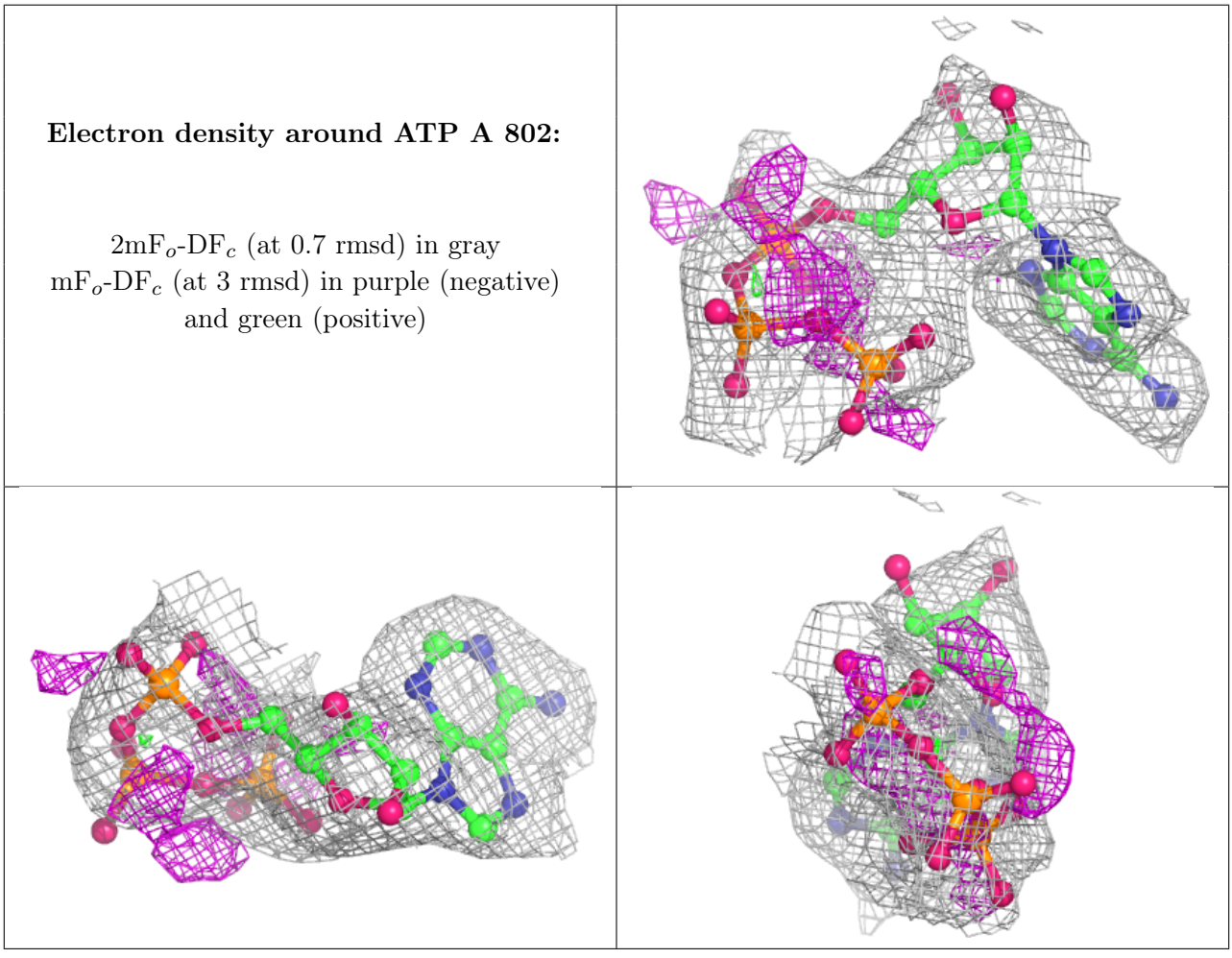
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ATP	A	802	31/31	0.82	0.20	25,66,106,112	0
3	ATP	B	802	31/31	0.88	0.15	25,55,88,96	0
6	ACT	B	806	4/4	0.89	0.17	28,34,36,39	0
4	MG	B	803	1/1	0.95	0.14	25,25,25,25	0
5	CA	A	804	1/1	0.95	0.11	24,24,24,24	0
6	ACT	A	806	4/4	0.95	0.15	30,33,34,44	0
4	MG	A	803	1/1	0.95	0.10	21,21,21,21	0
4	MG	B	807	1/1	0.97	0.06	12,12,12,12	0
2	PT1	A	801	23/23	0.97	0.12	9,10,12,15	0
6	ACT	A	805	4/4	0.98	0.10	18,20,21,23	0
2	PT1	B	801	23/23	0.98	0.11	8,9,11,12	0
5	CA	B	804	1/1	0.98	0.04	35,35,35,35	0
6	ACT	B	805	4/4	0.99	0.13	13,14,14,14	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.

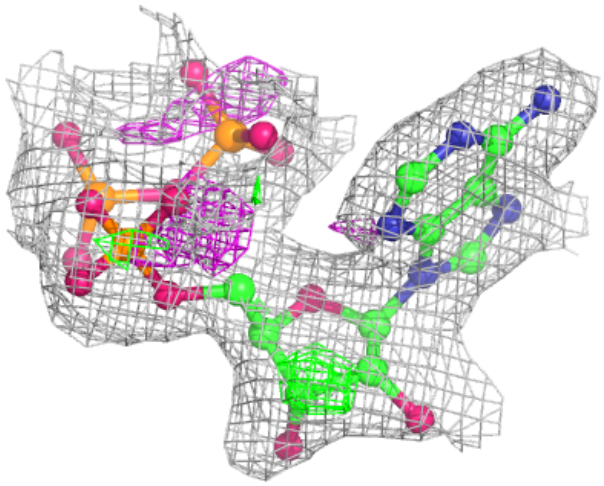
Electron density around ATP A 802:

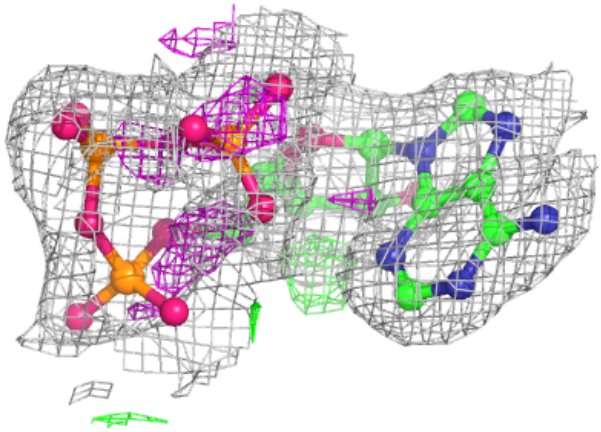
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

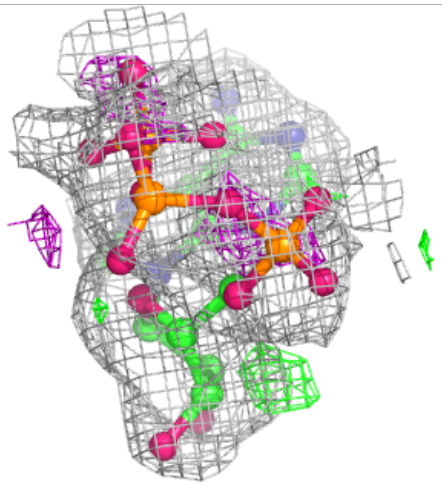


Electron density around ATP B 802:

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

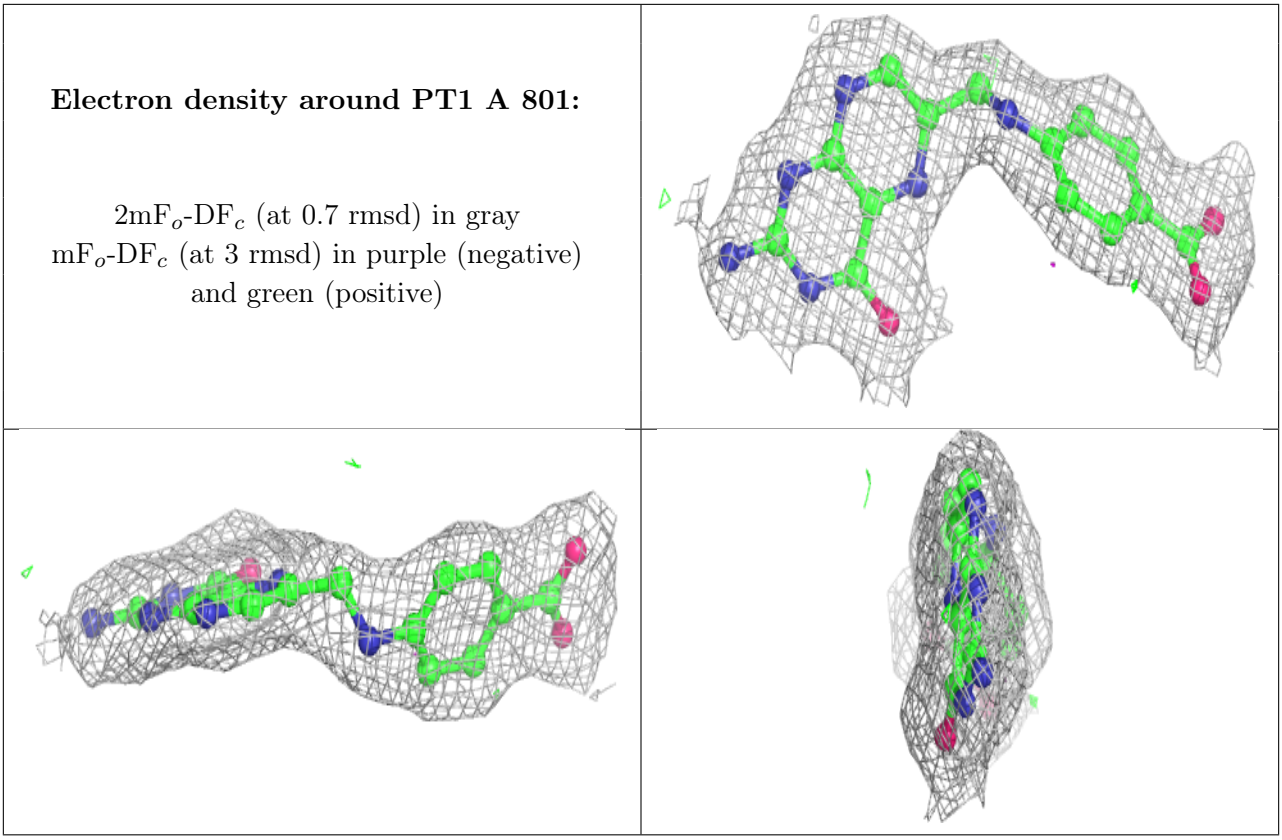






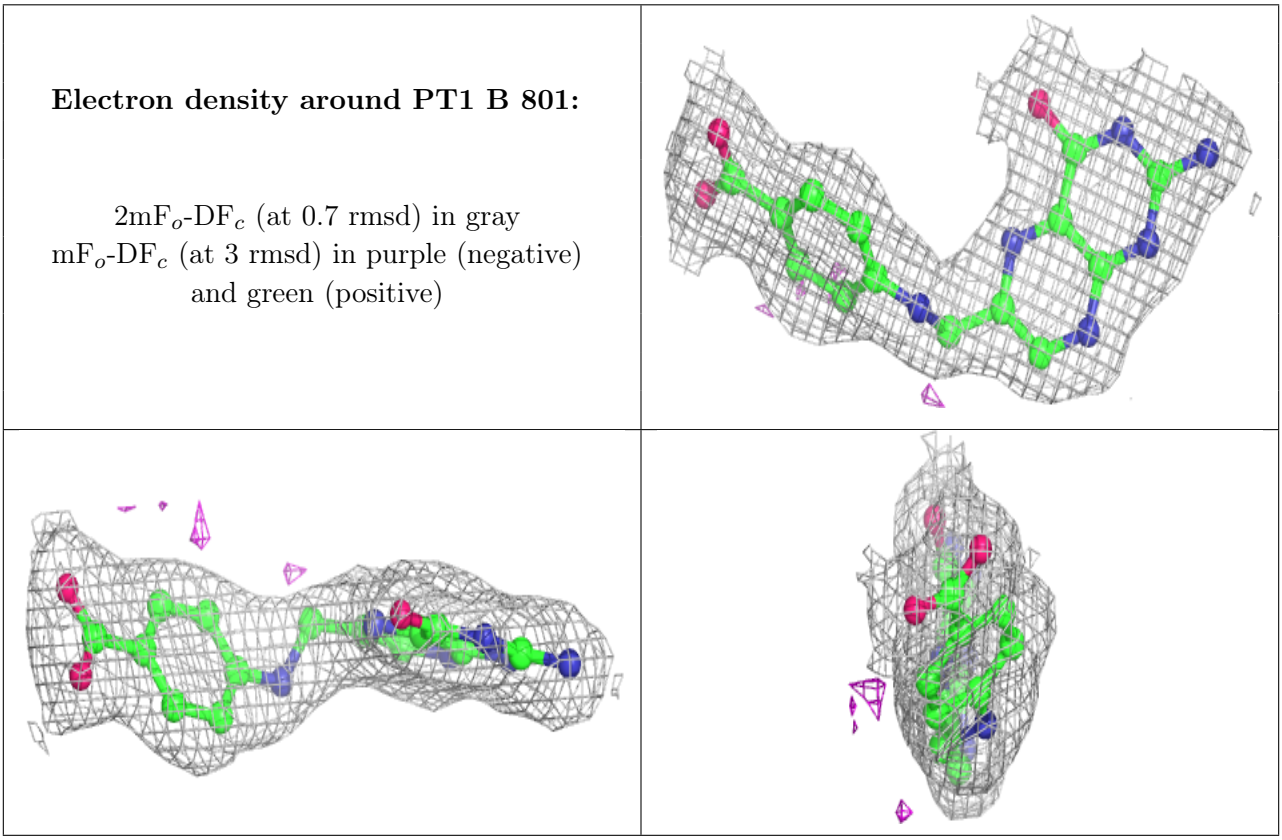
Electron density around PT1 A 801:

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



Electron density around PT1 B 801:

$2mF_o$-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.