



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:02 AM BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

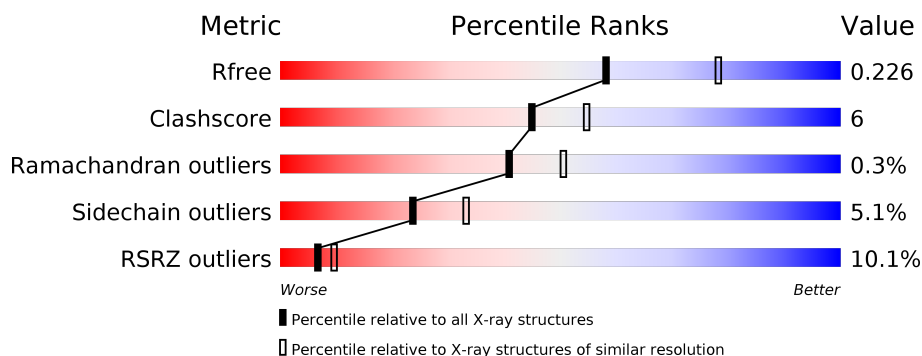
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>9%</div> <div>65%</div> <div>10%</div> <div>24%</div> </div>
1	B	728	<div> <div>7%</div> <div>67%</div> <div>12%</div> <div>19%</div> </div>

2 Entry composition

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-dihydropteroate 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:

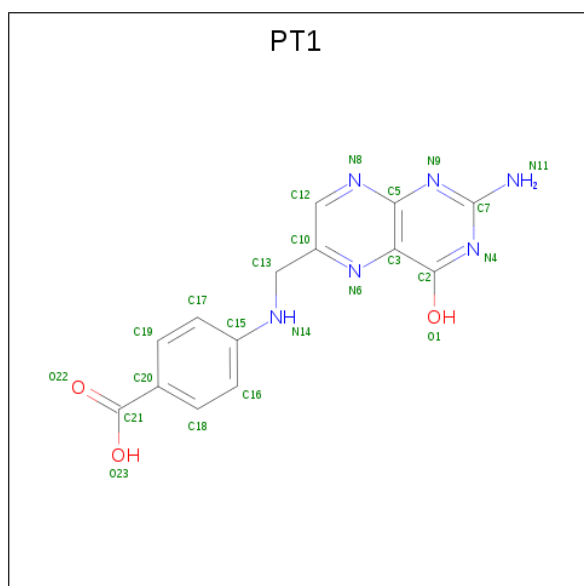
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression 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

Continued on next page...

Continued from previous page...

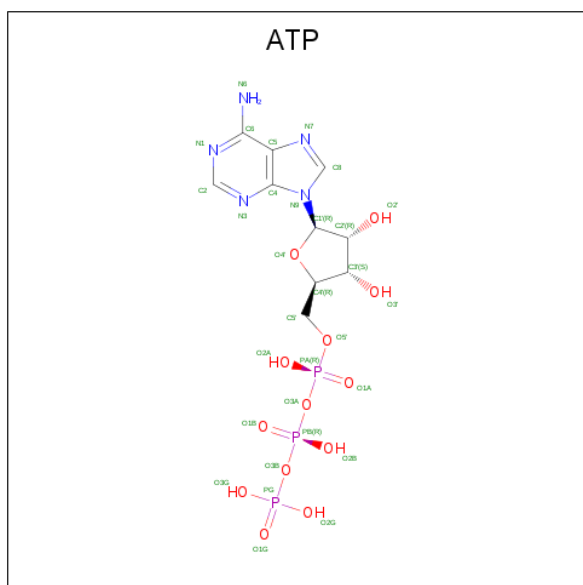
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	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: C₁₄H₁₂N₆O₃).



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	B	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		

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

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

Continued on next page...

Continued from previous page...

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

- 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	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

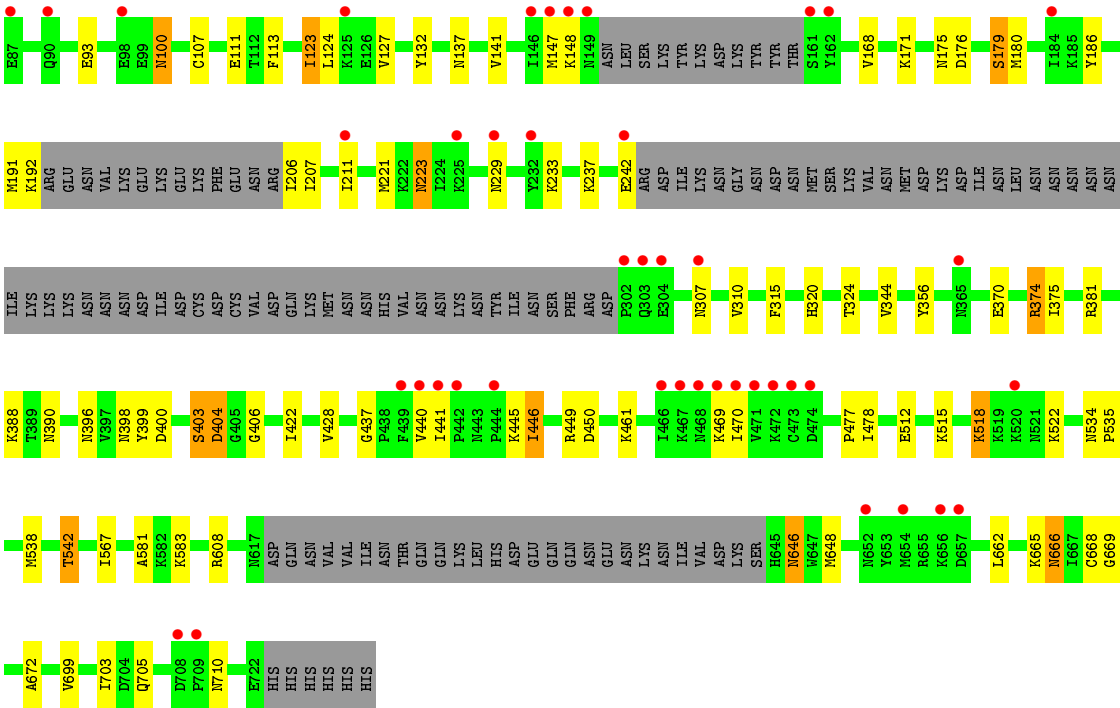
- Molecule 7 is water.

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

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.

- [illegible]

- Chain B:
-
- | Amino Acid | Category | Percentage |
|------------|----------|------------|
| NET | Grey | 19% |
| GLU | Grey | |
| THR | Grey | |
| ILE | Grey | |
| Q5 | Red | |
| I8 | Green | |
| L9 | Green | |
| S10 | Green | |
| E11 | Green | |
| E12 | Green | |
| N13 | Green | |
| K14 | Green | |
| T15 | Green | |
| N16 | Green | |
| I17 | Green | |
| A18 | Green | |
| V19 | Green | |
| L20 | Green | |
| R28 | Green | |
| A37 | Green | |
| L38 | Green | |
| V41 | Green | |
| Y53 | Green | |
| L54 | Yellow | |
| T57 | Green | |
| V58 | Green | |
| F59 | Green | |
| E60 | Green | |
| Y61 | Green | |
| I62 | Green | |
| VAL | Yellow | |
| LEU | Yellow | |
| ASP | Yellow | |
| LYS | Yellow | |
| LYS | Yellow | |
| GLU | Yellow | |
| SER | Yellow | |
| CYS | Yellow | |
| GLU | Yellow | |
| LYS | Yellow | |
| ILE | Yellow | |
| ASN | Yellow | |
| LYS | Yellow | |
| ASP | Yellow | |
| CYS | Yellow | |
| ARG | Yellow | |
| ILE | Yellow | |
| TYR | Yellow | |
| ASP | Yellow | |
| V82 | Green | |
| N83 | Green | |
| Y84 | Green | |
| I85 | Green | |
| I86 | Green | |



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PT1, MG, CA, ATP, ACT

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

Continued on next page...

Continued from previous page...

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.

All (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
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.69	0.75
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.53	0.74
1:B:5:GLN:N	7:B:901:HOH:O	2.23	0.70
1:A:51:THR:HG22	1:A:168:VAL:HG12	1.74	0.70
1:A:235:LEU:HB3	1:A:241:LEU:HD11	1.74	0.69
1:B:53:TYR:CG	1:B:374:ARG:HD2	2.27	0.69
1:B:518:LYS:HD3	1:B:567:ILE:HD13	1.72	0.69
1:B:53:TYR:CD2	1:B:374:ARG:HD2	2.28	0.68
1:B:422:ILE:CD1	1:B:477:PRO:HG3	2.24	0.67
1:B:648:MET:HE3	1:B:668:CYS:SG	2.35	0.67
1:B:176:ASP:OD1	1:B:179:SER:OG	2.11	0.67
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.24	0.66
1:B:404:ASP:HB3	1:B:406:GLY:H	1.60	0.66
1:B:18:ALA:CB	1:B:180:MET:HE1	2.26	0.65
1:B:648:MET:HE1	1:B:668:CYS:SG	2.35	0.65
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.78	0.64
7:A:1093:HOH:O	1:B:665:LYS:HD3	1.98	0.63
1:A:663:TYR:CE2	1:B:646:ASN:HB2	2.33	0.62
1:B:307:ASN:O	1:B:310:VAL:HG22	2.00	0.62
1:B:404:ASP:CB	1:B:406:GLY:H	2.13	0.61
1:B:608:ARG:HA	1:B:666:ASN:ND2	2.16	0.60
1:A:359:ARG:O	1:A:363:GLN:HB2	2.02	0.59
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.32	0.59
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.33	0.58
1:B:512:GLU:OE1	1:B:515:LYS:HE3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:TYR:CD2	1:B:646:ASN:OD1	2.58	0.57
1:B:461:LYS:NZ	7:B:908:HOH:O	2.38	0.56
1:A:29:ASN:ND2	7:A:901:HOH:O	2.23	0.56
1:A:206:ILE:HG22	1:A:207:ILE:HG22	1.88	0.56
1:A:374:ARG:NH1	1:A:374:ARG:HG3	2.21	0.55
1:A:616:MET:HE2	1:B:699:VAL:HG23	1.88	0.55
1:A:663:TYR:HE2	1:B:646:ASN:HB2	1.70	0.55
1:A:90:GLN:HE21	1:A:90:GLN:HA	1.72	0.54
1:A:39:HIS:HD2	7:A:1119:HOH:O	1.91	0.54
1:B:175:ASN:ND2	1:B:237:LYS:HE2	2.23	0.54
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.89	0.53
1:A:86:ASN:O	1:A:90:GLN:HG2	2.08	0.53
1:B:18:ALA:HB1	1:B:180:MET:HE1	1.90	0.53
1:B:18:ALA:HB2	1:B:180:MET:HE1	1.90	0.53
1:B:437:GLY:O	1:B:440:VAL:HG22	2.09	0.53
1:A:55:TYR:OH	1:A:374:ARG:NH1	2.42	0.53
1:B:132:TYR:CE2	1:B:344:VAL:HG11	2.43	0.53
1:A:54:LEU:HB3	1:A:375:ILE:HB	1.89	0.53
1:B:705:GLN:HG3	1:B:705:GLN:O	2.10	0.52
1:B:127:VAL:HG13	7:B:935:HOH:O	2.10	0.51
1:A:103:LEU:HD11	1:A:511:PRO:O	2.10	0.51
1:A:527:VAL:HG22	1:A:573:LEU:HD12	1.93	0.50
1:B:666:ASN:C	1:B:666:ASN:HD22	2.15	0.50
1:A:38:LEU:HD21	1:A:168:VAL:HG11	1.93	0.50
1:B:388:LYS:HD3	1:B:390:ASN:OD1	2.11	0.50
1:B:180:MET:HE2	1:B:211:ILE:HD13	1.93	0.49
1:A:302:PRO:O	1:A:306:ILE:HD12	2.12	0.49
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.78	0.49
1:A:522:LYS:HD3	1:A:524:TYR:CZ	2.47	0.49
1:A:663:TYR:HD2	1:B:646:ASN:OD1	1.95	0.49
1:A:388:LYS:HE3	1:A:390:ASN:OD1	2.12	0.48
1:A:53:TYR:CG	1:A:374:ARG:HD3	2.47	0.48
1:A:187:ILE:HG22	1:A:191:MET:CE	2.43	0.48
1:A:132:TYR:CZ	1:A:136:CYS:SG	3.06	0.48
1:B:705:GLN:HG3	7:B:970:HOH:O	2.13	0.48
1:A:180:MET:HE3	1:A:211:ILE:HG12	1.95	0.47
1:B:399:TYR:O	1:B:403:SER:HB2	2.14	0.47
1:B:422:ILE:HD11	1:B:477:PRO:HG3	1.95	0.47
1:B:608:ARG:HA	1:B:666:ASN:HD21	1.78	0.47
1:B:512:GLU:OE1	1:B:515:LYS:CE	2.62	0.47
1:A:56:GLU:HG3	1:A:164:TYR:CE1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:O	1:A:618:ASP:HB3	2.15	0.47
1:B:446:ILE:HD12	1:B:450:ASP:HB2	1.97	0.47
1:A:182:VAL:HG12	1:A:235:LEU:HD13	1.97	0.46
1:A:374:ARG:HD2	1:A:385:LEU:HD22	1.96	0.46
1:B:8:ILE:HG22	1:B:9:LEU:HG	1.96	0.46
1:B:137:ASN:O	1:B:141:VAL:HG13	2.15	0.46
1:A:466:ILE:O	1:A:466:ILE:HG22	2.16	0.45
1:A:39:HIS:HE1	7:A:1106:HOH:O	2.00	0.45
1:A:107:CYS:O	1:A:111:GLU:HG2	2.17	0.45
1:B:518:LYS:HD3	1:B:567:ILE:CD1	2.43	0.45
1:A:419:PHE:HA	1:A:422:ILE:HD12	1.99	0.44
1:B:223:ASN:HA	1:B:223:ASN:HD22	1.47	0.44
1:B:100:ASN:HD22	1:B:100:ASN:N	2.14	0.44
1:B:422:ILE:HG12	1:B:477:PRO:HG3	1.98	0.44
1:A:113:PHE:O	1:A:115:LYS:O	2.35	0.44
1:B:428:VAL:HG22	1:B:478:ILE:HB	2.00	0.44
1:A:327:TYR:CE2	1:A:331:LEU:HD22	2.53	0.44
1:A:191:MET:HE3	1:A:207:ILE:HG12	1.99	0.44
1:B:14:LYS:NZ	7:B:916:HOH:O	2.50	0.44
1:B:113:PHE:HB2	7:B:975:HOH:O	2.18	0.43
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.90	0.43
1:B:396:ASN:ND2	1:B:399:TYR:HB2	2.33	0.43
1:B:221:MET:O	1:B:315:PHE:HB2	2.19	0.43
1:B:542:THR:HG21	1:B:583:LYS:HE2	2.00	0.43
1:B:93:GLU:OE1	1:B:186:TYR:OH	2.26	0.43
1:A:191:MET:HE3	1:A:207:ILE:HG21	2.01	0.43
1:B:14:LYS:HD3	1:B:16:ASN:HD21	1.83	0.42
1:B:60:GLU:OE1	1:B:356:TYR:OH	2.36	0.42
1:A:534:ASN:CB	1:A:535:PRO:CD	2.93	0.42
1:A:592:GLN:HG2	1:B:703:ILE:O	2.20	0.42
1:B:191:MET:HE3	1:B:207:ILE:HG21	2.01	0.42
1:B:404:ASP:HB3	1:B:406:GLY:N	2.32	0.42
1:A:171:LYS:NZ	7:A:903:HOH:O	2.34	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.90	0.41
1:B:82:VAL:HG13	1:B:83:ASN:N	2.35	0.41
1:B:123:ILE:HG13	1:B:124:LEU:N	2.35	0.41
1:B:229:ASN:HD21	1:B:233:LYS:HE3	1.85	0.41
1:B:441:ILE:HG13	1:B:441:ILE:H	1.69	0.41
1:B:538:MET:O	1:B:581:ALA:HA	2.20	0.41
1:B:669:GLY:O	1:B:672:ALA:HB3	2.21	0.41
1:B:320:HIS:HE2	3:B:802:ATP:PG	2.43	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HB3	1:B:375:ILE:HB	2.03	0.41
1:A:59:PRO:HG3	1:A:163:PHE:CD1	2.55	0.41
1:A:696:VAL:HA	1:B:672:ALA:HB2	2.01	0.41
1:A:59:PRO:HG3	1:A:163:PHE:HD1	1.86	0.41
1:B:38:LEU:CD2	1:B:168:VAL:HG11	2.51	0.41
3:A:802:ATP:H5'2	3:A:802:ATP:PG	2.61	0.41
1:B:82:VAL:HG22	1:B:83:ASN:H	1.85	0.41
1:B:37:ALA:O	1:B:41:VAL:HG23	2.21	0.41
1:B:648:MET:HB2	1:B:648:MET:HE2	1.81	0.41
1:B:422:ILE:CG1	1:B:477:PRO:HG3	2.51	0.40
1:A:180:MET:HE3	1:A:211:ILE:CD1	2.52	0.40
1:A:428:VAL:O	1:A:429:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
1	B	404	ASP
1	A	466	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	8	ILE
1	A	85	ILE
1	A	90	GLN
1	A	192	LYS
1	A	206	ILE
1	A	225	LYS
1	A	227	GLU
1	A	235	LEU
1	A	302	PRO
1	A	304	GLU
1	A	306	ILE
1	A	324	THR
1	A	339	GLU
1	A	341	LYS
1	A	344	VAL
1	A	359	ARG
1	A	398	ASN
1	A	443	ASN
1	A	449	ARG
1	A	461	LYS
1	A	462	GLU
1	A	470	ILE
1	A	542	THR
1	B	5	GLN
1	B	54	LEU
1	B	57	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	100	ASN
1	B	111	GLU
1	B	123	ILE
1	B	147	MET
1	B	148	LYS
1	B	179	SER
1	B	192	LYS
1	B	206	ILE
1	B	223	ASN
1	B	242	GLU
1	B	324	THR
1	B	370	GLU
1	B	374	ARG
1	B	381	ARG
1	B	398	ASN
1	B	400	ASP
1	B	403	SER
1	B	445	LYS
1	B	446	ILE
1	B	449	ARG
1	B	469	LYS
1	B	518	LYS
1	B	522	LYS
1	B	542	THR
1	B	646	ASN
1	B	662	LEU
1	B	666	ASN
1	B	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	39	HIS
1	A	83	ASN
1	A	90	GLN
1	A	116	ASN
1	A	165	ASN
1	A	308	ASN
1	A	363	GLN
1	A	617	ASN
1	B	5	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	21	ASN
1	B	83	ASN
1	B	100	ASN
1	B	137	ASN
1	B	165	ASN
1	B	175	ASN
1	B	223	ASN
1	B	229	ASN
1	B	240	HIS
1	B	363	GLN
1	B	617	ASN
1	B	646	ASN
1	B	666	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	$\# Z > 2$
2	PT1	B	801	-	22,25,25	1.87	6 (27%)	28,35,35	2.48	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	805	-	1,3,3	4.66	1 (100%)	0,3,3	0.00	-
2	PT1	A	801	-	22,25,25	1.50	3 (13%)	28,35,35	2.00	8 (28%)
6	ACT	A	806	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
6	ACT	B	806	-	1,3,3	5.38	1 (100%)	0,3,3	0.00	-
6	ACT	B	805	-	1,3,3	3.72	1 (100%)	0,3,3	0.00	-
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

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	A	801	-	-	3/5/9/9	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	B	801	-	-	1/5/9/9	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	806	ACT	CH3-C	5.38	1.55	1.48
6	A	805	ACT	CH3-C	4.66	1.54	1.48
2	B	801	PT1	C20-C21	4.39	1.51	1.47
2	A	801	PT1	C3-C5	3.76	1.47	1.40
2	B	801	PT1	C3-C5	3.73	1.47	1.40
6	B	805	ACT	CH3-C	3.72	1.53	1.48
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
6	A	806	ACT	CH3-C	2.31	1.51	1.48
2	B	801	PT1	C12-N8	2.29	1.35	1.31
2	B	801	PT1	C10-N6	2.21	1.36	1.32
2	A	801	PT1	C5-N9	-2.11	1.32	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PT1	N8-C5-N9	6.99	123.80	115.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	A	801	PT1	N8-C5-N9	4.35	120.78	115.82
2	A	801	PT1	C12-N8-C5	3.77	120.48	116.69
2	A	801	PT1	N9-C7-N4	-3.33	122.79	127.22
2	A	801	PT1	C10-C13-N14	-2.50	107.55	113.07
2	A	801	PT1	C13-C10-N6	2.42	120.95	116.66
2	B	801	PT1	C10-C12-N8	-2.28	120.89	123.13
2	A	801	PT1	C7-N4-C2	2.23	122.05	116.43
2	A	801	PT1	C16-C18-C20	-2.20	117.97	121.13
2	B	801	PT1	C7-N4-C2	2.18	121.94	116.43
2	B	801	PT1	C10-C13-N14	-2.10	108.44	113.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

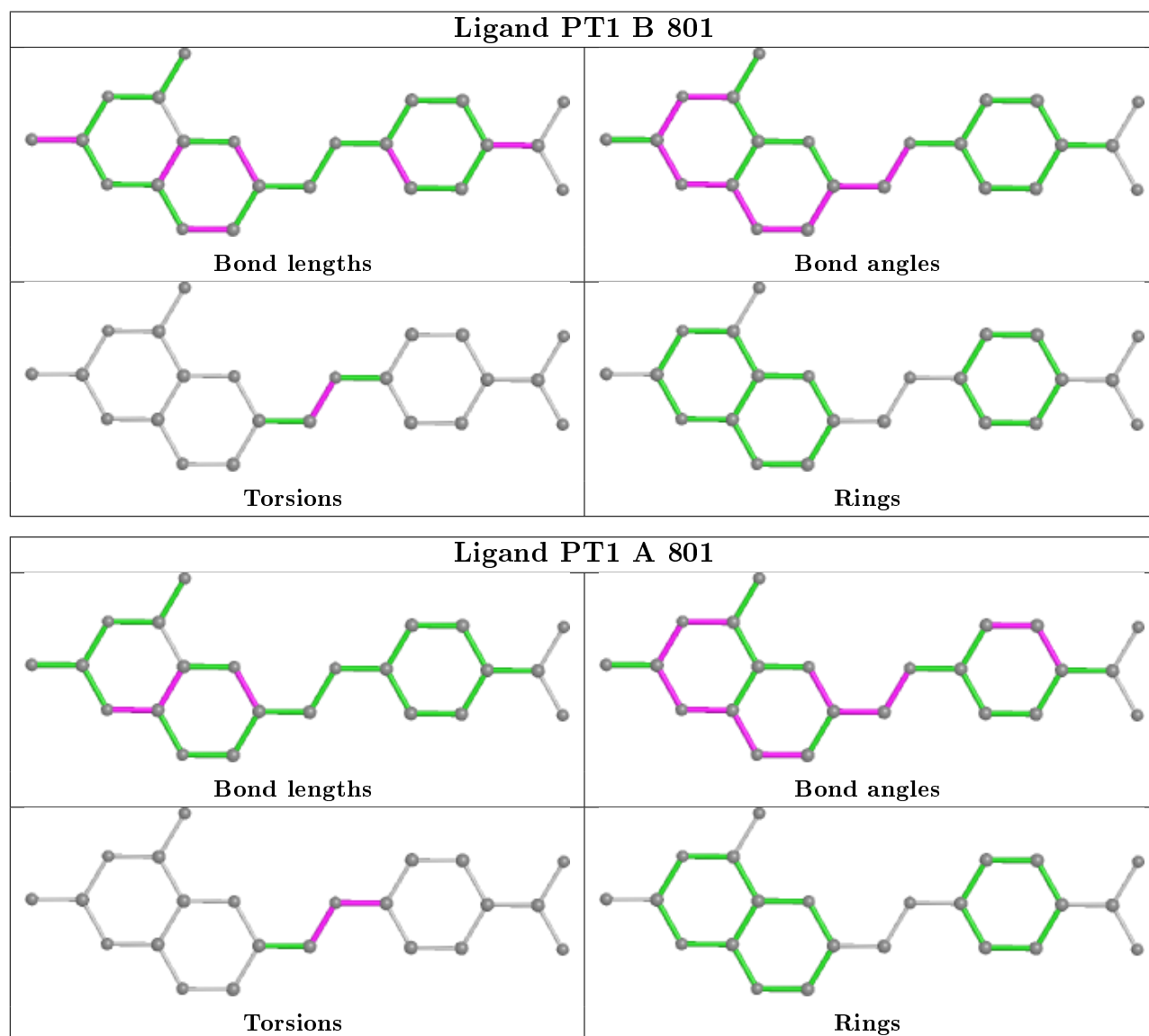
Mol	Chain	Res	Type	Atoms
3	A	802	ATP	C5'-O5'-PA-O1A
3	A	802	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	C3'-C4'-C5'-O5'
3	B	802	ATP	PB-O3B-PG-O2G
3	B	802	ATP	C5'-O5'-PA-O1A
3	B	802	ATP	O4'-C4'-C5'-O5'
3	B	802	ATP	C3'-C4'-C5'-O5'
3	A	802	ATP	O4'-C4'-C5'-O5'
3	B	802	ATP	PB-O3A-PA-O5'
2	B	801	PT1	C10-C13-N14-C15
2	A	801	PT1	C10-C13-N14-C15
3	B	802	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	PG-O3B-PB-O2B
3	A	802	ATP	PA-O3A-PB-O1B
2	A	801	PT1	C16-C15-N14-C13
3	A	802	ATP	C5'-O5'-PA-O3A
3	B	802	ATP	C5'-O5'-PA-O3A
2	A	801	PT1	C17-C15-N14-C13
3	A	802	ATP	PA-O3A-PB-O3B

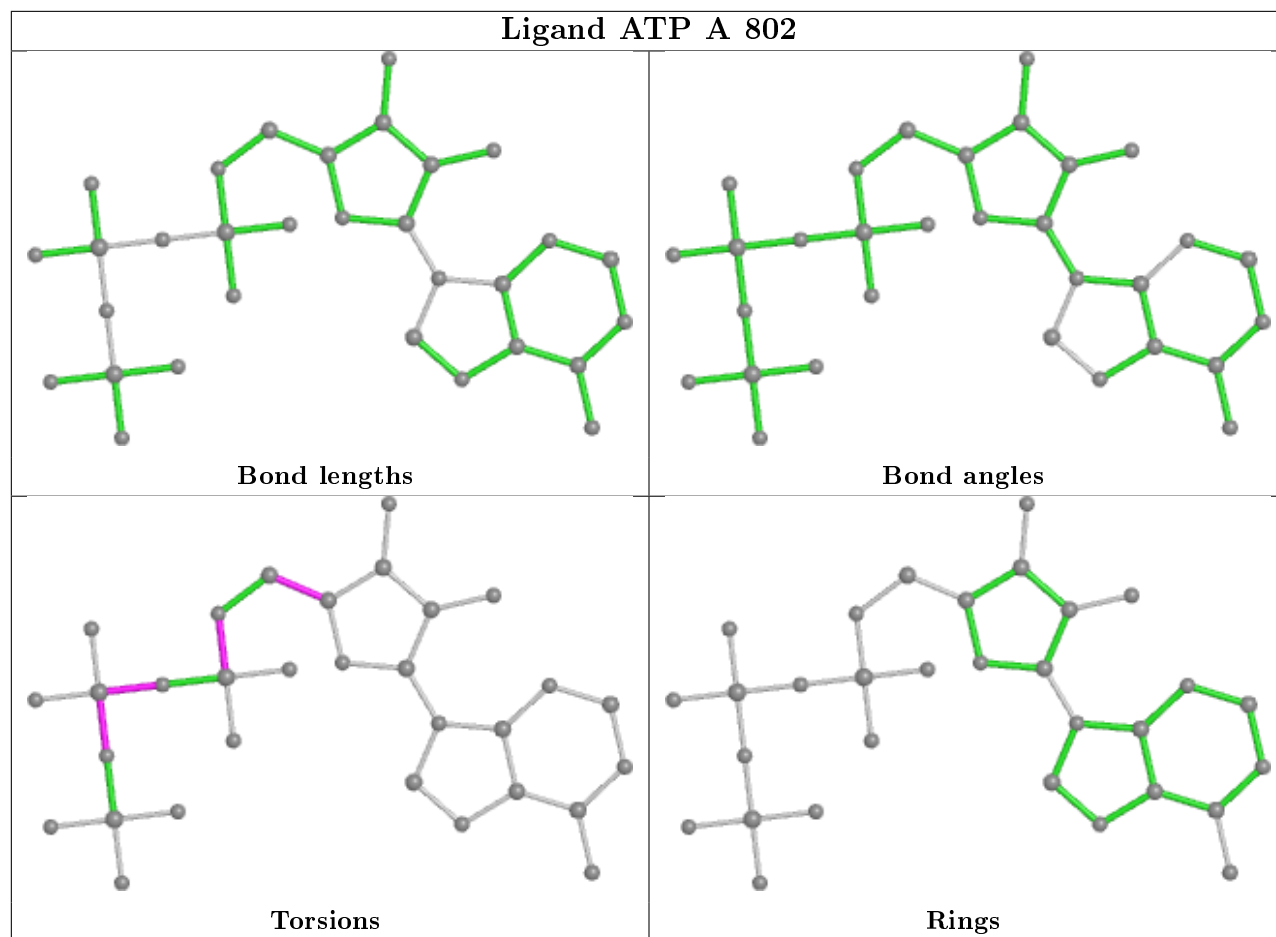
There are no ring outliers.

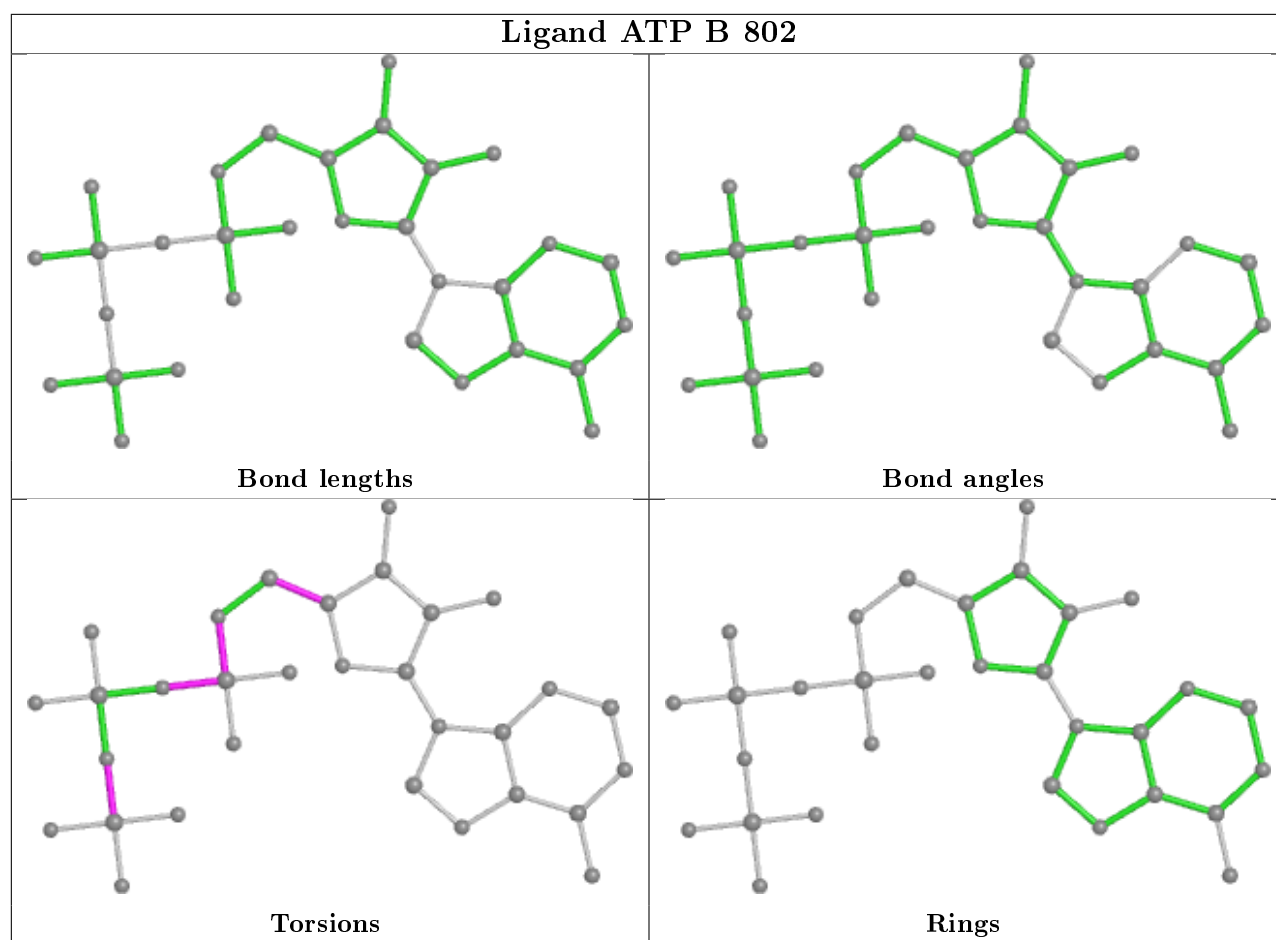
2 monomers are involved in 2 short contacts:

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

All (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
1	B	471	VAL	8.3
1	A	473	CYS	7.6
1	A	146	ILE	7.6
1	A	468	ASN	7.1
1	B	84	TYR	6.8
1	A	443	ASN	6.7
1	A	708	ASP	6.5
1	B	469	LYS	6.4
1	B	474	ASP	6.2
1	B	11	GLU	6.2
1	B	467	LYS	6.2
1	B	441	ILE	5.9
1	A	301	ASP	5.9
1	A	470	ILE	5.7
1	A	84	TYR	5.6
1	A	161	SER	5.4
1	A	657	ASP	5.1
1	A	442	PRO	5.0
1	B	472	LYS	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	707	LYS	4.7
1	A	618	ASP	4.3
1	A	439	PHE	4.2
1	A	367	ASN	4.2
1	A	302	PRO	4.1
1	B	442	PRO	4.0
1	B	87	GLU	4.0
1	A	303	GLN	3.8
1	B	58	VAL	3.8
1	A	365	ASN	3.7
1	B	444	PRO	3.7
1	A	148	LYS	3.7
1	B	468	ASN	3.6
1	A	145	GLU	3.6
1	A	469	LYS	3.6
1	A	162	TYR	3.6
1	A	706	VAL	3.6
1	A	472	LYS	3.5
1	A	658	LYS	3.5
1	A	361	LYS	3.5
1	B	656	LYS	3.5
1	A	445	LYS	3.5
1	B	147	MET	3.5
1	B	98	GLU	3.5
1	B	440	VAL	3.5
1	B	161	SER	3.4
1	A	11	GLU	3.4
1	A	444	PRO	3.4
1	B	709	PRO	3.3
1	B	439	PHE	3.3
1	B	146	ILE	3.3
1	B	90	GLN	3.2
1	A	58	VAL	3.2
1	A	617	ASN	3.2
1	A	87	GLU	3.1
1	B	83	ASN	3.1
1	B	652	ASN	3.1
1	A	446	ILE	3.1
1	A	366	ILE	3.0
1	A	28	ARG	3.0
1	B	148	LYS	3.0
1	A	661	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	83	ASN	2.9
1	B	304	GLU	2.9
1	B	62	ILE	2.9
1	A	474	ASP	2.9
1	B	302	PRO	2.9
1	A	440	VAL	2.9
1	A	206	ILE	2.8
1	B	466	ILE	2.8
1	A	659	ASP	2.8
1	A	467	LYS	2.8
1	A	59	PRO	2.8
1	B	303	GLN	2.8
1	B	162	TYR	2.7
1	B	13	ASN	2.7
1	A	242	GLU	2.6
1	A	362	GLU	2.6
1	A	311	ASP	2.6
1	B	225	LYS	2.5
1	A	20	LEU	2.5
1	A	144	ASP	2.5
1	B	85	ILE	2.5
1	B	184	ILE	2.5
1	B	654	MET	2.4
1	A	358	SER	2.4
1	A	305	ILE	2.4
1	B	307	ASN	2.4
1	B	5	GLN	2.4
1	A	142	LYS	2.4
1	A	357	VAL	2.4
1	A	19	VAL	2.3
1	A	304	GLU	2.3
1	B	149	ASN	2.3
1	A	184	ILE	2.3
1	B	28	ARG	2.2
1	B	211	ILE	2.2
1	B	242	GLU	2.2
1	B	708	ASP	2.2
1	B	232	TYR	2.2
1	B	520	LYS	2.1
1	A	6	GLU	2.1
1	A	120	ASP	2.1
1	B	20	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	657	ASP	2.1
1	B	12	GLU	2.1
1	A	115	LYS	2.1
1	B	125	LYS	2.0
1	A	662	LEU	2.0
1	B	229	ASN	2.0
1	B	365	ASN	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

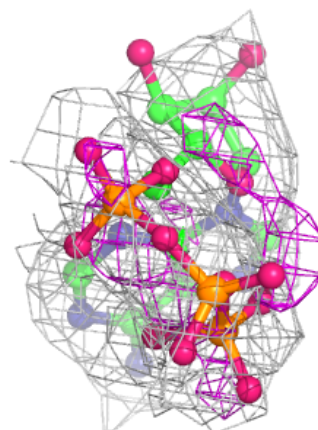
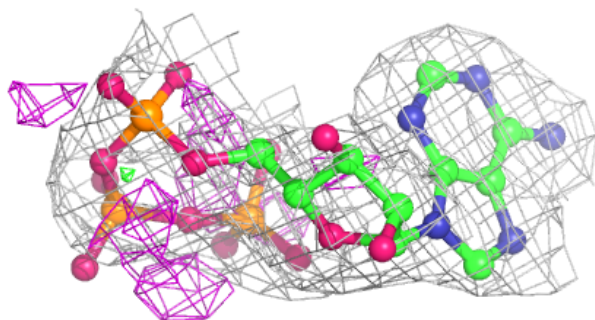
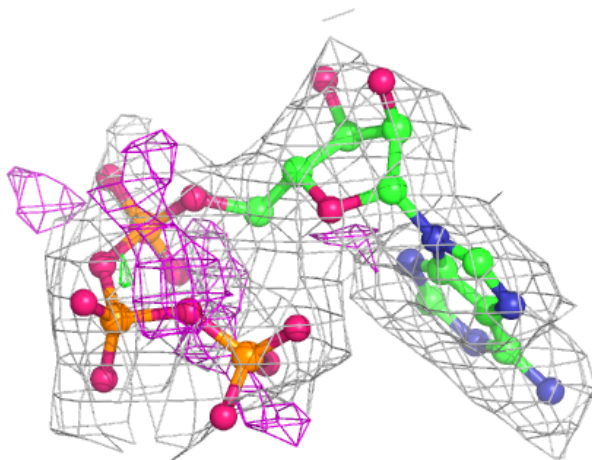
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ATP	A	802	31/31	0.82	0.20	25,66,106,112	0
3	ATP	B	802	31/31	0.88	0.15	25,55,88,96	0
6	ACT	B	806	4/4	0.89	0.17	28,34,36,39	0
4	MG	B	803	1/1	0.95	0.14	25,25,25,25	0
4	MG	A	803	1/1	0.95	0.10	21,21,21,21	0
6	ACT	A	806	4/4	0.95	0.15	30,33,34,44	0
5	CA	A	804	1/1	0.95	0.11	24,24,24,24	0
2	PT1	A	801	23/23	0.97	0.12	9,10,12,15	0
4	MG	B	807	1/1	0.97	0.06	12,12,12,12	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.

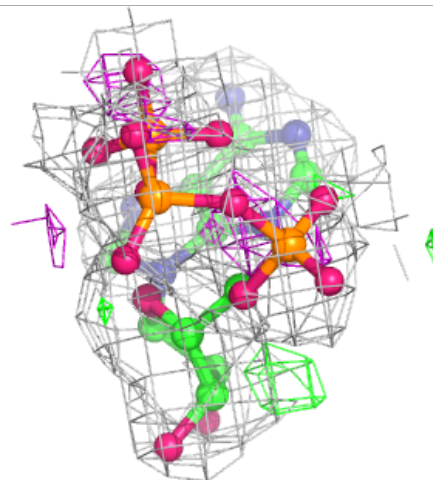
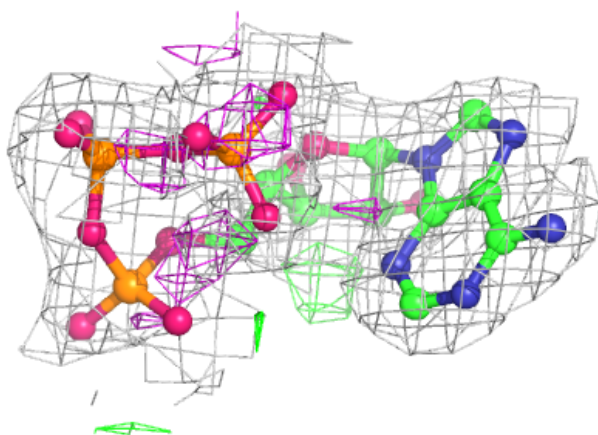
Electron density around ATP A 802:

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



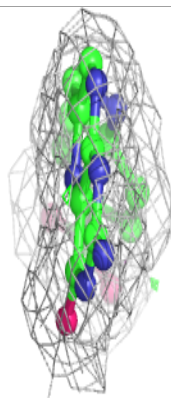
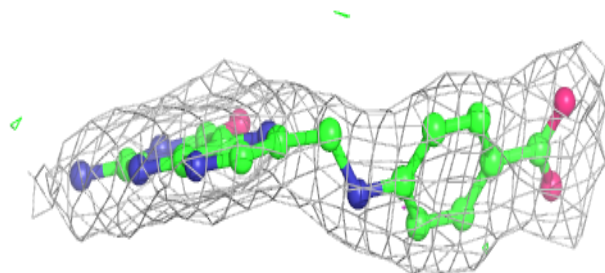
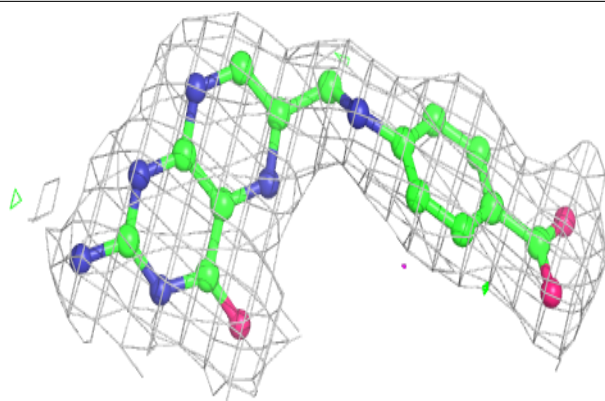
Electron density around ATP B 802:

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

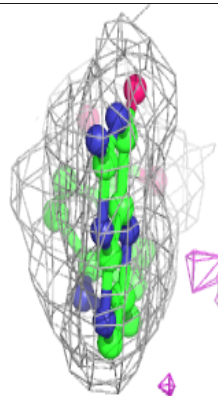
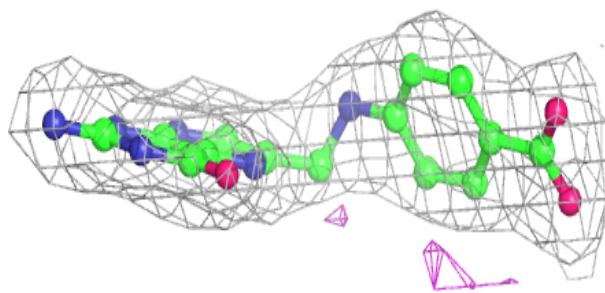
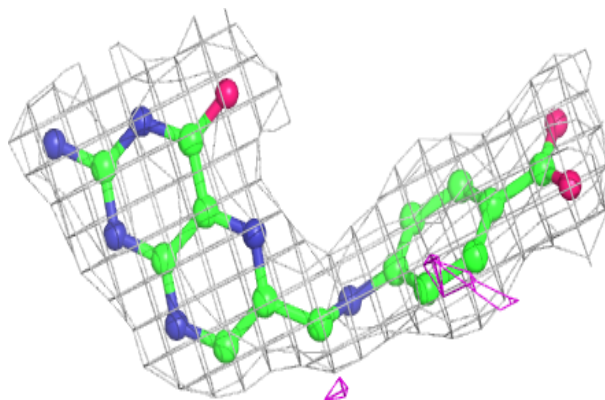


Electron density around PT1 A 801:

$2mF_o-DF_c$ (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.