



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:02 AM BST

PDB ID : 6KCM
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS
S436F/A437G/A613S with pterin and p-hydrobenzoate
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-06-28
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

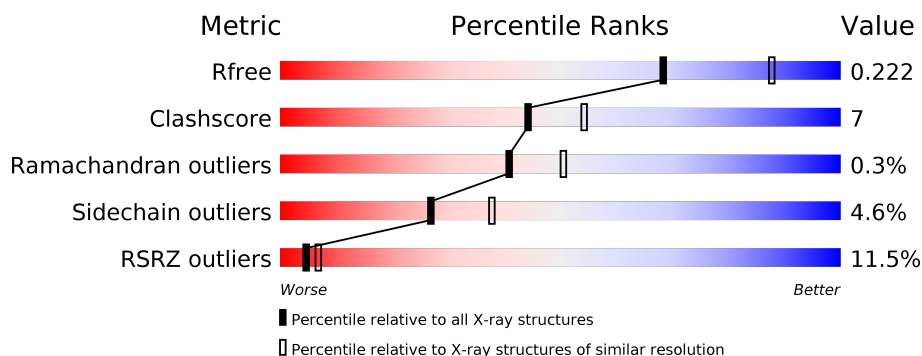
1 Overall quality at a glance

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>61%</div> <div>13%</div> <div>•</div> <div>25%</div> </div>
1	B	728	<div> <div>8%</div> <div>69%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PHB	A	802	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9766 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	543	Total	C	N	O	S	0	0	0
			4497	2894	746	834	23			
1	B	590	Total	C	N	O	S	0	0	0
			4880	3140	806	909	25			

There are 50 discrepancies between the modelled and reference sequences:

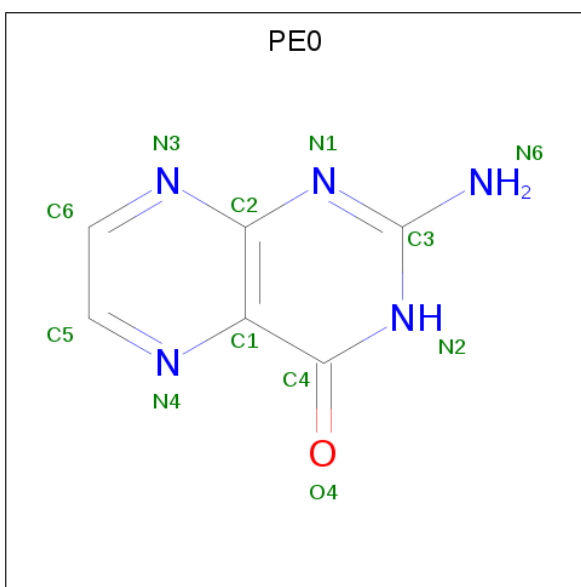
Chain	Residue	Modelled	Actual	Comment	Reference
A	436	PHE	SER	engineered mutation	UNP Q25704
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	613	SER	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	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

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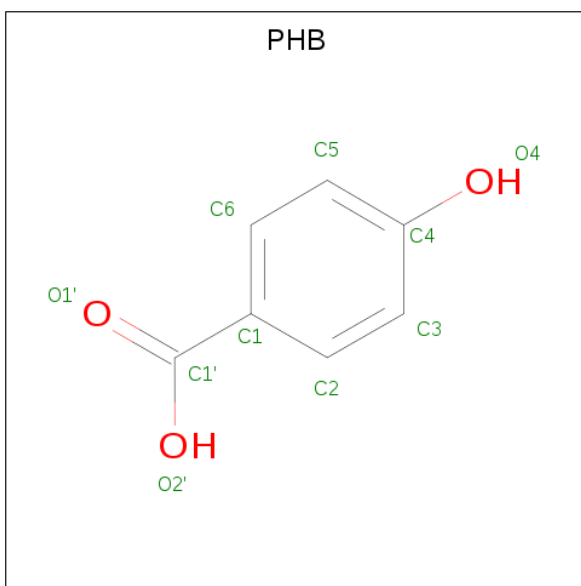
Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q25704
B	436	PHE	SER	engineered mutation	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704
B	613	SER	ALA	engineered mutation	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	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 PTERINE (three-letter code: PE0) (formula: C₆H₅N₅O) (labeled as "Ligand of Interest" by author).



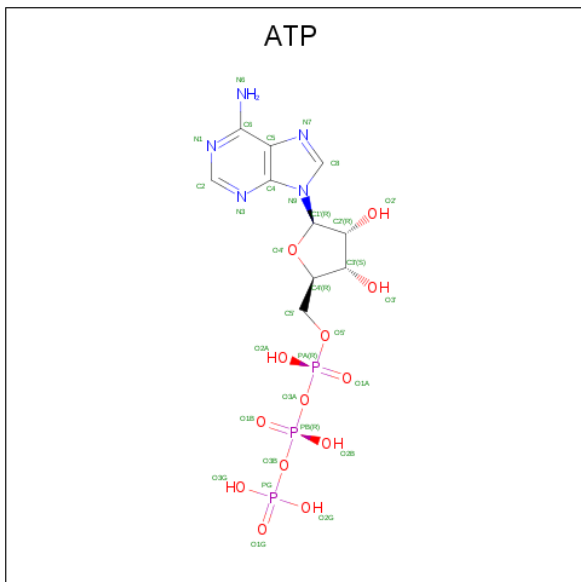
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	5	1		
2	B	1	Total	C	N	O	0	0
			12	6	5	1		

- Molecule 3 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula: $C_7H_6O_3$).



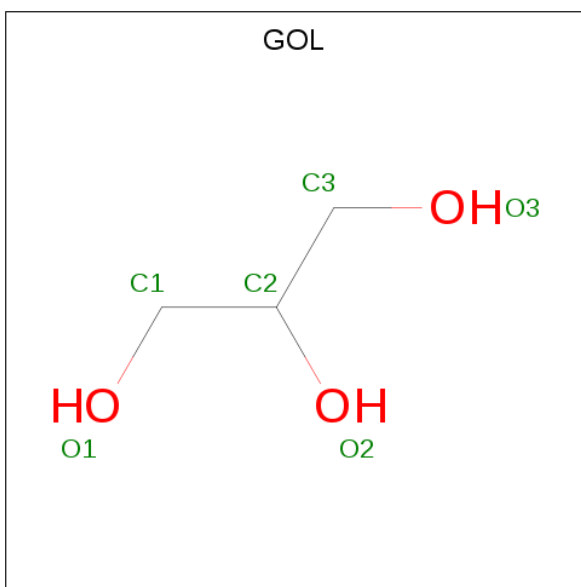
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

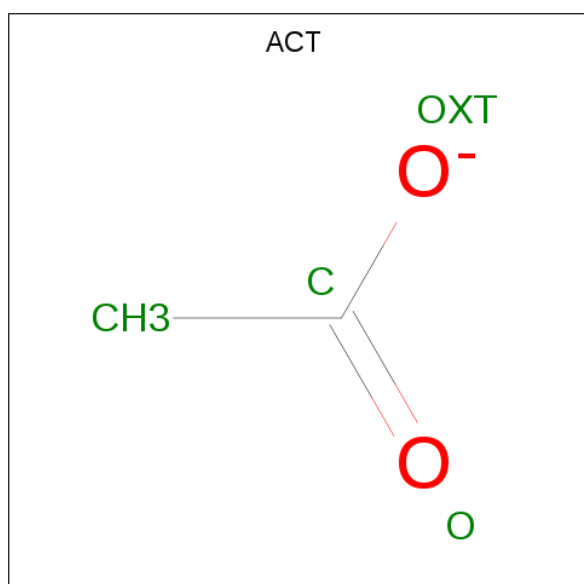
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

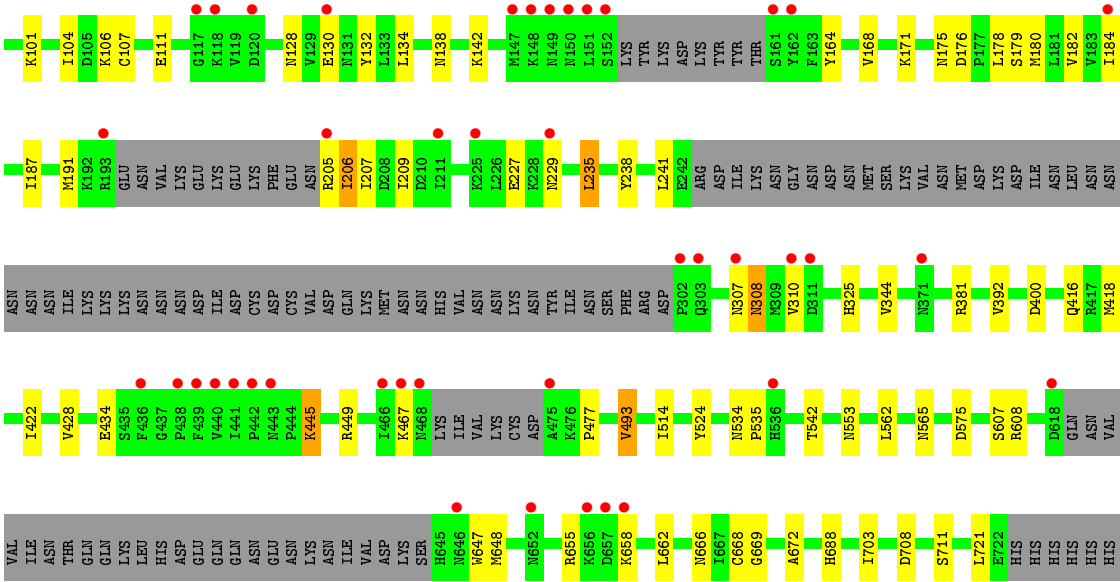
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	137	Total	O	0	0
			137	137		
9	B	122	Total	O	0	0
			122	122		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.47Å 136.36Å 139.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (30.00-2.30) 93.3 (29.28-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.226 0.192 , 0.222	Depositor DCC
R_{free} test set	8016 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9766	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PHB, CA, PE0, 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	0.58	0/4565	0.71	1/6152 (0.0%)
1	B	0.58	1/4964 (0.0%)	0.67	1/6696 (0.0%)
All	All	0.58	1/9529 (0.0%)	0.69	2/12848 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	647	TRP	CD2-CE2	5.89	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	575	ASP	CB-CG-OD1	5.23	123.01	118.30

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	4497	0	4605	62	0
1	B	4880	0	4945	59	0
2	A	12	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	5	0	0
3	A	10	0	5	5	0
3	B	10	0	5	0	0
4	A	31	0	12	1	0
4	B	31	0	12	2	0
5	A	6	0	8	3	0
5	B	6	0	8	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
9	A	137	0	0	3	0
9	B	122	0	0	5	0
All	All	9766	0	9616	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (126) 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:A:107:CYS:SG	1:A:171:LYS:HE3	1.90	1.09
1:B:688:HIS:HE1	5:B:804:GOL:H32	1.19	1.04
1:B:648:MET:HE1	1:B:668:CYS:SG	2.00	1.01
1:B:688:HIS:CE1	5:B:804:GOL:H32	2.00	0.96
1:B:648:MET:CE	1:B:668:CYS:SG	2.55	0.94
3:A:802:PHB:H3	5:A:804:GOL:H32	1.51	0.90
1:A:227:GLU:HG2	1:A:230:MET:HB2	1.52	0.90
1:B:104:ILE:H	1:B:565:ASN:HD21	1.19	0.90
1:A:25:ASN:HD22	1:A:25:ASN:H	1.17	0.89
1:B:107:CYS:SG	1:B:171:LYS:HE3	2.12	0.89
1:A:107:CYS:SG	1:A:171:LYS:CE	2.62	0.87
1:A:104:ILE:H	1:A:565:ASN:HD21	1.20	0.85
3:A:802:PHB:C3	5:A:804:GOL:H32	2.05	0.85
1:B:14:LYS:H	1:B:14:LYS:HE3	1.39	0.85
1:A:607:SER:OG	1:A:688:HIS:HD2	1.64	0.80
2:A:801:PEO:H5	3:A:802:PHB:O4	1.85	0.77
1:A:342:HIS:HD2	1:A:344:VAL:H	1.33	0.74
1:B:688:HIS:HE1	5:B:804:GOL:C3	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HB2	1:A:8:ILE:HG22	1.69	0.72
1:B:12:GLU:O	1:B:14:LYS:HE3	1.92	0.69
1:A:466:ILE:CG2	1:A:466:ILE:O	2.40	0.69
1:B:178:LEU:O	1:B:182:VAL:HG23	1.94	0.68
1:B:422:ILE:CD1	1:B:477:PRO:HG3	2.25	0.66
1:B:648:MET:HE2	1:B:668:CYS:SG	2.35	0.65
1:A:607:SER:OG	1:A:688:HIS:CD2	2.49	0.65
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.26	0.65
1:B:107:CYS:SG	1:B:171:LYS:CE	2.83	0.65
1:B:51:THR:HG22	1:B:168:VAL:HG12	1.77	0.65
1:A:342:HIS:CD2	1:A:344:VAL:H	2.15	0.64
1:B:83:ASN:HA	1:B:86:ASN:HD22	1.63	0.64
1:A:358:SER:HA	1:A:361:LYS:HE2	1.81	0.63
1:B:708:ASP:HB3	1:B:711:SER:HB3	1.82	0.62
1:A:608:ARG:HA	1:A:666:ASN:OD1	1.98	0.62
1:B:607:SER:OG	1:B:688:HIS:HD2	1.82	0.62
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.74	0.60
1:A:101:LYS:HE2	9:A:1023:HOH:O	2.01	0.59
1:A:107:CYS:HG	1:A:171:LYS:HE3	1.63	0.59
1:B:307:ASN:O	1:B:310:VAL:HG22	2.01	0.58
1:B:308:ASN:OD1	1:B:308:ASN:N	2.36	0.58
1:A:466:ILE:HG23	1:A:466:ILE:O	2.04	0.58
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.84	0.58
1:B:608:ARG:HA	1:B:666:ASN:OD1	2.04	0.57
1:A:364:TYR:HB2	1:A:366:ILE:HG13	1.86	0.57
1:B:18:ALA:CB	1:B:180:MET:HE1	2.36	0.56
1:B:171:LYS:NZ	9:B:905:HOH:O	2.37	0.55
1:B:235:LEU:HB3	1:B:241:LEU:HD11	1.88	0.55
1:A:14:LYS:HE3	1:A:175:ASN:HA	1.88	0.55
1:B:132:TYR:CE2	1:B:344:VAL:HG11	2.40	0.55
1:A:359:ARG:O	1:A:363:GLN:HB2	2.08	0.54
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.37	0.54
1:A:347:ASN:ND2	1:A:351:CYS:SG	2.81	0.53
1:B:176:ASP:OD2	1:B:179:SER:OG	2.27	0.53
1:B:205:ARG:HH12	4:B:803:ATP:PA	2.33	0.52
1:A:25:ASN:ND2	1:A:25:ASN:H	1.96	0.52
1:A:34:LEU:HD12	1:A:54:LEU:HD11	1.91	0.52
1:B:187:ILE:HG22	1:B:191:MET:CE	2.39	0.52
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.39	0.52
2:A:801:PEO:C5	3:A:802:PHB:O4	2.58	0.52
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ILE:HG22	1:B:191:MET:HE2	1.92	0.51
1:B:325:HIS:HD2	9:B:912:HOH:O	1.93	0.51
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.92	0.51
1:A:227:GLU:CD	1:A:227:GLU:H	2.13	0.51
1:B:422:ILE:HD11	1:B:477:PRO:HG3	1.92	0.51
1:A:408:PHE:HB2	1:A:413:ARG:HH12	1.77	0.50
1:B:106:LYS:HE2	1:B:111:GLU:HG3	1.92	0.50
1:A:93:GLU:OE1	1:A:186:TYR:OH	2.30	0.49
1:A:165:ASN:HB2	9:A:928:HOH:O	2.12	0.49
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.94	0.49
1:B:514:ILE:CD1	1:B:562:LEU:HD22	2.43	0.49
1:B:38:LEU:CD2	1:B:168:VAL:HG11	2.44	0.48
1:A:465:ASP:C	1:A:467:LYS:H	2.15	0.48
1:A:347:ASN:HD22	1:A:351:CYS:CB	2.27	0.48
1:A:146:ILE:HG22	1:A:146:ILE:O	2.14	0.47
1:B:206:ILE:HG13	1:B:207:ILE:N	2.28	0.47
1:A:469:LYS:CB	1:A:472:LYS:HE3	2.44	0.47
1:A:592:GLN:HG2	1:B:703:ILE:O	2.14	0.47
1:B:184:ILE:HG23	1:B:209:ILE:HB	1.97	0.47
1:B:101:LYS:NZ	9:B:911:HOH:O	2.48	0.47
1:B:60:GLU:HA	1:B:60:GLU:OE2	2.16	0.46
1:B:138:ASN:HD21	1:B:142:LYS:HE3	1.80	0.46
1:A:191:MET:HB3	1:A:206:ILE:HD11	1.98	0.46
1:A:410:GLU:HG2	1:A:411:PRO:HD2	1.97	0.46
1:A:467:LYS:HD2	1:A:467:LYS:HA	1.52	0.45
1:B:18:ALA:HB2	1:B:180:MET:HE1	1.97	0.45
1:B:26:ASP:HB2	1:B:80:TYR:HE2	1.81	0.45
1:A:25:ASN:HD22	1:A:25:ASN:N	1.96	0.45
1:A:146:ILE:HG23	1:A:149:ASN:HD22	1.81	0.45
5:A:804:GOL:H31	9:A:997:HOH:O	2.16	0.45
1:B:418:MET:O	1:B:422:ILE:HG13	2.16	0.44
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.99	0.44
1:A:342:HIS:CD2	1:A:344:VAL:HB	2.53	0.44
1:A:103:LEU:HD11	1:A:511:PRO:O	2.18	0.44
1:A:431:ILE:HG21	1:A:456:LEU:HD21	2.00	0.44
1:B:12:GLU:O	1:B:14:LYS:CE	2.65	0.44
1:A:344:VAL:O	1:A:344:VAL:HG13	2.18	0.44
1:A:20:LEU:HB2	1:A:168:VAL:HG22	1.99	0.43
1:A:312:ASN:O	4:A:803:ATP:H3'	2.17	0.43
1:A:469:LYS:O	1:A:472:LYS:HG2	2.17	0.43
1:B:182:VAL:HG12	1:B:235:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:GLY:O	1:B:672:ALA:HB3	2.19	0.43
1:B:128:ASN:HB2	9:B:942:HOH:O	2.17	0.43
1:B:130:GLU:O	1:B:134:LEU:HD23	2.18	0.43
1:A:186:TYR:HE1	1:A:305:ILE:HD13	1.84	0.42
1:B:553:ASN:OD1	9:B:901:HOH:O	2.21	0.42
1:B:55:TYR:O	1:B:164:TYR:HA	2.19	0.42
1:A:410:GLU:O	1:A:411:PRO:C	2.58	0.42
4:B:803:ATP:O3B	4:B:803:ATP:O5'	2.38	0.42
1:A:306:ILE:O	1:A:310:VAL:HG23	2.20	0.42
1:A:493:VAL:HG13	1:A:519:LYS:HE3	2.01	0.42
1:A:580:PHE:CE1	3:A:802:PHB:H5	2.55	0.42
1:B:18:ALA:HB1	1:B:180:MET:HE1	2.01	0.42
1:B:445:LYS:HB2	1:B:445:LYS:HE2	1.95	0.42
1:B:655:ARG:HH11	1:B:655:ARG:HG2	1.84	0.42
1:B:493:VAL:HG22	1:B:524:TYR:CZ	2.55	0.42
1:A:353:TYR:O	1:A:357:VAL:HG23	2.20	0.41
1:A:504:ILE:HA	1:A:529:MET:HB3	2.02	0.41
1:B:416:GLN:OE1	1:B:416:GLN:HA	2.20	0.41
1:A:422:ILE:HD11	1:A:477:PRO:HG3	2.01	0.41
1:A:8:ILE:HG23	1:A:9:LEU:HG	2.03	0.41
1:A:551:ILE:HD12	1:A:590:LEU:HD21	2.02	0.41
1:B:175:ASN:ND2	1:B:238:TYR:OH	2.52	0.41
1:A:326:ARG:HB2	1:A:329:ILE:HD12	2.03	0.41
1:B:534:ASN:HB2	1:B:535:PRO:HD2	2.02	0.40
1:A:227:GLU:CG	1:A:230:MET:HB2	2.38	0.40
1:A:103:LEU:HD11	1:A:511:PRO:HB2	2.03	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	527/728 (72%)	506 (96%)	18 (3%)	3 (1%)	25	31
1	B	576/728 (79%)	554 (96%)	22 (4%)	0	100	100
All	All	1103/1456 (76%)	1060 (96%)	40 (4%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	A	466	ILE
1	A	146	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	519/697 (74%)	490 (94%)	29 (6%)	21	29
1	B	560/697 (80%)	539 (96%)	21 (4%)	33	47
All	All	1079/1394 (77%)	1029 (95%)	50 (5%)	27	38

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	25	ASN
1	A	82	VAL
1	A	87	GLU
1	A	88	LEU
1	A	120	ASP
1	A	134	LEU
1	A	162	TYR
1	A	205	ARG
1	A	225	LYS
1	A	229	ASN
1	A	305	ILE
1	A	314	GLU

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Mol	Chain	Res	Type
1	A	324	THR
1	A	344	VAL
1	A	360	MET
1	A	408	PHE
1	A	412	LYS
1	A	413	ARG
1	A	449	ARG
1	A	473	CYS
1	A	522	LYS
1	A	542	THR
1	A	618	ASP
1	A	658	LYS
1	A	659	ASP
1	A	660	GLN
1	A	661	LEU
1	A	705	GLN
1	B	14	LYS
1	B	27	ARG
1	B	28	ARG
1	B	54	LEU
1	B	60	GLU
1	B	206	ILE
1	B	227	GLU
1	B	229	ASN
1	B	235	LEU
1	B	308	ASN
1	B	381	ARG
1	B	400	ASP
1	B	434	GLU
1	B	445	LYS
1	B	449	ARG
1	B	467	LYS
1	B	493	VAL
1	B	542	THR
1	B	658	LYS
1	B	662	LEU
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN

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Mol	Chain	Res	Type
1	A	25	ASN
1	A	86	ASN
1	A	165	ASN
1	A	303	GLN
1	A	342	HIS
1	A	347	ASN
1	A	363	GLN
1	A	553	ASN
1	A	565	ASN
1	A	584	HIS
1	A	593	ASN
1	A	664	GLN
1	A	688	HIS
1	A	705	GLN
1	B	5	GLN
1	B	21	ASN
1	B	83	ASN
1	B	86	ASN
1	B	90	GLN
1	B	116	ASN
1	B	137	ASN
1	B	138	ASN
1	B	165	ASN
1	B	175	ASN
1	B	363	GLN
1	B	468	ASN
1	B	565	ASN
1	B	688	HIS

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
5	GOL	A	804	-	5,5,5	0.43	0	5,5,5	0.42	0
2	PE0	B	801	-	13,13,13	2.57	4 (30%)	15,18,18	4.02	9 (60%)
4	ATP	B	803	6	26,33,33	0.98	2 (7%)	31,52,52	1.35	4 (12%)
8	ACT	A	807	-	1,3,3	1.93	0	0,3,3	0.00	-
3	PHB	A	802	-	8,10,10	1.24	1 (12%)	10,13,13	1.10	1 (10%)
4	ATP	A	803	6	26,33,33	1.13	2 (7%)	31,52,52	1.23	2 (6%)
8	ACT	B	807	-	1,3,3	0.89	0	0,3,3	0.00	-
2	PE0	A	801	-	13,13,13	2.37	3 (23%)	15,18,18	3.74	10 (66%)
3	PHB	B	802	-	8,10,10	1.60	1 (12%)	10,13,13	0.85	0
5	GOL	B	804	-	5,5,5	0.45	0	5,5,5	0.65	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
5	GOL	A	804	-	-	2/4/4/4	-
2	PE0	B	801	-	-	-	0/2/2/2
4	ATP	B	803	6	-	8/18/38/38	0/3/3/3
3	PHB	A	802	-	-	0/0/4/4	0/1/1/1
4	ATP	A	803	6	-	7/18/38/38	0/3/3/3
2	PE0	A	801	-	-	-	0/2/2/2
3	PHB	B	802	-	-	0/0/4/4	0/1/1/1
5	GOL	B	804	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	PE0	C4-C1	5.99	1.51	1.41
2	A	801	PE0	C4-C1	5.53	1.50	1.41
2	B	801	PE0	C1-C2	4.91	1.50	1.40
2	A	801	PE0	C1-C2	4.61	1.49	1.40
3	B	802	PHB	C1-C1'	3.84	1.51	1.47
2	B	801	PE0	C1-N4	3.06	1.37	1.33
3	A	802	PHB	C1-C1'	2.83	1.50	1.47
4	A	803	ATP	C5-C4	2.75	1.48	1.40
2	A	801	PE0	C1-N4	2.73	1.37	1.33
4	B	803	ATP	C2-N3	2.38	1.35	1.32
2	B	801	PE0	C3-N6	2.24	1.38	1.33
4	A	803	ATP	O4'-C1'	2.22	1.44	1.41
4	B	803	ATP	C5-C4	2.20	1.46	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PE0	C3-N1-C2	6.89	123.22	115.36
2	B	801	PE0	N3-C2-N1	6.71	123.48	115.82
2	B	801	PE0	C4-C1-C2	-6.57	115.60	119.95
2	A	801	PE0	C3-N1-C2	6.48	122.76	115.36
2	A	801	PE0	N3-C2-N1	6.32	123.04	115.82
2	B	801	PE0	C4-C1-N4	5.16	124.67	118.24
2	B	801	PE0	N1-C3-N2	-5.08	120.45	127.22
2	A	801	PE0	C4-C1-N4	5.04	124.52	118.24
2	A	801	PE0	C4-C1-C2	-4.84	116.75	119.95
2	B	801	PE0	C4-N2-C3	4.40	122.92	115.93
2	A	801	PE0	C4-N2-C3	4.20	122.60	115.93
2	A	801	PE0	N1-C3-N2	-4.20	121.62	127.22
2	A	801	PE0	C1-C4-N2	-3.87	118.14	123.43
4	B	803	ATP	N3-C2-N1	-3.17	123.73	128.68
2	B	801	PE0	C6-N3-C2	3.14	120.48	116.60
4	A	803	ATP	N3-C2-N1	-3.12	123.80	128.68
2	A	801	PE0	C2-C1-N4	-3.10	118.73	122.32
2	B	801	PE0	C1-C4-N2	-3.04	119.28	123.43
2	A	801	PE0	C6-N3-C2	2.79	120.05	116.60
4	B	803	ATP	PA-O3A-PB	-2.51	124.22	132.83
4	B	803	ATP	C5'-C4'-C3'	-2.45	106.00	115.18
4	A	803	ATP	PA-O3A-PB	-2.43	124.48	132.83
2	B	801	PE0	C2-C1-N4	-2.24	119.73	122.32
2	A	801	PE0	C1-C2-N1	-2.22	118.07	121.80
3	A	802	PHB	C2-C1-C1'	-2.13	117.50	120.37
4	B	803	ATP	N6-C6-N1	2.08	122.89	118.57

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	GOL	O1-C1-C2-C3
4	B	803	ATP	C5'-O5'-PA-O3A
4	B	803	ATP	C3'-C4'-C5'-O5'
4	A	803	ATP	C5'-O5'-PA-O1A
4	A	803	ATP	O4'-C4'-C5'-O5'
4	A	803	ATP	C3'-C4'-C5'-O5'
4	B	803	ATP	O4'-C4'-C5'-O5'
5	B	804	GOL	O1-C1-C2-C3
5	B	804	GOL	O1-C1-C2-O2
5	A	804	GOL	O1-C1-C2-O2
4	B	803	ATP	PB-O3A-PA-O5'
4	A	803	ATP	C5'-O5'-PA-O3A
4	B	803	ATP	C5'-O5'-PA-O1A
4	A	803	ATP	C5'-O5'-PA-O2A
4	B	803	ATP	PA-O3A-PB-O1B
4	B	803	ATP	PB-O3A-PA-O1A
4	A	803	ATP	PG-O3B-PB-O1B
4	A	803	ATP	PG-O3B-PB-O2B
4	B	803	ATP	PA-O3A-PB-O3B

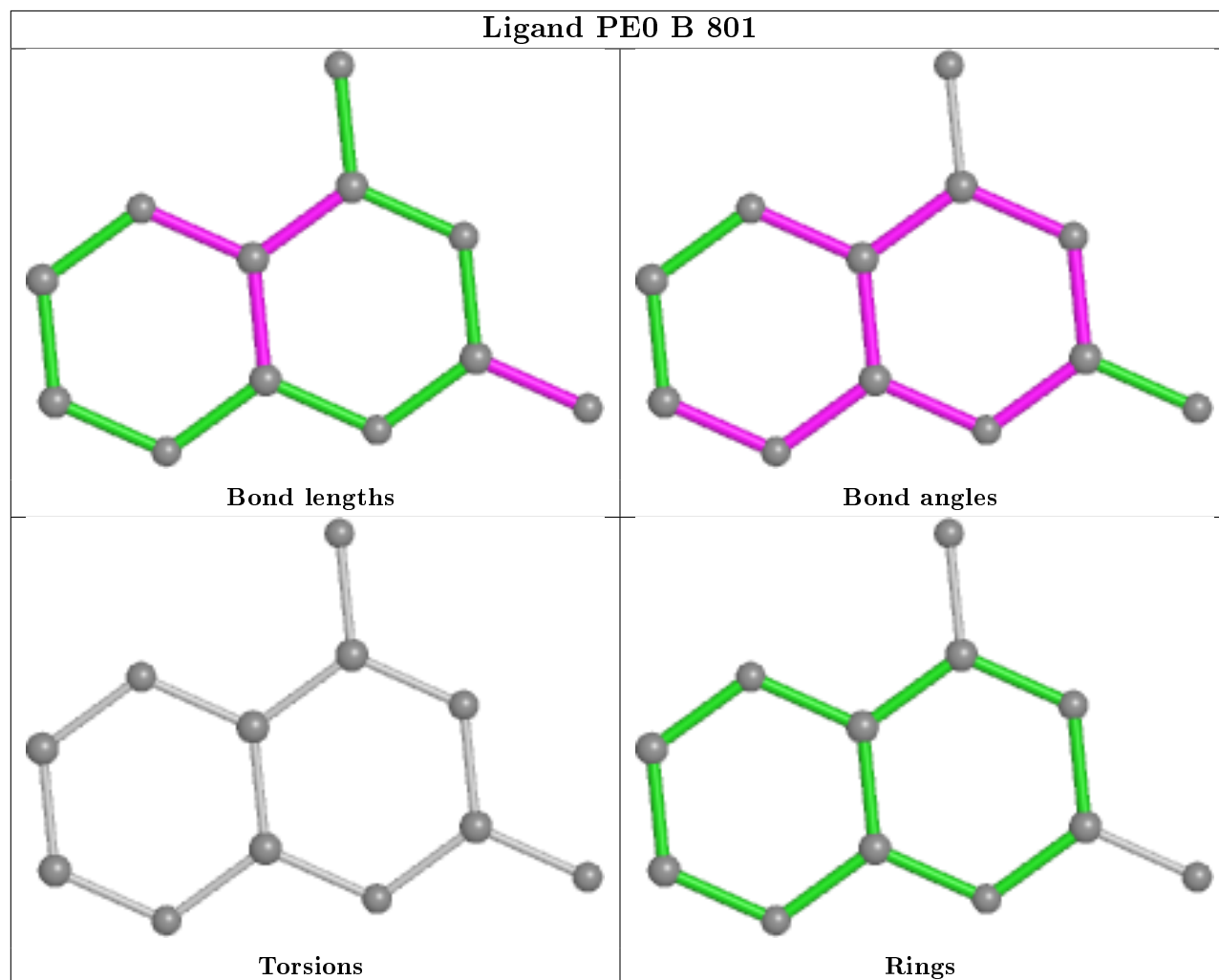
There are no ring outliers.

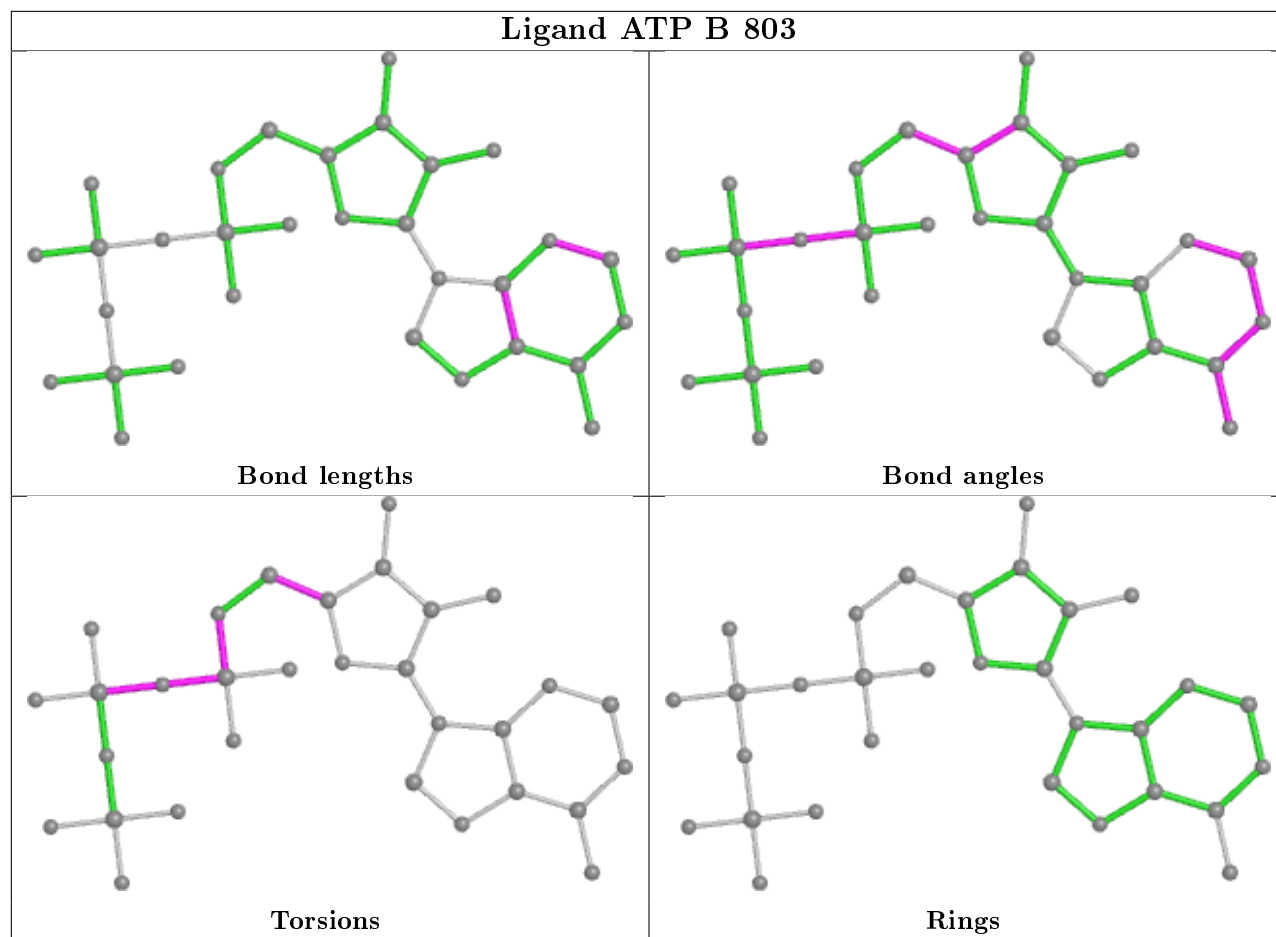
6 monomers are involved in 12 short contacts:

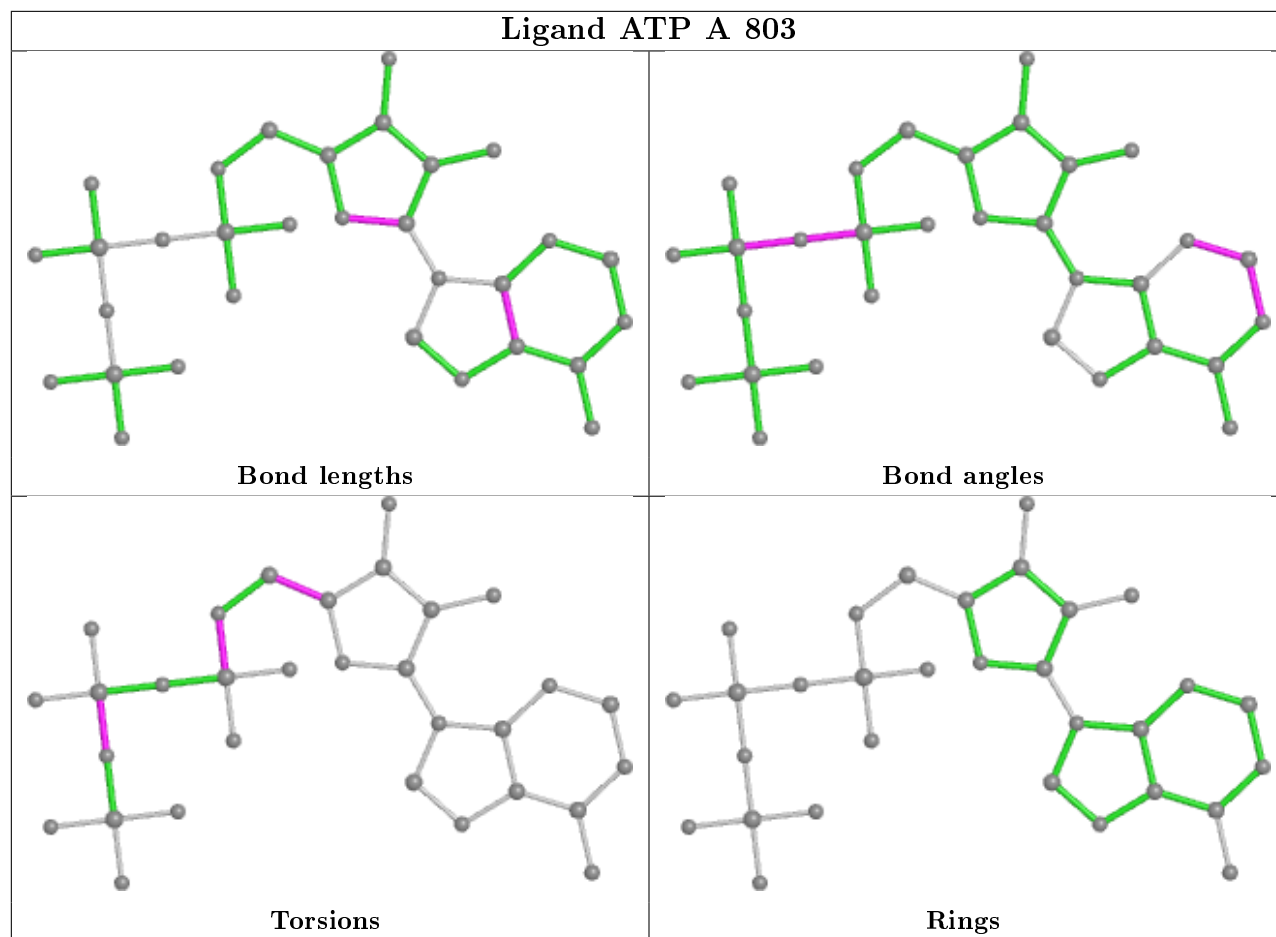
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	GOL	3	0
4	B	803	ATP	2	0
3	A	802	PHB	5	0
4	A	803	ATP	1	0
2	A	801	PE0	2	0
5	B	804	GOL	3	0

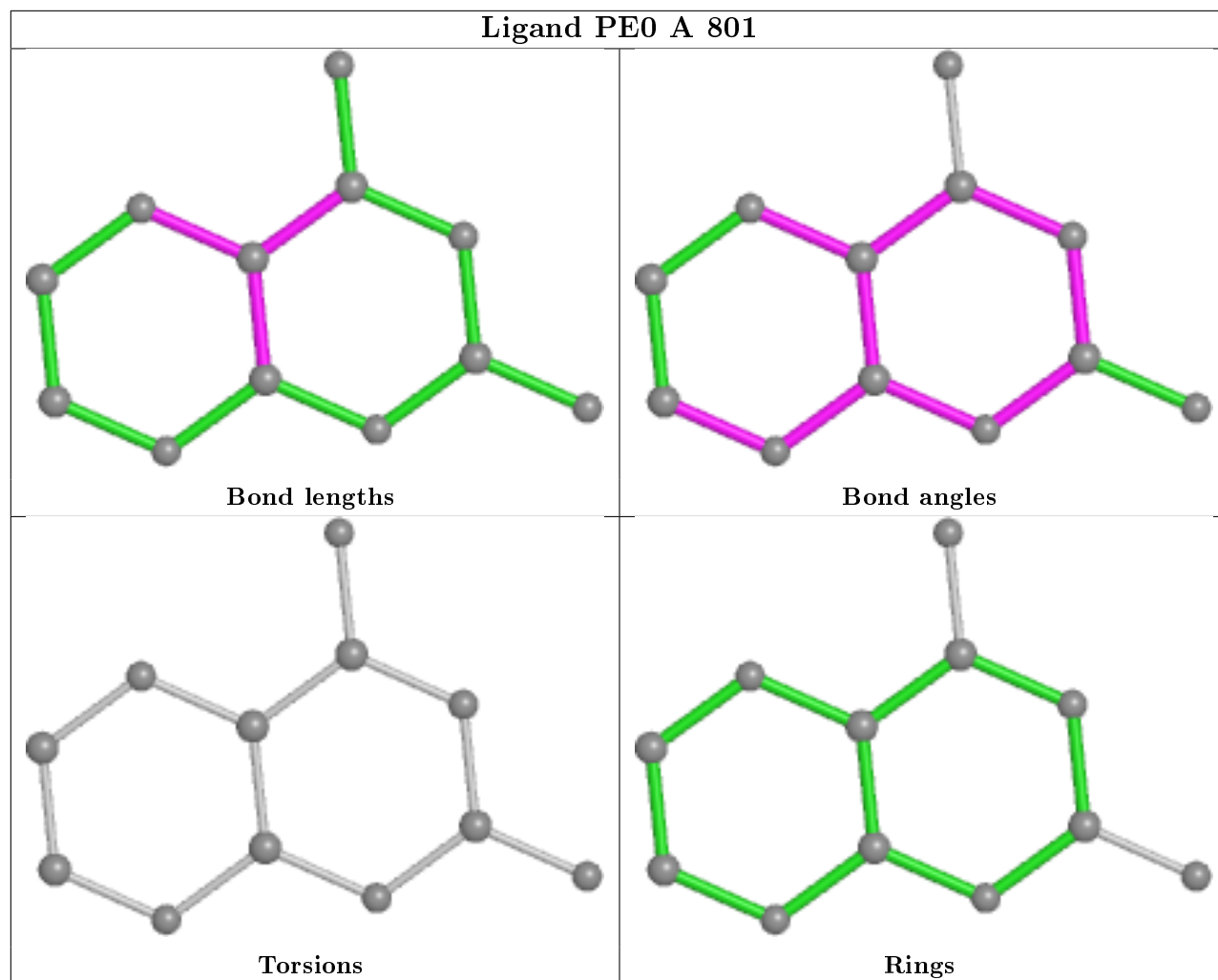
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	543/728 (74%)	0.41	69 (12%) 3 5	12, 30, 91, 117	0
1	B	590/728 (81%)	0.33	61 (10%) 6 9	10, 34, 90, 117	0
All	All	1133/1456 (77%)	0.37	130 (11%) 4 7	10, 32, 91, 117	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	11.7
1	B	80	TYR	10.3
1	A	149	ASN	8.6
1	A	161	SER	6.2
1	A	470	ILE	6.2
1	A	146	ILE	5.9
1	A	147	MET	5.8
1	A	84	TYR	5.8
1	A	473	CYS	5.7
1	B	442	PRO	5.6
1	A	468	ASN	5.6
1	B	443	ASN	5.5
1	B	84	TYR	5.4
1	A	300	ARG	5.4
1	B	83	ASN	5.3
1	B	81	ASP	5.3
1	B	151	LEU	5.3
1	A	446	ILE	5.2
1	B	90	GLN	5.1
1	A	408	PHE	5.0
1	B	13	ASN	4.8
1	B	152	SER	4.8
1	B	468	ASN	4.8
1	A	301	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLU	4.7
1	A	618	ASP	4.7
1	B	193	ARG	4.6
1	A	162	TYR	4.6
1	A	361	LYS	4.5
1	B	150	ASN	4.3
1	A	365	ASN	4.2
1	A	205	ARG	4.2
1	B	466	ILE	4.2
1	B	467	LYS	4.2
1	A	409	VAL	4.1
1	A	619	GLN	4.1
1	B	11	GLU	4.1
1	A	303	GLN	4.1
1	A	311	ASP	4.1
1	B	87	GLU	4.1
1	A	148	LYS	4.0
1	B	652	ASN	3.9
1	A	366	ILE	3.8
1	A	304	GLU	3.7
1	A	474	ASP	3.7
1	B	12	GLU	3.5
1	A	658	LYS	3.5
1	A	445	LYS	3.5
1	B	303	GLN	3.5
1	B	536	HIS	3.5
1	A	144	ASP	3.5
1	A	362	GLU	3.4
1	B	311	ASP	3.4
1	B	60	GLU	3.4
1	A	370	GLU	3.4
1	A	398	ASN	3.4
1	B	85	ILE	3.3
1	A	367	ASN	3.3
1	A	469	LYS	3.3
1	A	20	LEU	3.2
1	A	206	ILE	3.2
1	A	11	GLU	3.2
1	B	229	ASN	3.2
1	B	82	VAL	3.1
1	A	59	PRO	3.1
1	B	441	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	VAL	3.0
1	B	149	ASN	3.0
1	A	472	LYS	3.0
1	A	83	ASN	3.0
1	A	7	LEU	3.0
1	A	617	ASN	2.9
1	B	211	ILE	2.9
1	B	59	PRO	2.9
1	A	307	ASN	2.8
1	B	307	ASN	2.8
1	B	302	PRO	2.8
1	B	118	LYS	2.8
1	B	646	ASN	2.8
1	A	228	LYS	2.8
1	B	440	VAL	2.7
1	A	163	PHE	2.7
1	B	439	PHE	2.7
1	A	227	GLU	2.7
1	B	656	LYS	2.6
1	B	436	PHE	2.6
1	A	659	ASP	2.6
1	B	438	PRO	2.6
1	B	184	ILE	2.6
1	B	120	ASP	2.6
1	B	162	TYR	2.6
1	A	90	GLN	2.5
1	A	87	GLU	2.5
1	B	657	ASP	2.5
1	A	184	ILE	2.5
1	B	20	LEU	2.5
1	A	663	TYR	2.4
1	B	475	ALA	2.4
1	A	302	PRO	2.4
1	A	28	ARG	2.4
1	B	6	GLU	2.4
1	B	161	SER	2.4
1	B	28	ARG	2.4
1	A	412	LYS	2.4
1	B	148	LYS	2.4
1	A	82	VAL	2.4
1	A	410	GLU	2.3
1	A	19	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	310	VAL	2.3
1	A	143	ASN	2.3
1	B	225	LYS	2.3
1	A	661	LEU	2.3
1	A	142	LYS	2.3
1	A	467	LYS	2.3
1	A	536	HIS	2.2
1	A	706	VAL	2.2
1	B	61	TYR	2.2
1	B	658	LYS	2.2
1	B	7	LEU	2.1
1	A	435	SER	2.1
1	B	117	GLY	2.1
1	B	130	GLU	2.1
1	B	371	ASN	2.1
1	B	37	ALA	2.1
1	A	358	SER	2.1
1	B	618	ASP	2.1
1	B	147	MET	2.1
1	A	166	LEU	2.0
1	A	211	ILE	2.0
1	B	205	ARG	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(Å ²)	Q<0.9
2	PE0	B	801	12/12	0.80	0.24	34,44,47,47	0

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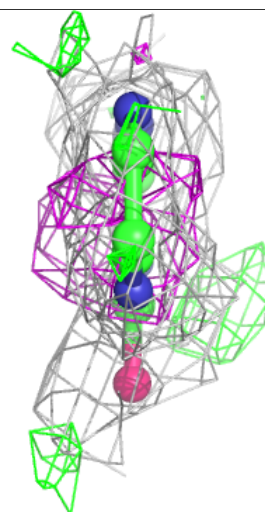
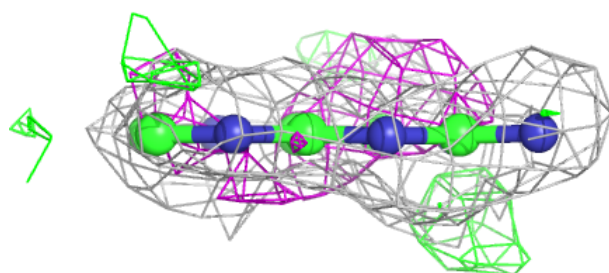
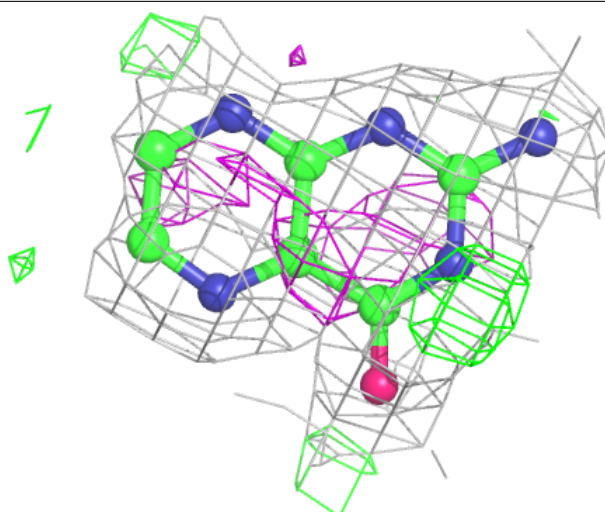
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	A	803	31/31	0.85	0.16	33,62,93,94	0
6	MG	A	805	1/1	0.86	0.11	30,30,30,30	0
4	ATP	B	803	31/31	0.86	0.16	29,59,83,84	0
5	GOL	A	804	6/6	0.89	0.23	36,39,43,43	0
2	PE0	A	801	12/12	0.90	0.15	30,34,38,38	0
3	PHB	B	802	10/10	0.90	0.15	42,46,54,57	0
5	GOL	B	804	6/6	0.91	0.17	43,46,48,49	0
3	PHB	A	802	10/10	0.92	0.16	37,40,44,51	0
6	MG	B	805	1/1	0.95	0.11	30,30,30,30	0
8	ACT	A	807	4/4	0.98	0.08	24,26,28,29	0
7	CA	A	806	1/1	0.98	0.08	28,28,28,28	0
8	ACT	B	807	4/4	0.98	0.12	15,15,16,16	0
7	CA	B	806	1/1	0.99	0.06	40,40,40,40	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.

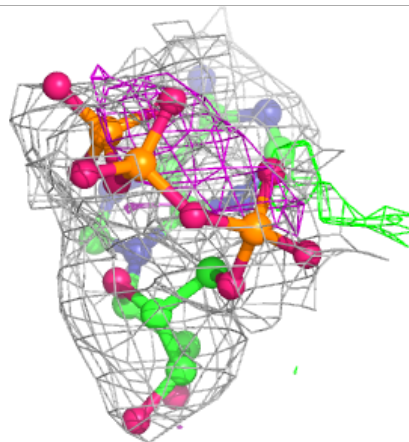
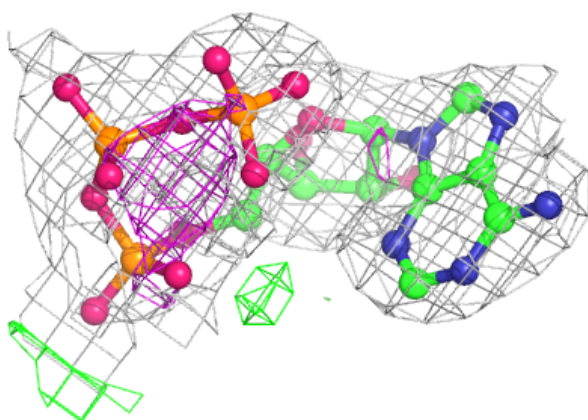
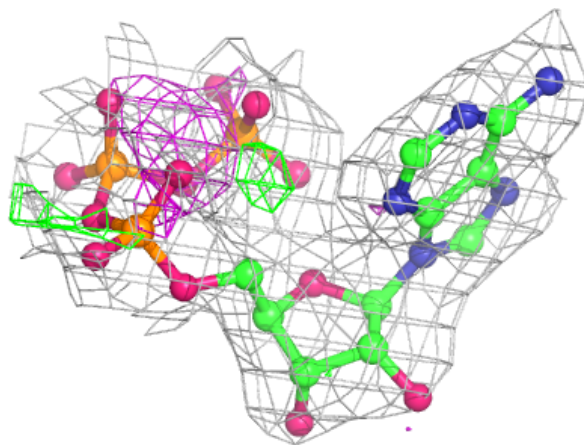
Electron density around PE0 B 801:

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



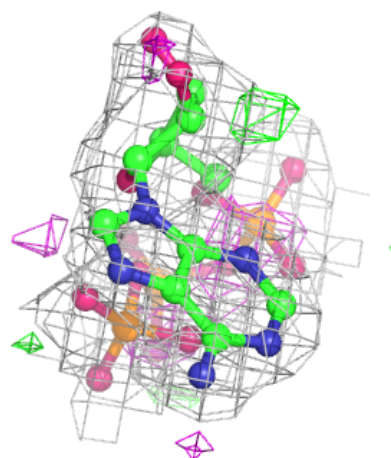
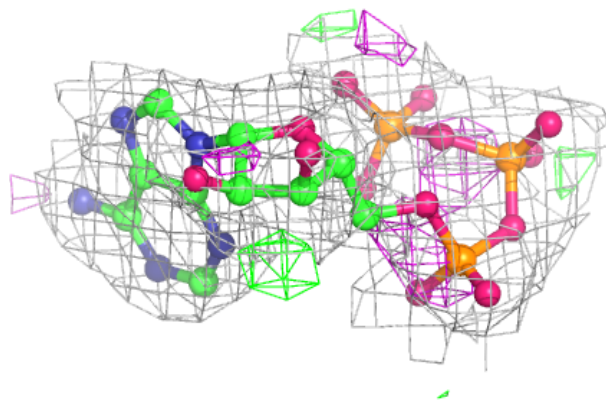
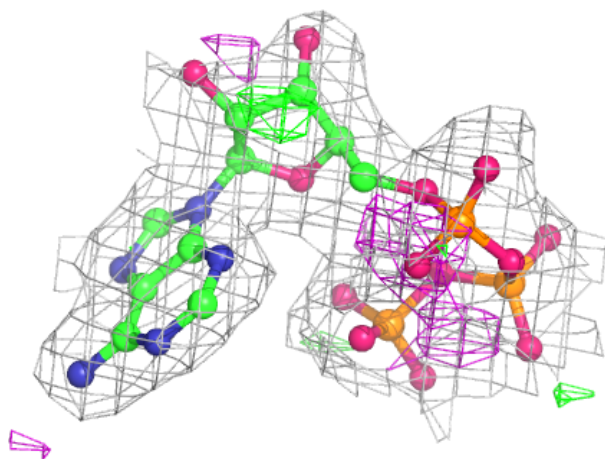
Electron density around ATP A 803:

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



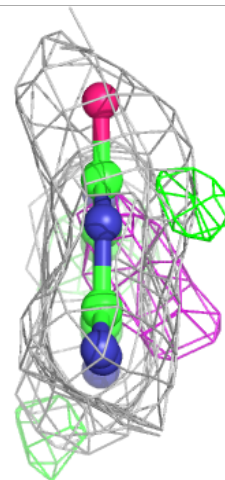
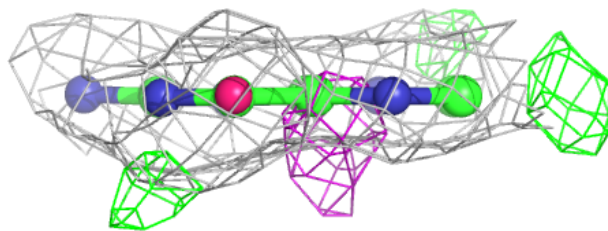
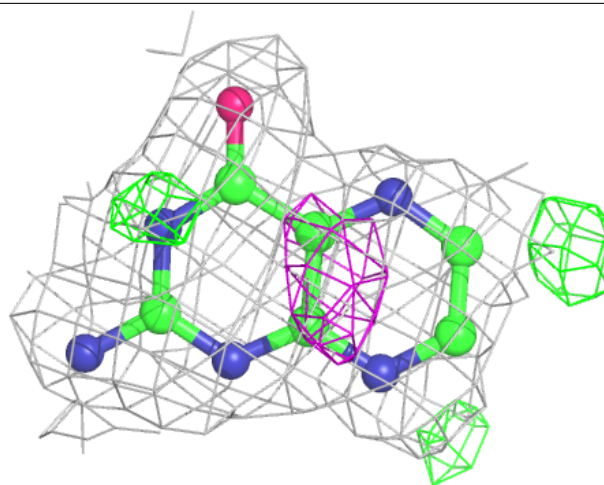
Electron density around ATP B 803:

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



Electron density around PE0 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.