wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 01:27 AM JST

PDB ID	:	6KCK
Title	:	Crystal structure of Plasmodium falciparum HPPK-DHPS wild type with pterin and p-hydroxybenzoate
Authors	:	Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on	:	2019-06-28
Resolution	:	2.50 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:

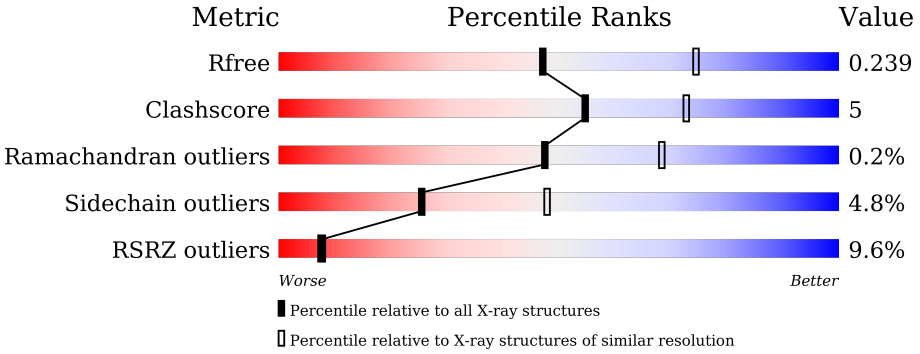
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	7% 66% 9% • 24%
1	B	728	8% 63% 14% • 23%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9536 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
			Total	C	N	O	S			
1	A	551	4554	2934	754	844	22	0	0	0
			Total	C	N	O	S			
1	B	562	4615	2973	760	860	22	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

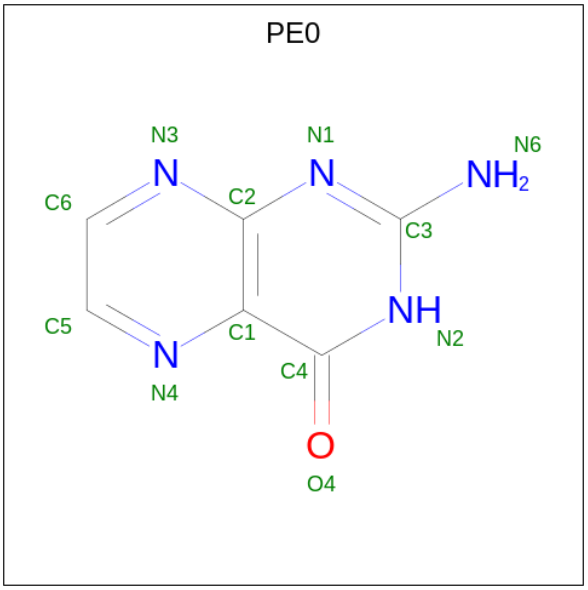
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_6H_5N_5O$) (labeled as "Ligand of Interest" by depositor).



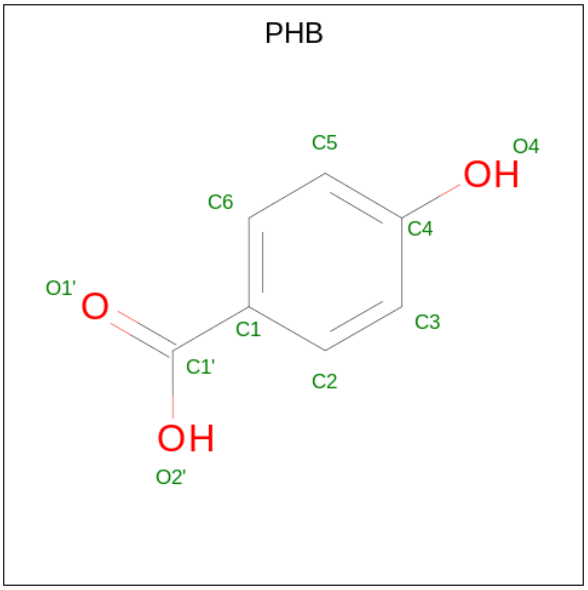
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	6	5	1	0	0

Continued on next page...

Continued from previous page...

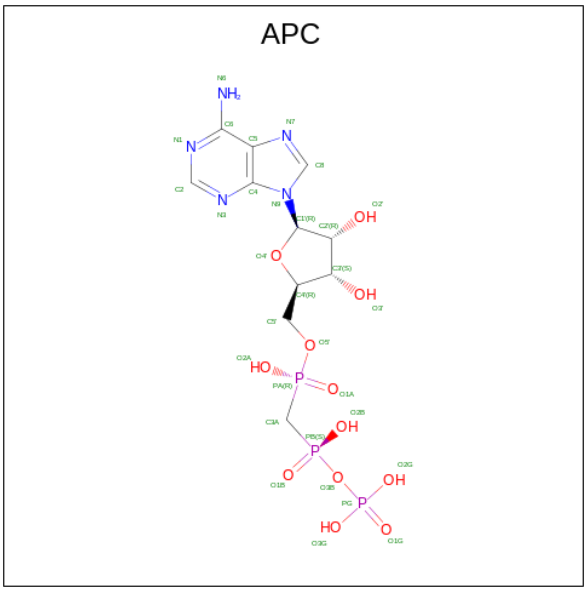
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	12	6	5	1	0	0

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



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

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
4	B	1	31	11	5	12	3	0	0

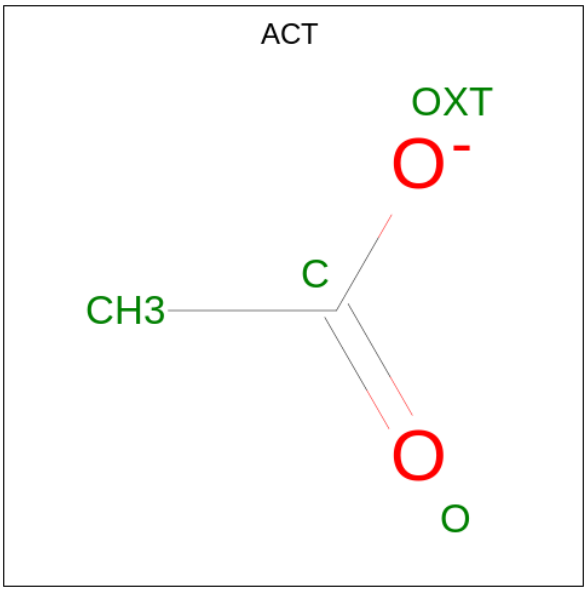
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

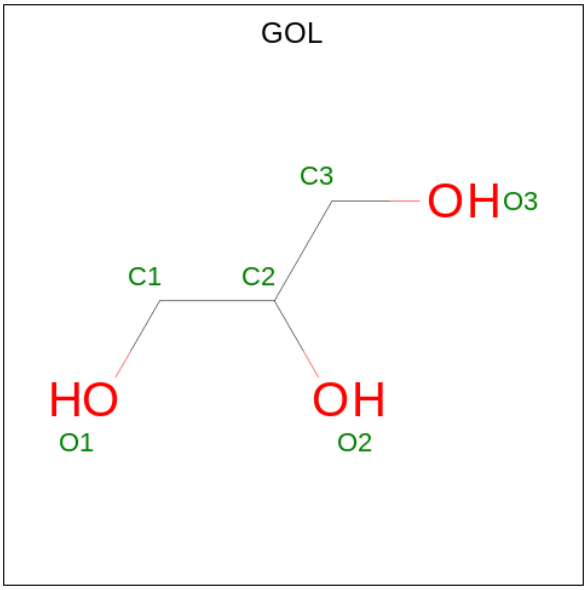
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0
			Total	Ca		
6	B	1	1	1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

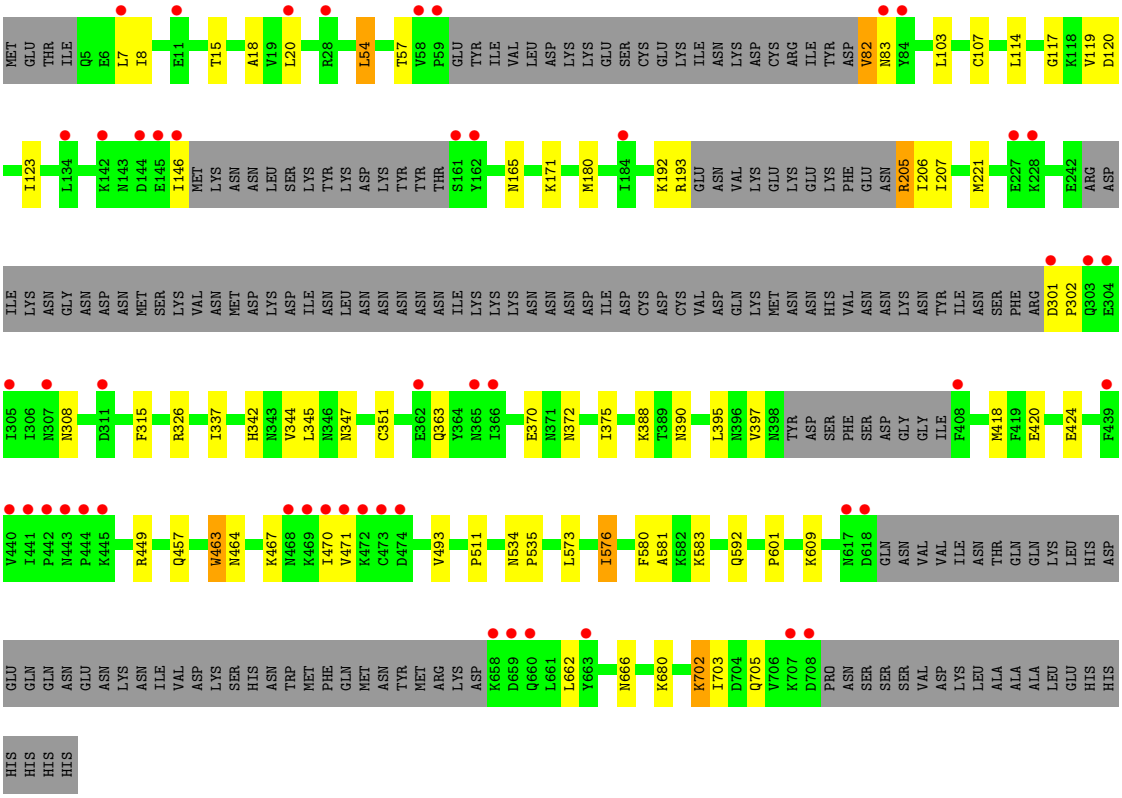
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	137	137	137	0	0
			Total	O		
9	B	99	99	99	0	0

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.

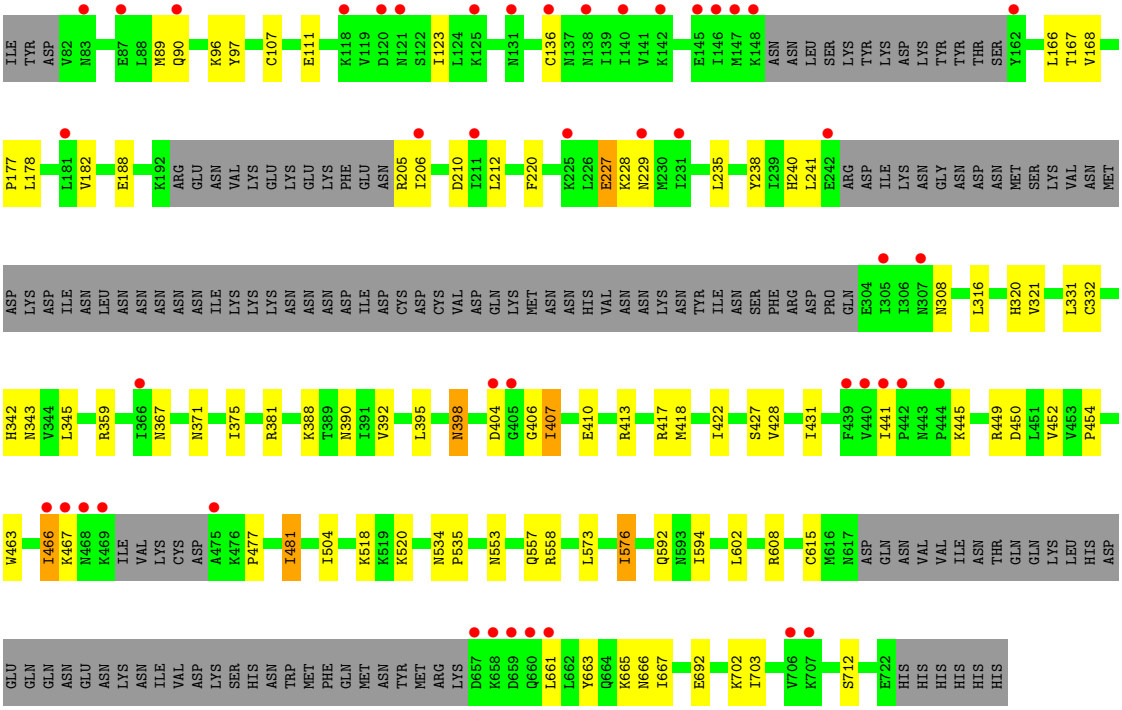
• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase

Chain A:



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

Chain B:


ILE TYR ASP V82 N83 E87 L88 M89 Q90 K96 Y97 C107 E111 K118 V119 D120 N121 S122 I123 L124 K125 N131 C136 N137 N138 I139 I140 V141 K142 E145 I146 M147 K148 ASN ASN LEU SER LYS TYR LYS ASP LYS TYR TYR THR SER Y162 L166 T167 V168
P177 L178 L181 V182 E188 K192 ARG GLU ASN VAL LYS GLU LYS GLU LYS PHE GLU ASN R205 I206 D210 I211 L212 F220 K225 L226 E227 K228 N229 M230 I231 L235 Y238 I239 H240 L241 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 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 PRO GLN E304 I305 I306 N307 N308 L316 H320 V321 L331 C332
H342 N343 V344 L345 R359 I366 N367 N371 I375 R381 K388 T389 N390 I391 V392 L395 N398 D404 G405 G406 I407 E410 R413 R417 M418 I422 S427 V428 I431 F439 V440 I441 P442 N443 P444 K445 R449 D450 L451 V452 V453 P454
W463 I466 K467 N468 K469 ILE VAL LYS CYS ASP A475 K476 P477 I481 I504 K518 K519 K520 N534 P535 N553 Q557 R558 L573 I576 Q592 N593 I594 L602 R608 C615 M616 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 HIS ASN TRP MET PHE GLN MET ASN TYR MET ARG LYS D657 K658 D659 Q660 L661 L662 Y663 Q664 K665 N666 I667 E692 K702 I703 V706 K707 S712 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	101.49Å 137.22Å 139.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 27.59 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-2.50) 91.3 (27.59-2.49)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.245 0.191 , 0.239	Depositor DCC
R_{free} test set	6351 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9536	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, ACT, APC, PHB, PE0, MG

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	1/4627 (0.0%)	0.70	0/6243
1	B	0.54	1/4690 (0.0%)	0.66	0/6329
All	All	0.56	2/9317 (0.0%)	0.68	0/12572

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	TRP	CD2-CE2	5.10	1.47	1.41
1	B	463	TRP	CD2-CE2	5.07	1.47	1.41

There are no bond angle outliers.

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	4554	0	4661	40	0
1	B	4615	0	4703	59	0
2	A	12	0	5	1	0
2	B	12	0	5	0	0
3	A	10	0	5	0	0
3	B	10	0	4	2	0
4	A	31	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	14	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
8	A	6	0	8	0	0
8	B	6	0	8	2	0
9	A	137	0	0	1	0
9	B	99	0	0	3	0
All	All	9536	0	9433	98	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 5.

The worst 5 of 98 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:20:LEU:HD21	1:A:180:MET:HE1	1.47	0.92
1:A:192:LYS:HE3	1:A:205:ARG:HG3	1.50	0.91
1:A:20:LEU:HD21	1:A:180:MET:CE	2.10	0.81
1:B:407:ILE:H	1:B:407:ILE:HD13	1.43	0.81
3:B:802:PHB:H5	8:B:808:GOL:H11	1.61	0.81

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 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	548/728 (75%)	519 (95%)	28 (5%)	1 (0%)	47	68
All	All	1085/1456 (74%)	1036 (96%)	47 (4%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	LYS
1	A	117	GLY

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%)	502 (96%)	23 (4%)	28	52
1	B	529/696 (76%)	501 (95%)	28 (5%)	22	43
All	All	1054/1392 (76%)	1003 (95%)	51 (5%)	25	48

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	206	ILE
1	B	407	ILE
1	B	702	LYS
1	B	220	PHE
1	B	343	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	GLN
1	B	398	ASN
1	B	553	ASN
1	A	343	ASN
1	A	91	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 15 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
7	ACT	A	806	-	3,3,3	0.86	0	3,3,3	0.21	0
2	PE0	A	801	-	13,13,13	1.66	2 (15%)	15,18,18	3.04	8 (53%)
8	GOL	B	808	-	5,5,5	0.57	0	5,5,5	1.31	0
4	APC	B	803	5	27,33,33	1.51	5 (18%)	31,52,52	1.39	4 (12%)
7	ACT	B	807	-	3,3,3	0.86	0	3,3,3	0.68	0
8	GOL	A	807	-	5,5,5	0.41	0	5,5,5	1.21	1 (20%)
3	PHB	B	802	-	10,10,10	0.84	0	13,13,13	1.34	2 (15%)
2	PE0	B	801	-	13,13,13	2.06	3 (23%)	15,18,18	3.46	10 (66%)
4	APC	A	803	5	27,33,33	1.43	5 (18%)	31,52,52	1.38	4 (12%)
3	PHB	A	802	-	10,10,10	0.84	0	13,13,13	0.96	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
8	GOL	B	808	-	-	2/4/4/4	-
2	PE0	A	801	-	-	-	0/2/2/2
4	APC	B	803	5	-	6/15/38/38	0/3/3/3
8	GOL	A	807	-	-	2/4/4/4	-
3	PHB	B	802	-	-	0/4/4/4	0/1/1/1
2	PE0	B	801	-	-	-	0/2/2/2
4	APC	A	803	5	-	5/15/38/38	0/3/3/3
3	PHB	A	802	-	-	0/4/4/4	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	PE0	C1-C4	4.74	1.49	1.41
2	A	801	PE0	C1-C2	3.95	1.48	1.40
2	B	801	PE0	C1-C2	3.73	1.47	1.40
4	B	803	APC	PA-O5'	3.64	1.62	1.57
4	A	803	APC	PB-O3B	3.09	1.61	1.58

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	PE0	N3-C2-N1	6.44	123.17	115.82
2	B	801	PE0	C3-N1-C2	6.07	122.30	115.36
2	B	801	PE0	N3-C2-N1	5.54	122.14	115.82
2	B	801	PE0	C4-C1-N4	4.69	124.08	118.24
2	A	801	PE0	C3-N2-C4	4.43	122.97	115.93

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	APC	PA-C3A-PB-O1B
4	A	803	APC	PA-C3A-PB-O2B
4	A	803	APC	PA-C3A-PB-O3B
4	A	803	APC	C3'-C4'-C5'-O5'
4	B	803	APC	PA-C3A-PB-O1B

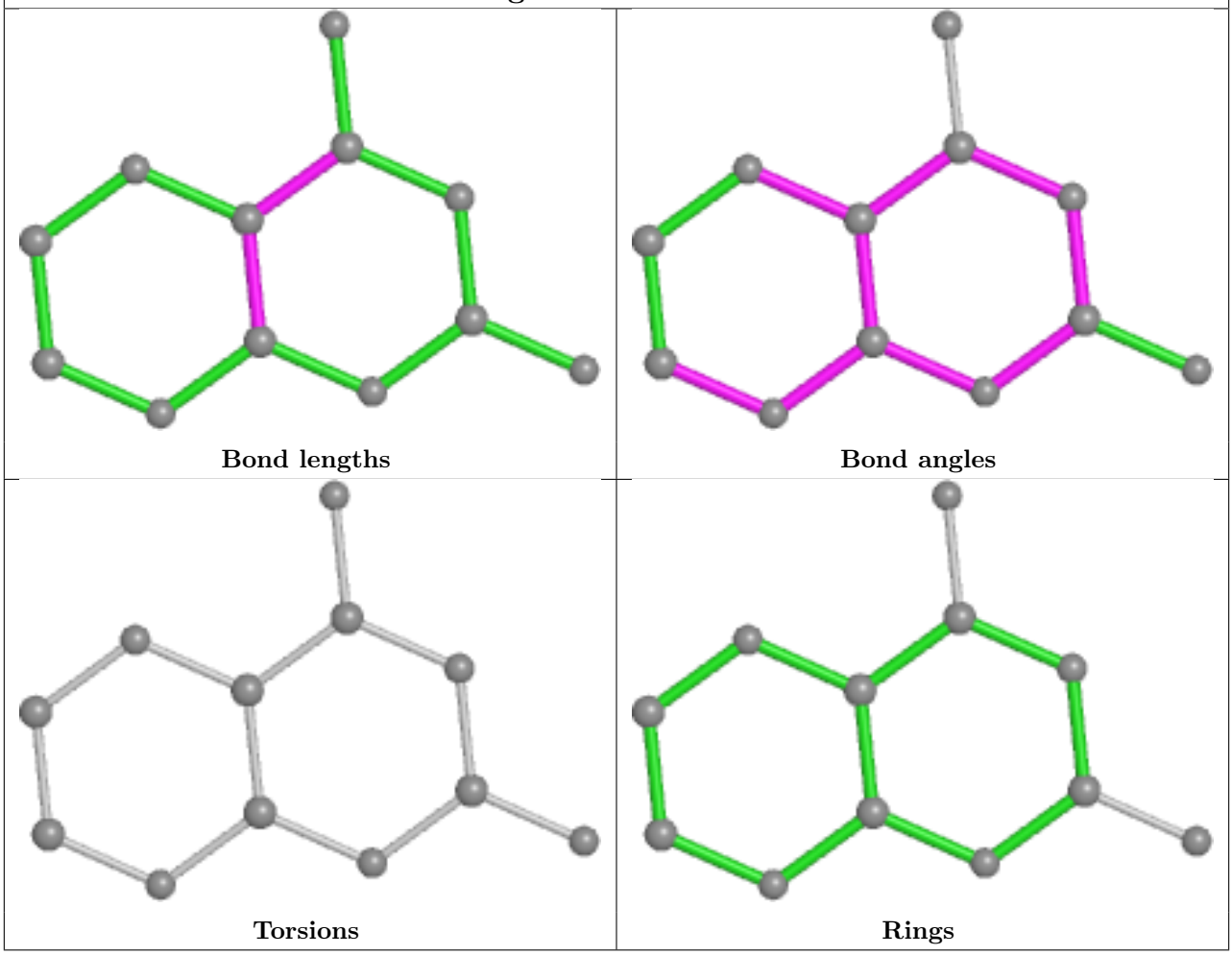
There are no ring outliers.

3 monomers are involved in 3 short contacts:

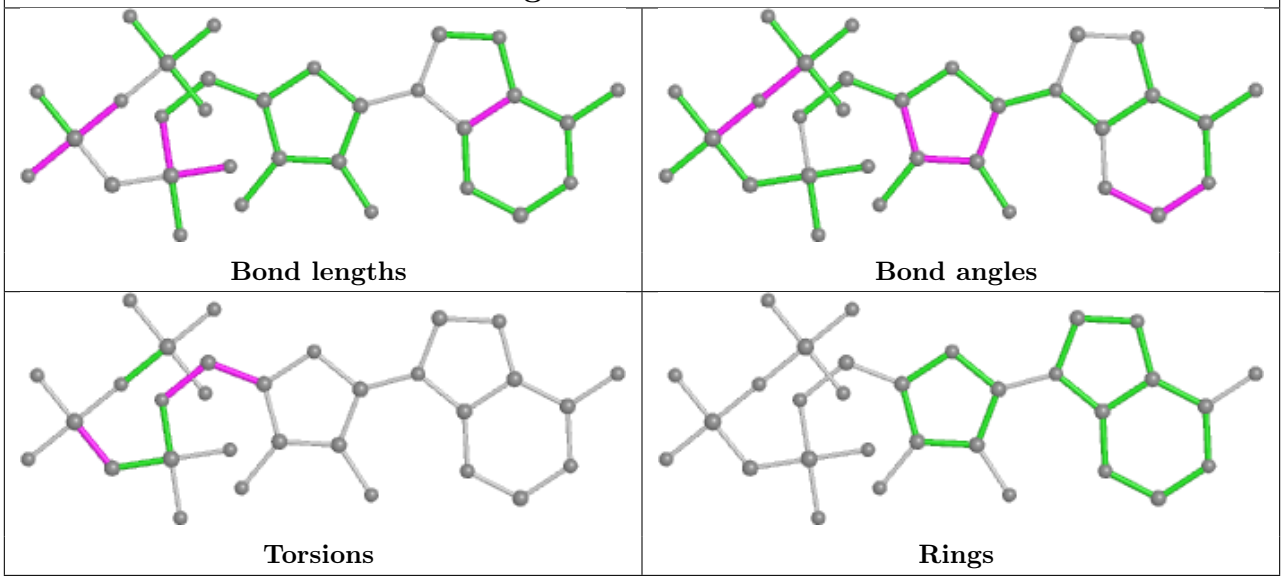
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PE0	1	0
8	B	808	GOL	2	0
3	B	802	PHB	2	0

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.

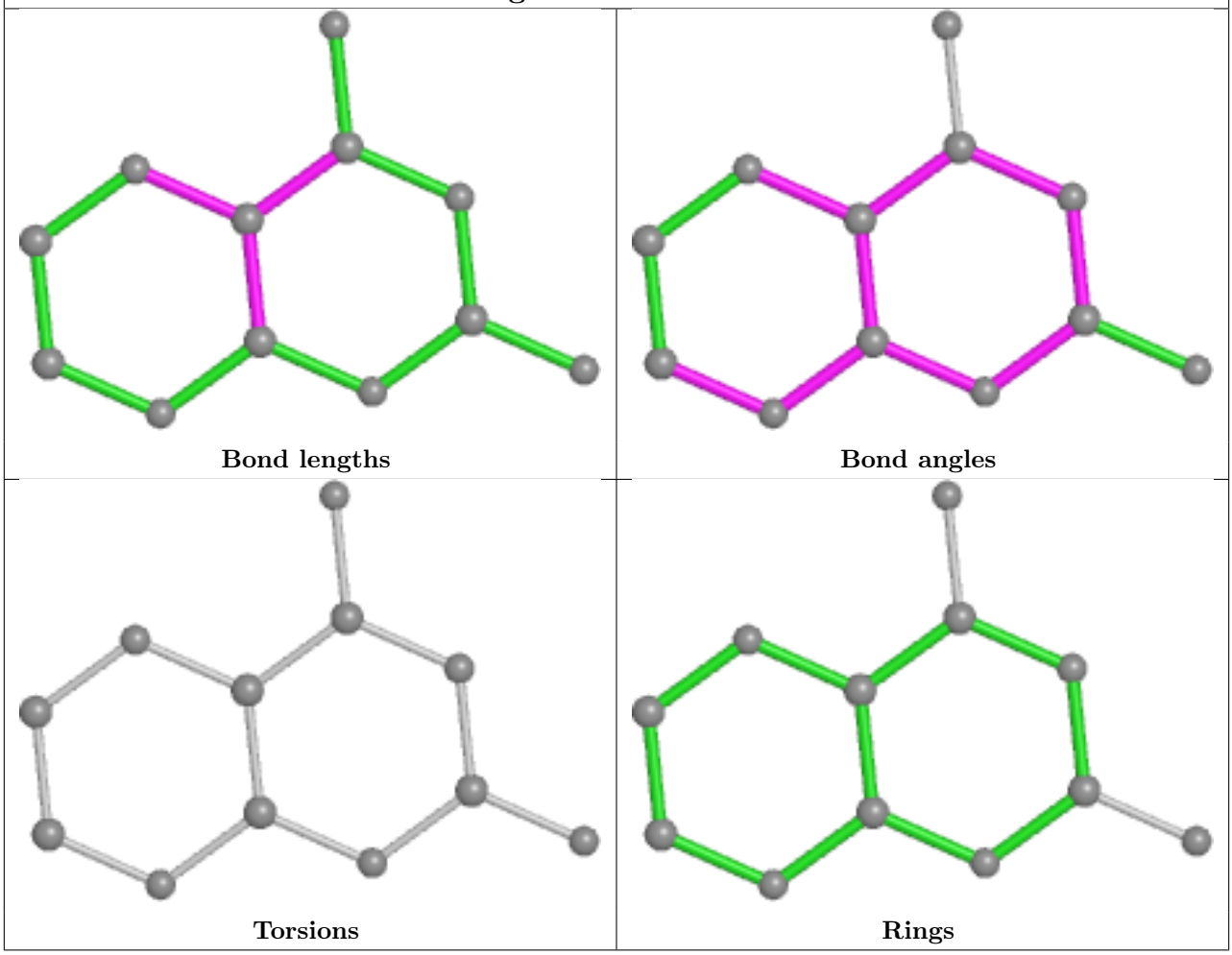
Ligand PE0 A 801

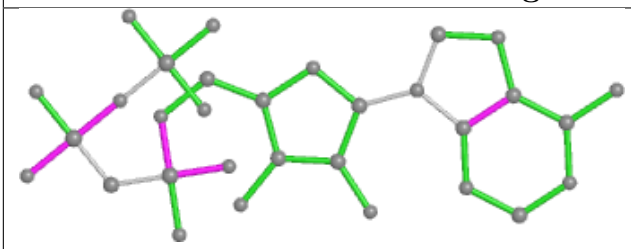
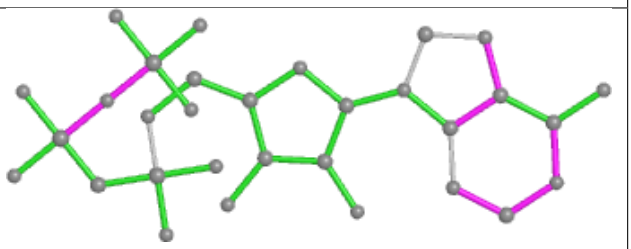
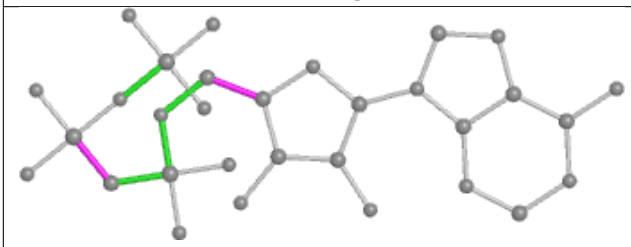
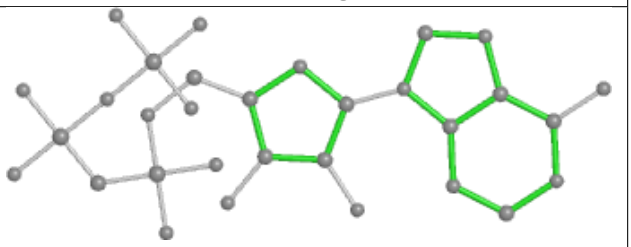


Ligand APC B 803



Ligand PE0 B 801



Ligand APC A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.07	50 (9%)	9	9	10, 31, 96, 120	0
1	B	562/728 (77%)	0.32	57 (10%)	7	6	9, 44, 106, 120	0
All	All	1113/1456 (76%)	0.19	107 (9%)	8	7	9, 37, 103, 120	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	CYS	5.6
1	A	84	TYR	5.2
1	A	468	ASN	5.0
1	A	708	ASP	4.9
1	A	366	ILE	4.9

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)

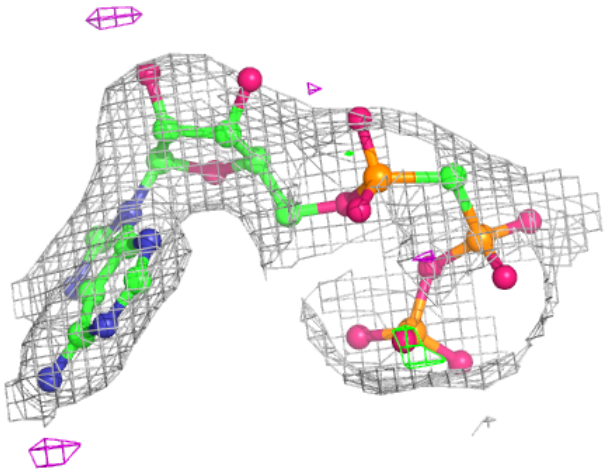
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

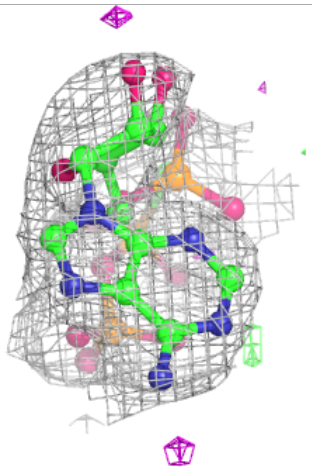
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	APC	B	803	31/31	0.90	0.13	42,73,100,105	0
4	APC	A	803	31/31	0.91	0.13	36,56,101,104	0
8	GOL	B	808	6/6	0.92	0.16	28,32,35,39	0
5	MG	B	805	1/1	0.93	0.17	50,50,50,50	0
6	CA	B	806	1/1	0.94	0.09	67,67,67,67	0
5	MG	B	804	1/1	0.94	0.13	61,61,61,61	0
8	GOL	A	807	6/6	0.95	0.13	21,23,24,25	0
5	MG	A	804	1/1	0.95	0.13	32,32,32,32	0
7	ACT	A	806	4/4	0.96	0.16	24,25,27,29	0
3	PHB	A	802	10/10	0.97	0.13	18,19,21,24	0
6	CA	A	805	1/1	0.97	0.08	34,34,34,34	0
2	PE0	B	801	12/12	0.98	0.12	14,15,16,16	0
3	PHB	B	802	10/10	0.98	0.09	20,21,23,25	0
2	PE0	A	801	12/12	0.99	0.16	12,13,13,13	0
7	ACT	B	807	4/4	0.99	0.12	15,16,17,17	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 APC B 803:

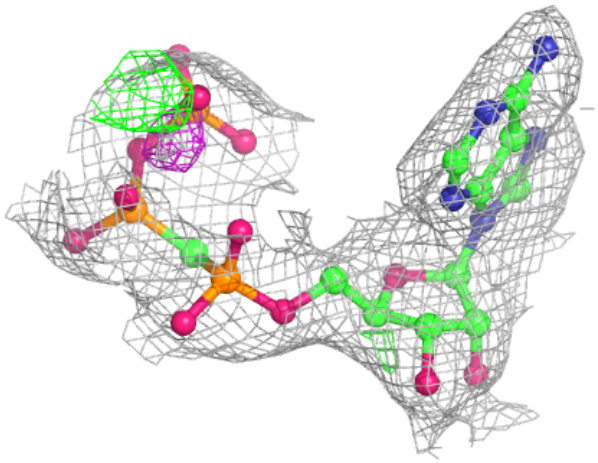
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

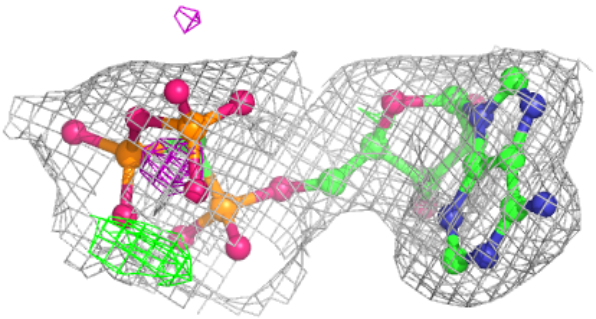


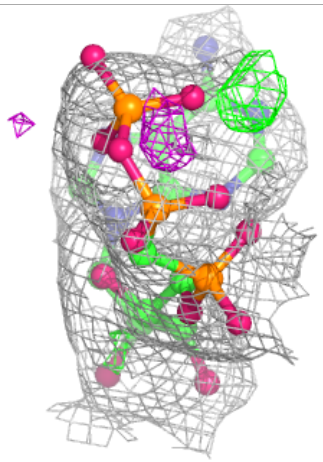


Electron density around APC A 803:

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

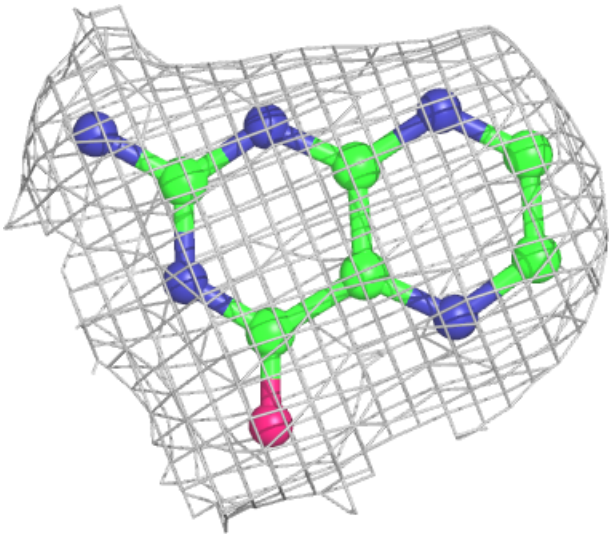


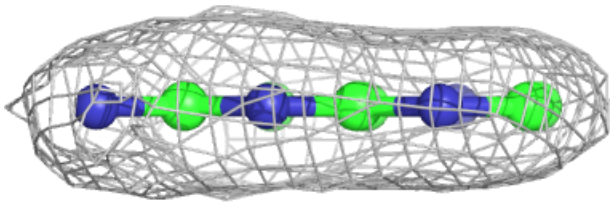


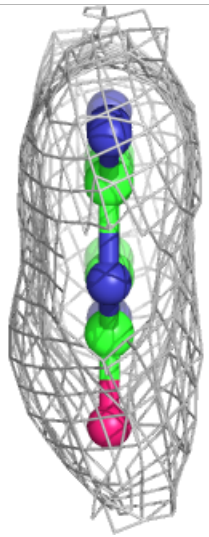


Electron density around PE0 B 801:

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

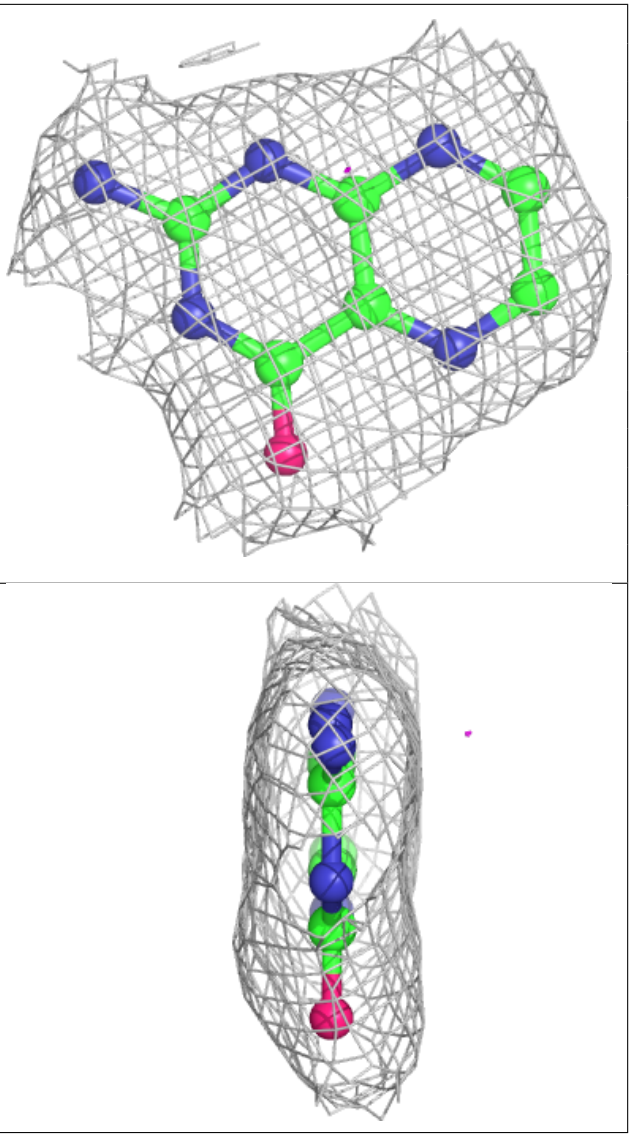






Electron density around PE0 A 801:

$2mF_o$-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.