



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:03 AM BST

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 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

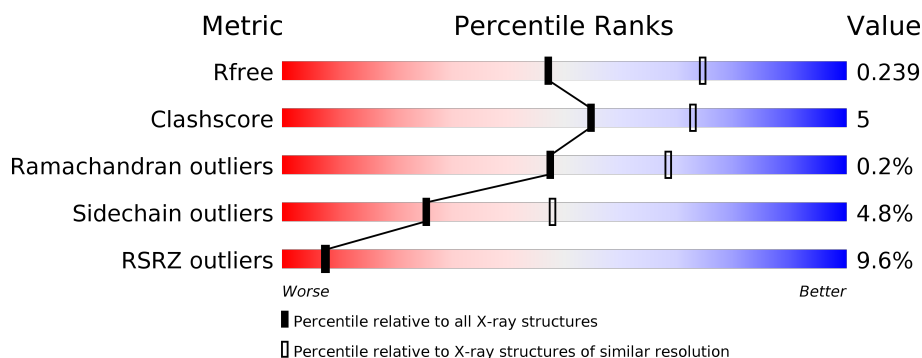
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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 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>7%</div> <div> <div></div> <div>66%</div> <div>9%</div> <div>24%</div> </div> </div>
1	B	728	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>14%</div> <div>23%</div> </div> </div>

2 Entry composition

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-dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4554	2934	754	844	22			
1	B	562	Total	C	N	O	S	0	0	0
			4615	2973	760	860	22			

There are 44 discrepancies between the modelled and reference sequences:

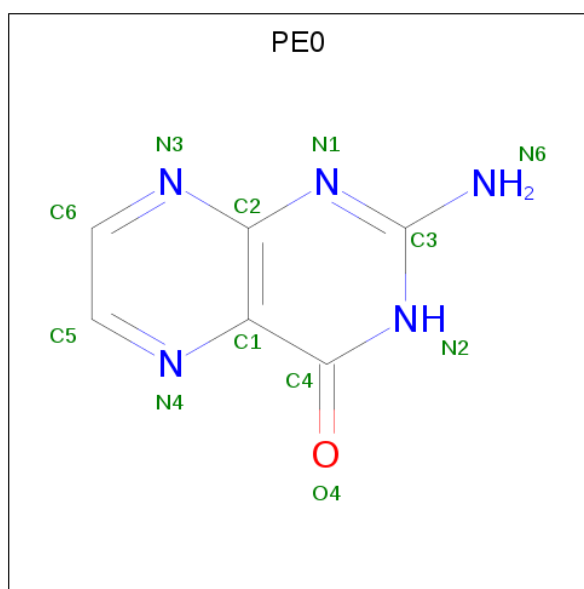
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag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

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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: C₆H₅N₅O) (labeled as "Ligand of Interest" by author).



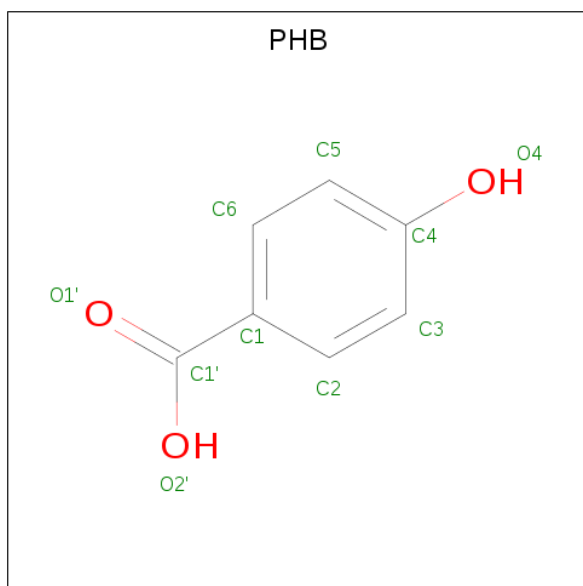
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	5	1		

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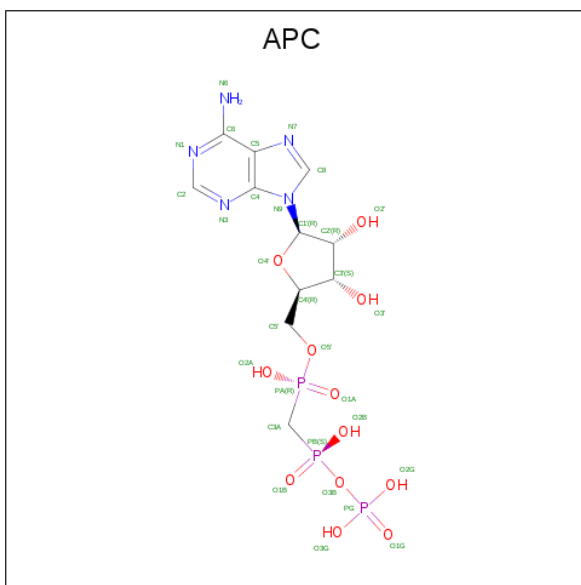
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			12	6	5	1		

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



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

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

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

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

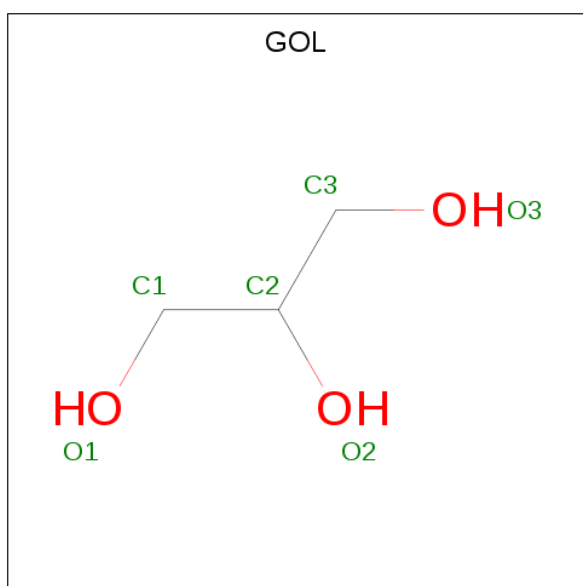
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

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



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

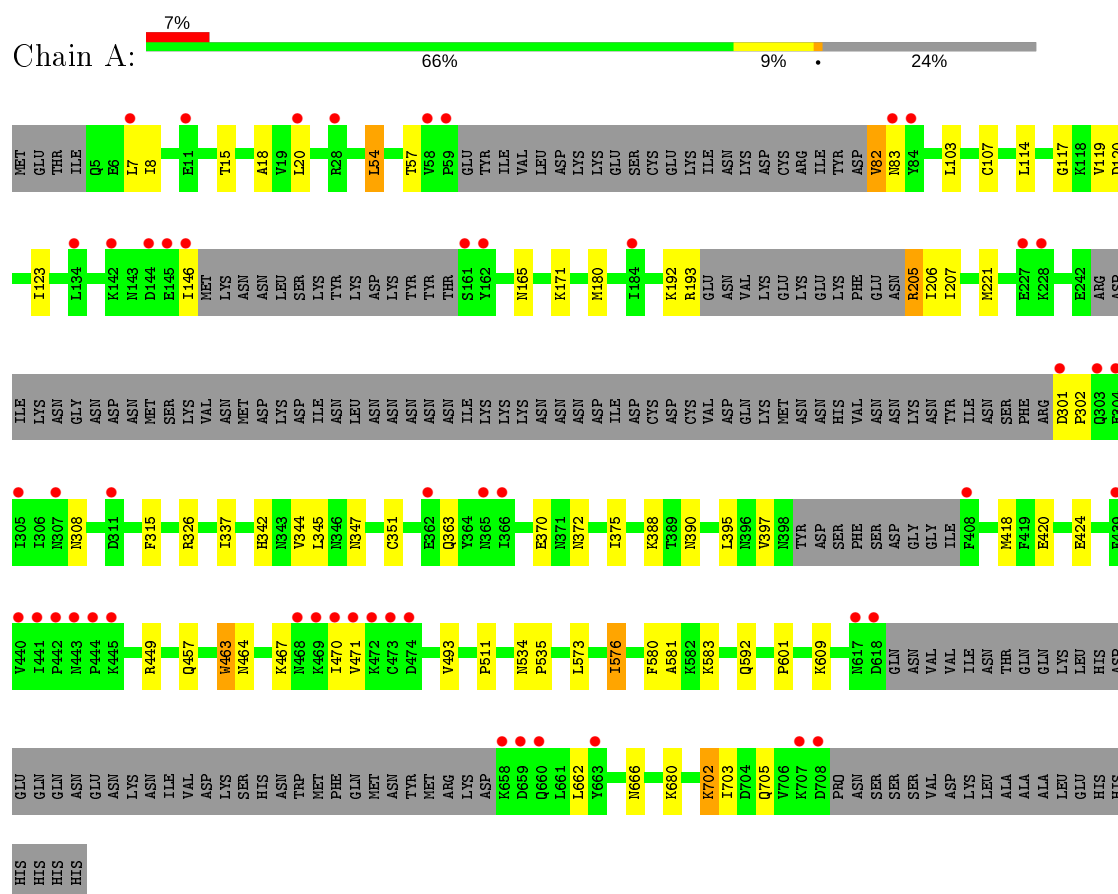
- Molecule 9 is water.

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

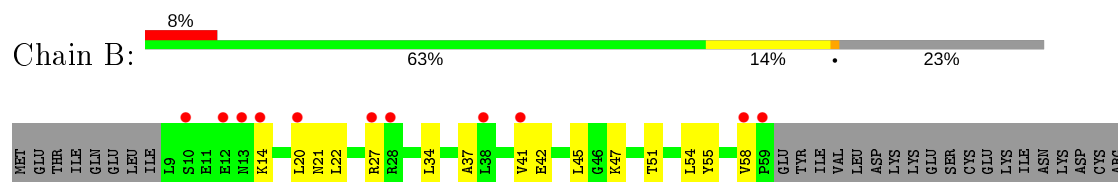
3 Residue-property plots

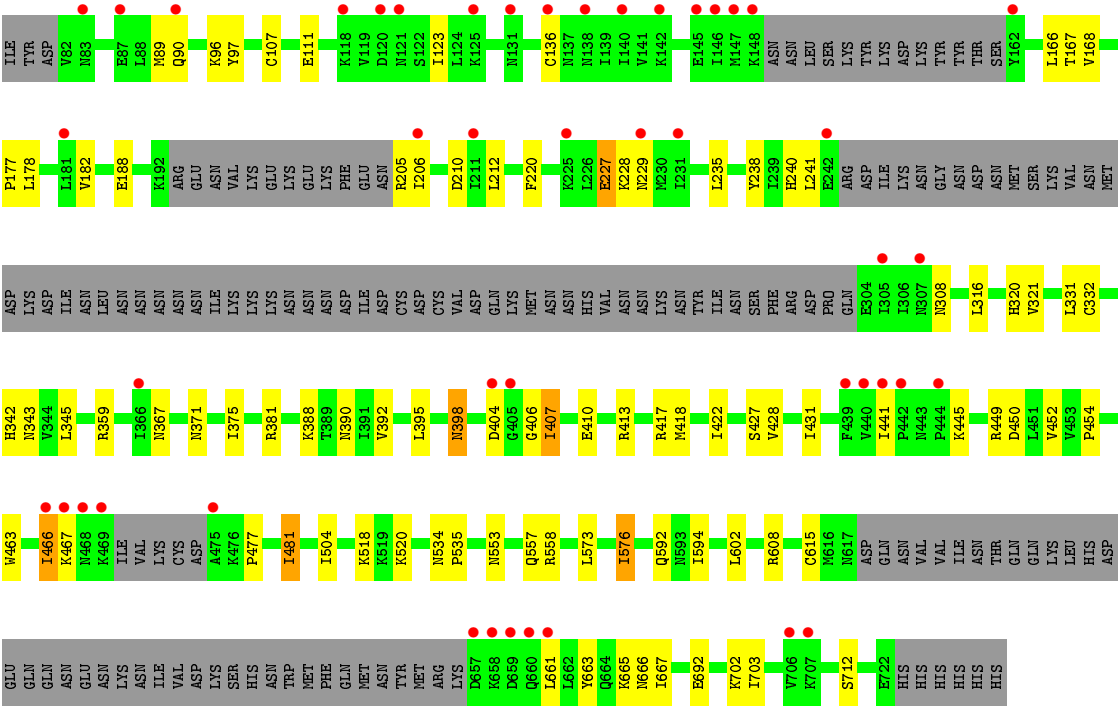
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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, ACT, APC

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

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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.

All (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
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.63	0.80
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.53	0.80
1:B:58:VAL:HG22	1:B:371:ASN:HB3	1.68	0.75
1:A:420:GLU:O	1:A:424:GLU:HG3	1.88	0.73
1:B:395:LEU:HD23	1:B:431:ILE:HD12	1.74	0.69
1:B:418:MET:O	1:B:422:ILE:HD12	1.94	0.68
3:B:802:PHB:C5	8:B:808:GOL:H11	2.25	0.67
1:B:553:ASN:O	1:B:557:GLN:HG2	1.96	0.65
1:B:608:ARG:HA	1:B:666:ASN:OD1	1.99	0.63
1:A:8:ILE:HG13	1:A:123:ILE:HD11	1.79	0.63
1:A:342:HIS:HB3	1:A:345:LEU:HG	1.81	0.62
1:A:592:GLN:HG2	1:B:703:ILE:O	1.99	0.62
1:B:21:ASN:HB2	1:B:212:LEU:HD11	1.83	0.61
1:B:398:ASN:H	1:B:398:ASN:HD22	1.47	0.61
1:B:407:ILE:HD13	1:B:407:ILE:N	2.17	0.59
1:B:51:THR:HG22	1:B:168:VAL:HG12	1.85	0.58
1:B:41:VAL:HG13	1:B:45:LEU:HD12	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:TRP:O	1:A:467:LYS:HB2	2.04	0.57
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.87	0.57
1:B:553:ASN:ND2	9:B:902:HOH:O	2.38	0.56
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.35	0.56
1:B:54:LEU:HD12	1:B:166:LEU:HB2	1.88	0.56
1:B:96:LYS:HE3	1:B:240:HIS:CE1	2.40	0.56
1:A:57:THR:HB	1:A:372:ASN:OD1	2.06	0.56
1:B:34:LEU:HD13	1:B:54:LEU:HD11	1.90	0.54
1:A:221:MET:O	1:A:315:PHE:HB2	2.08	0.54
1:B:367:ASN:HB2	9:B:988:HOH:O	2.08	0.53
1:B:594:ILE:HD11	1:B:602:LEU:HD21	1.90	0.53
1:B:692:GLU:N	1:B:692:GLU:OE1	2.40	0.53
1:B:177:PRO:HB2	1:B:316:LEU:HD21	1.91	0.53
1:B:342:HIS:HB3	1:B:345:LEU:HG	1.90	0.52
1:B:235:LEU:HB3	1:B:241:LEU:HD11	1.91	0.52
1:B:188:GLU:OE1	1:B:205:ARG:NH1	2.43	0.52
1:B:42:GLU:OE2	1:B:47:LYS:HA	2.10	0.52
1:B:452:VAL:HG11	1:B:481:ILE:CD1	2.40	0.51
1:B:404:ASP:HB2	1:B:406:GLY:H	1.76	0.51
1:B:21:ASN:C	1:B:22:LEU:HD12	2.31	0.51
1:B:210:ASP:HB3	1:B:320:HIS:CD2	2.46	0.51
1:A:470:ILE:HG22	1:A:471:VAL:N	2.27	0.50
1:A:471:VAL:HG13	1:A:471:VAL:O	2.12	0.50
1:B:410:GLU:HG3	1:B:413:ARG:HB2	1.94	0.50
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.43	0.49
1:B:37:ALA:O	1:B:41:VAL:HG23	2.12	0.49
1:B:54:LEU:CD1	1:B:166:LEU:HB2	2.42	0.49
1:A:107:CYS:SG	1:A:171:LYS:HD3	2.53	0.48
1:A:703:ILE:O	1:B:592:GLN:HG2	2.13	0.48
1:A:470:ILE:HG22	1:A:471:VAL:H	1.78	0.48
1:B:407:ILE:CD1	1:B:407:ILE:N	2.77	0.47
1:B:398:ASN:H	1:B:398:ASN:ND2	2.10	0.47
1:B:407:ILE:CD1	1:B:407:ILE:H	2.22	0.47
1:A:580:PHE:O	1:A:581:ALA:HB3	2.16	0.45
1:A:15:THR:CG2	1:A:171:LYS:HG3	2.46	0.45
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.99	0.45
1:A:464:ASN:OD1	1:A:467:LYS:NZ	2.50	0.45
1:A:54:LEU:HB3	1:A:375:ILE:HB	1.98	0.45
1:B:576:ILE:H	1:B:576:ILE:HD13	1.82	0.45
1:B:388:LYS:NZ	1:B:390:ASN:OD1	2.45	0.45
1:A:680:LYS:HA	1:A:680:LYS:HD3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:CG2	1:B:371:ASN:HB3	2.43	0.45
1:A:103:LEU:HD11	1:A:511:PRO:O	2.17	0.45
1:A:114:LEU:HD21	1:A:337:ILE:HG22	1.99	0.45
1:A:395:LEU:HD22	1:A:418:MET:CG	2.48	0.44
1:B:558:ARG:HD2	1:B:558:ARG:HA	1.67	0.44
1:A:576:ILE:H	1:A:576:ILE:HD13	1.83	0.44
1:B:55:TYR:CD2	1:B:331:LEU:HD21	2.53	0.44
1:A:301:ASP:HA	1:A:302:PRO:HD3	1.76	0.43
1:B:20:LEU:HB2	1:B:168:VAL:CG2	2.48	0.43
1:A:702:LYS:HG2	1:B:615:CYS:SG	2.58	0.43
1:A:609:LYS:NZ	2:A:801:PE0:O4	2.51	0.43
1:B:450:ASP:O	1:B:454:PRO:HG2	2.19	0.42
1:B:97:TYR:HE1	1:B:238:TYR:HD1	1.66	0.42
1:A:583:LYS:HE2	1:A:583:LYS:HB2	1.68	0.42
1:B:504:ILE:HG12	9:B:959:HOH:O	2.18	0.42
1:A:388:LYS:HD3	1:A:390:ASN:OD1	2.20	0.42
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.50	0.42
1:A:82:VAL:HB	1:A:83:ASN:H	1.68	0.42
1:B:395:LEU:HD23	1:B:431:ILE:CD1	2.46	0.42
1:B:167:THR:HG23	1:B:332:CYS:HB3	2.02	0.41
1:B:661:LEU:O	1:B:665:LYS:HG3	2.19	0.41
1:B:381:ARG:HA	1:B:381:ARG:HD3	1.81	0.41
1:A:206:ILE:HG23	1:A:207:ILE:HG22	2.02	0.41
1:B:392:VAL:HG22	1:B:428:VAL:HB	2.03	0.41
1:B:466:ILE:HG23	1:B:466:ILE:O	2.20	0.41
1:A:165:ASN:HB3	9:A:913:HOH:O	2.20	0.41
1:A:15:THR:HG21	1:A:171:LYS:HD2	2.03	0.40
1:B:107:CYS:O	1:B:111:GLU:HG2	2.22	0.40
1:B:178:LEU:O	1:B:182:VAL:HG23	2.21	0.40
1:B:227:GLU:C	1:B:229:ASN:H	2.24	0.40
1:B:54:LEU:HB3	1:B:375:ILE:HB	2.02	0.40
1:B:136:CYS:SG	1:B:321:VAL:HG13	2.60	0.40
1:B:422:ILE:HG12	1:B:477:PRO:HG3	2.02	0.40
1:A:397:VAL:HG23	1:A:397:VAL:O	2.22	0.40
1:B:667:ILE:N	1:B:667:ILE:HD13	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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

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

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	54	LEU
1	A	82	VAL
1	A	119	VAL

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Mol	Chain	Res	Type
1	A	120	ASP
1	A	146	ILE
1	A	193	ARG
1	A	205	ARG
1	A	308	ASN
1	A	326	ARG
1	A	344	VAL
1	A	347	ASN
1	A	351	CYS
1	A	363	GLN
1	A	370	GLU
1	A	449	ARG
1	A	457	GLN
1	A	493	VAL
1	A	576	ILE
1	A	662	LEU
1	A	666	ASN
1	A	702	LYS
1	A	705	GLN
1	B	14	LYS
1	B	27	ARG
1	B	89	MET
1	B	90	GLN
1	B	123	ILE
1	B	206	ILE
1	B	220	PHE
1	B	227	GLU
1	B	308	ASN
1	B	343	ASN
1	B	359	ARG
1	B	398	ASN
1	B	407	ILE
1	B	417	ARG
1	B	427	SER
1	B	441	ILE
1	B	445	LYS
1	B	449	ARG
1	B	466	ILE
1	B	467	LYS
1	B	481	ILE
1	B	518	LYS
1	B	520	LYS

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Mol	Chain	Res	Type
1	B	573	LEU
1	B	576	ILE
1	B	663	TYR
1	B	702	LYS
1	B	712	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	343	ASN
1	A	457	GLN
1	A	660	GLN
1	B	398	ASN
1	B	553	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
2	PE0	B	801	-	13,13,13	2.06	3 (23%)	15,18,18	3.46	10 (66%)
8	GOL	B	808	-	5,5,5	0.57	0	5,5,5	1.31	0
3	PHB	A	802	-	8,10,10	1.10	1 (12%)	10,13,13	1.02	0
8	GOL	A	807	-	5,5,5	0.41	0	5,5,5	1.21	1 (20%)
4	APC	A	803	5	27,33,33	1.43	5 (18%)	31,52,52	1.38	4 (12%)
4	APC	B	803	5	27,33,33	1.51	5 (18%)	31,52,52	1.39	4 (12%)
3	PHB	B	802	-	8,10,10	0.78	0	10,13,13	1.40	3 (30%)
7	ACT	B	807	-	1,3,3	1.03	0	0,3,3	0.00	-
2	PE0	A	801	-	13,13,13	1.66	2 (15%)	15,18,18	3.04	8 (53%)
7	ACT	A	806	-	1,3,3	0.78	0	0,3,3	0.00	-

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	PE0	B	801	-	-	-	0/2/2/2
8	GOL	B	808	-	-	2/4/4/4	-
3	PHB	A	802	-	-	0/0/4/4	0/1/1/1
8	GOL	A	807	-	-	2/4/4/4	-
4	APC	A	803	5	-	5/15/38/38	0/3/3/3
4	APC	B	803	5	-	6/15/38/38	0/3/3/3
3	PHB	B	802	-	-	0/0/4/4	0/1/1/1
2	PE0	A	801	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	PE0	C4-C1	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
4	B	803	APC	PB-O3B	2.99	1.61	1.58
2	A	801	PE0	C4-C1	2.99	1.46	1.41
4	B	803	APC	C5-C4	2.84	1.48	1.40
4	A	803	APC	C5-C4	2.80	1.48	1.40
2	B	801	PE0	C1-N4	2.80	1.37	1.33
3	A	802	PHB	C1-C1'	2.76	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	APC	PA-O5'	2.63	1.61	1.57
4	B	803	APC	PA-O2A	2.47	1.62	1.56
4	A	803	APC	PB-O2B	2.22	1.61	1.56
4	A	803	APC	PA-O2A	2.18	1.61	1.56
4	B	803	APC	PB-O2B	2.18	1.61	1.56

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C4-N2-C3	4.43	122.97	115.93
2	B	801	PE0	C4-C1-C2	-4.33	117.08	119.95
2	A	801	PE0	C1-C4-N2	-4.10	117.83	123.43
4	A	803	APC	N3-C2-N1	-3.98	122.46	128.68
2	B	801	PE0	C1-C4-N2	-3.97	118.00	123.43
2	A	801	PE0	C3-N1-C2	3.84	119.74	115.36
2	B	801	PE0	C4-N2-C3	3.81	121.97	115.93
2	A	801	PE0	C4-C1-C2	-3.72	117.49	119.95
2	B	801	PE0	N1-C3-N2	-3.68	122.31	127.22
2	A	801	PE0	N1-C3-N2	-3.56	122.48	127.22
4	B	803	APC	N3-C2-N1	-3.54	123.14	128.68
4	B	803	APC	C3'-C2'-C1'	3.13	105.68	100.98
2	B	801	PE0	C2-C1-N4	-3.01	118.84	122.32
4	A	803	APC	PG-O3B-PB	-2.92	122.33	132.62
2	B	801	PE0	C6-N3-C2	2.79	120.05	116.60
4	B	803	APC	PG-O3B-PB	-2.52	123.75	132.62
2	A	801	PE0	C6-N3-C2	2.51	119.69	116.60
3	B	802	PHB	C5-C6-C1	-2.47	117.58	121.13
4	A	803	APC	C2-N1-C6	2.32	122.72	118.75
4	A	803	APC	C4-C5-N7	-2.27	107.03	109.40
4	B	803	APC	C2'-C3'-C4'	2.16	106.84	102.64
3	B	802	PHB	C2-C1-C1'	-2.16	117.47	120.37
2	A	801	PE0	C4-C1-N4	2.10	120.86	118.24
8	A	807	GOL	O1-C1-C2	-2.10	100.12	110.20
3	B	802	PHB	C6-C1-C2	2.08	121.73	117.59
2	B	801	PE0	C1-C2-N1	-2.07	118.33	121.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	808	GOL	C1-C2-C3-O3
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
4	B	803	APC	PA-C3A-PB-O2B
4	A	803	APC	O4'-C4'-C5'-O5'
4	B	803	APC	O4'-C4'-C5'-O5'
4	B	803	APC	C3'-C4'-C5'-O5'
8	B	808	GOL	O2-C2-C3-O3
4	B	803	APC	C4'-C5'-O5'-PA
8	A	807	GOL	O1-C1-C2-O2
4	B	803	APC	PA-C3A-PB-O3B
8	A	807	GOL	O1-C1-C2-C3

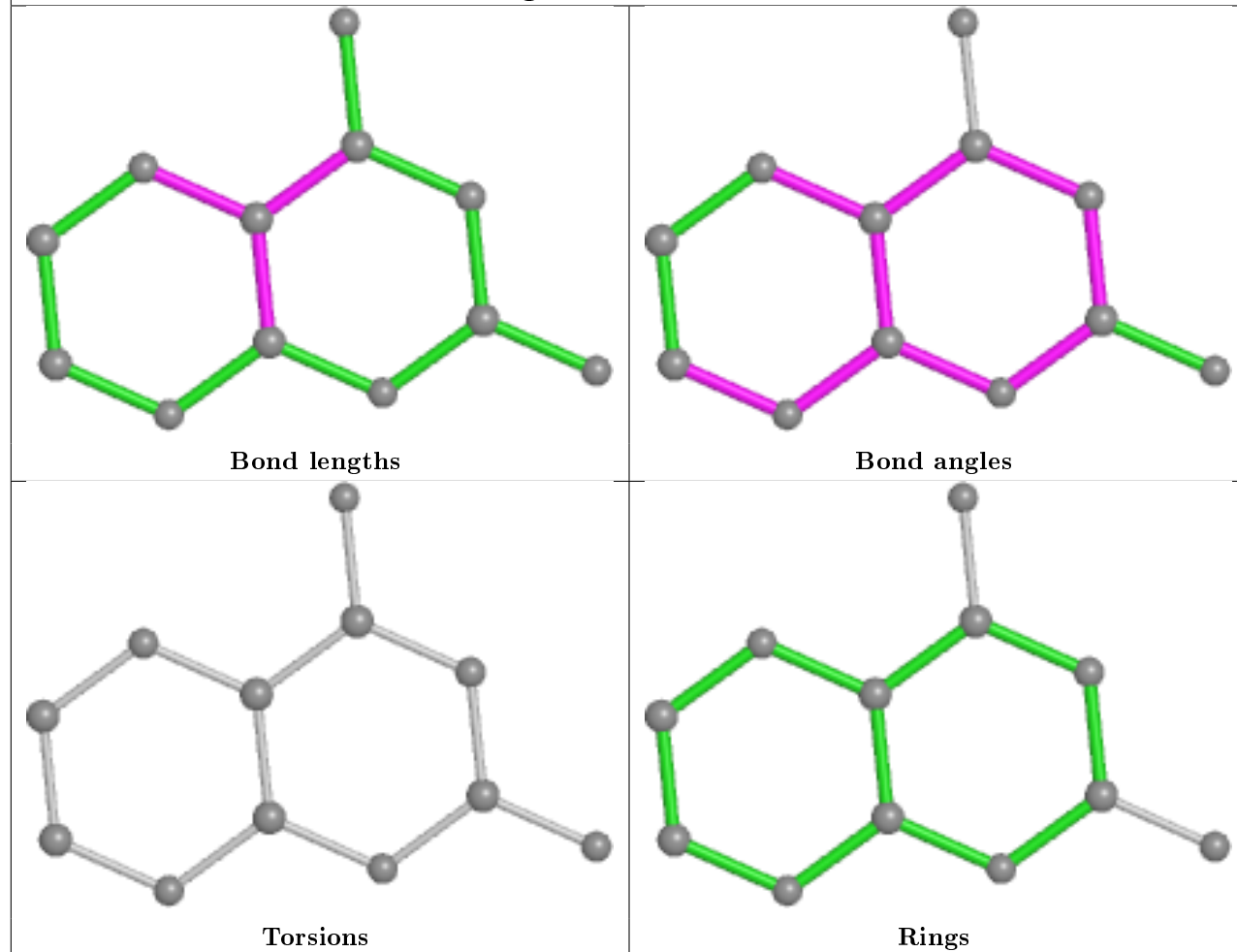
There are no ring outliers.

3 monomers are involved in 3 short contacts:

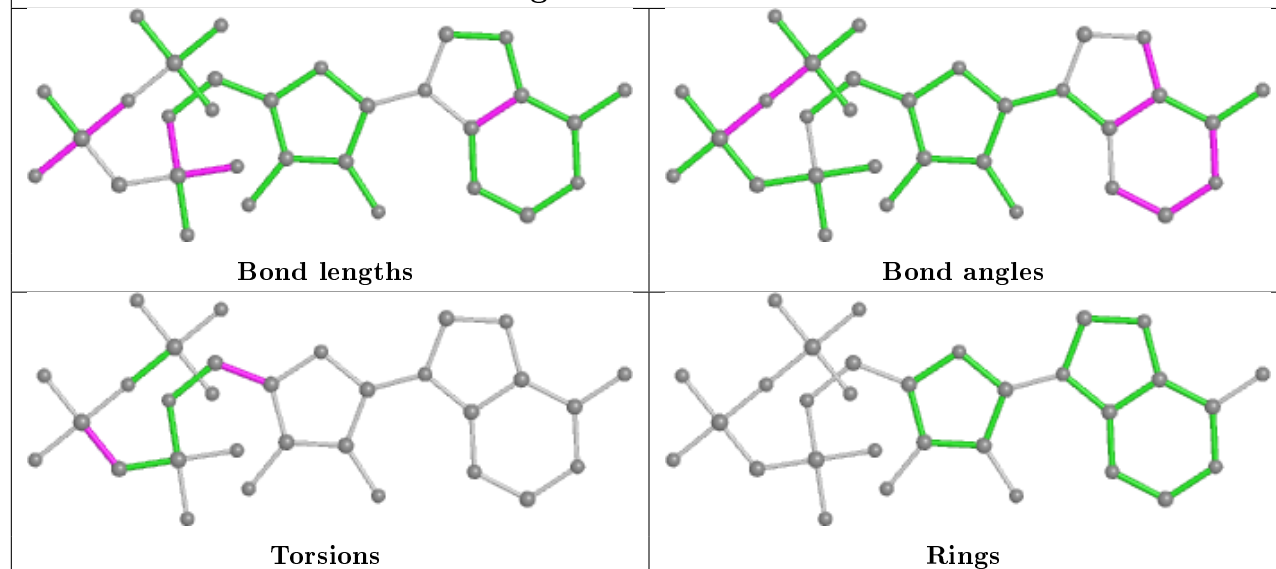
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	808	GOL	2	0
3	B	802	PHB	2	0
2	A	801	PE0	1	0

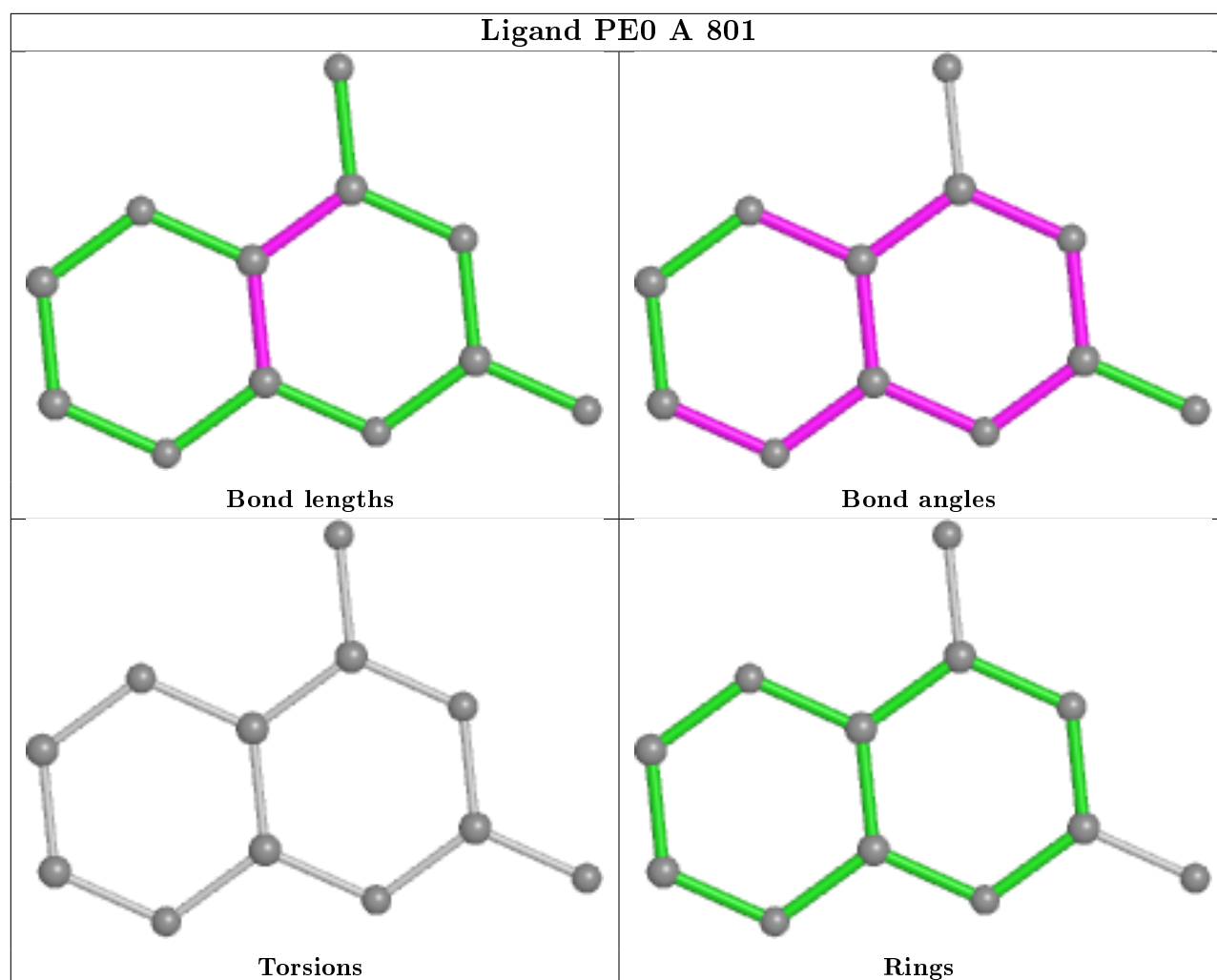
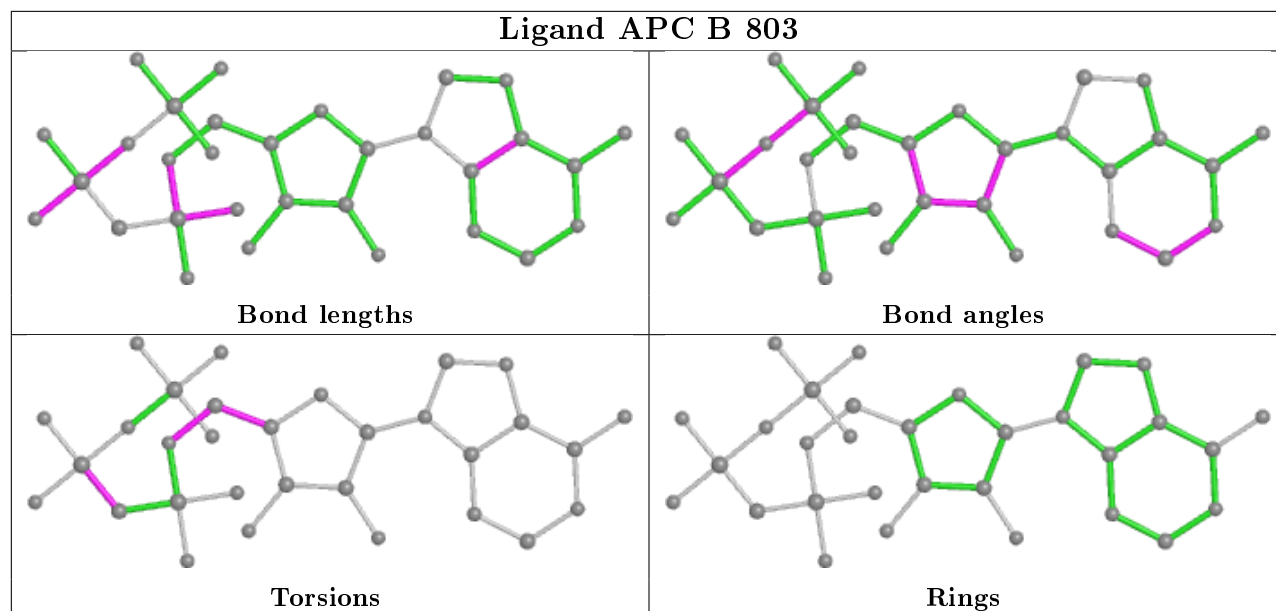
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PE0 B 801



Ligand APC A 803





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%)	0.07	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

All (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
1	B	146	ILE	4.6
1	B	404	ASP	4.5
1	B	468	ASN	4.5
1	B	444	PRO	4.3
1	A	658	LYS	4.2
1	B	87	GLU	4.2
1	B	136	CYS	4.2
1	B	658	LYS	4.1
1	B	147	MET	4.0
1	A	469	LYS	3.9
1	B	405	GLY	3.9
1	A	618	ASP	3.9
1	A	444	PRO	3.9
1	B	441	ILE	3.7
1	A	470	ILE	3.7
1	B	206	ILE	3.6
1	A	28	ARG	3.6
1	B	162	TYR	3.6
1	A	303	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLN	3.5
1	B	120	ASP	3.5
1	A	146	ILE	3.5
1	A	442	PRO	3.5
1	B	225	LYS	3.4
1	A	471	VAL	3.4
1	A	408	PHE	3.4
1	A	162	TYR	3.4
1	B	13	ASN	3.3
1	A	659	ASP	3.3
1	A	445	LYS	3.2
1	B	466	ILE	3.2
1	A	439	PHE	3.2
1	A	472	LYS	3.2
1	B	10	SER	3.2
1	B	242	GLU	3.1
1	B	307	ASN	3.1
1	B	83	ASN	3.0
1	B	145	GLU	3.0
1	B	12	GLU	3.0
1	A	301	ASP	2.9
1	B	231	ILE	2.9
1	B	440	VAL	2.8
1	B	125	LYS	2.8
1	A	311	ASP	2.8
1	B	14	LYS	2.8
1	B	148	LYS	2.8
1	A	7	LEU	2.8
1	B	467	LYS	2.8
1	A	304	GLU	2.7
1	B	475	ALA	2.7
1	A	228	LYS	2.7
1	A	20	LEU	2.7
1	B	706	VAL	2.6
1	A	441	ILE	2.6
1	B	59	PRO	2.6
1	B	659	ASP	2.6
1	B	142	LYS	2.6
1	B	28	ARG	2.6
1	A	142	LYS	2.6
1	A	161	SER	2.6
1	A	59	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	660	GLN	2.6
1	B	366	ILE	2.5
1	B	442	PRO	2.5
1	B	41	VAL	2.5
1	A	707	LYS	2.5
1	B	118	LYS	2.5
1	A	144	ASP	2.5
1	A	134	LEU	2.4
1	B	469	LYS	2.4
1	B	138	ASN	2.4
1	A	145	GLU	2.4
1	B	121	ASN	2.4
1	B	131	ASN	2.3
1	B	58	VAL	2.3
1	A	443	ASN	2.3
1	B	661	LEU	2.3
1	A	184	ILE	2.2
1	A	362	GLU	2.2
1	B	305	ILE	2.2
1	B	439	PHE	2.2
1	A	11	GLU	2.2
1	B	211	ILE	2.2
1	A	58	VAL	2.2
1	A	305	ILE	2.2
1	A	474	ASP	2.2
1	A	440	VAL	2.1
1	A	617	ASN	2.1
1	A	227	GLU	2.1
1	A	365	ASN	2.1
1	A	83	ASN	2.1
1	B	140	ILE	2.1
1	B	707	LYS	2.1
1	B	20	LEU	2.1
1	B	38	LEU	2.1
1	B	229	ASN	2.1
1	B	660	GLN	2.1
1	B	27	ARG	2.1
1	B	657	ASP	2.0
1	A	663	TYR	2.0
1	B	181	LEU	2.0
1	A	307	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](#)

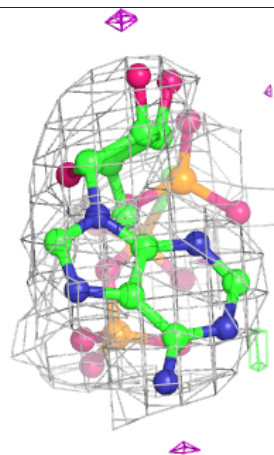
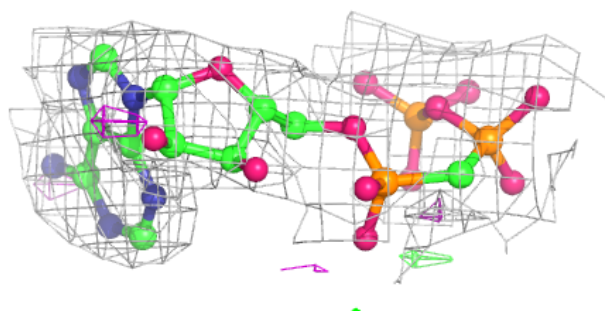
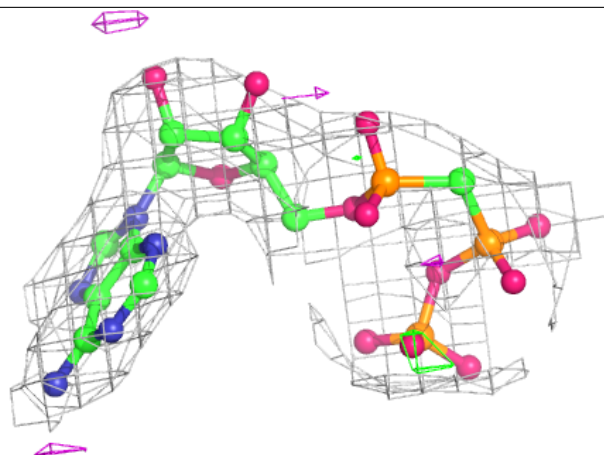
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
5	MG	A	804	1/1	0.95	0.13	32,32,32,32	0
8	GOL	A	807	6/6	0.95	0.13	21,23,24,25	0
7	ACT	A	806	4/4	0.96	0.16	24,25,27,29	0
6	CA	A	805	1/1	0.97	0.08	34,34,34,34	0
3	PHB	A	802	10/10	0.97	0.13	18,19,21,24	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.

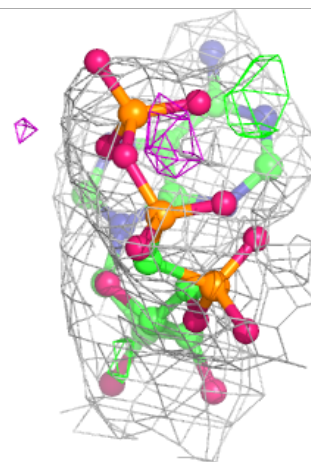
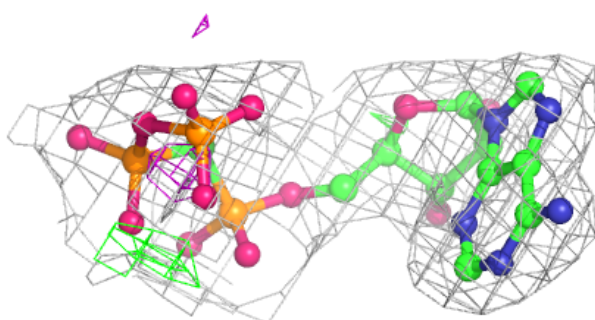
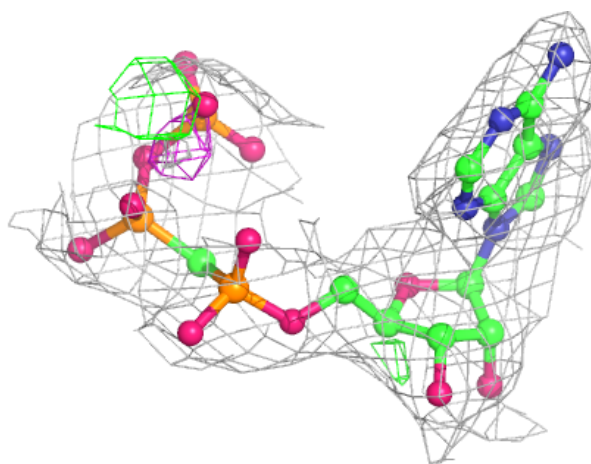
Electron density around APC B 803:

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



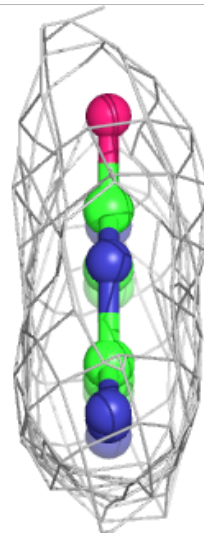
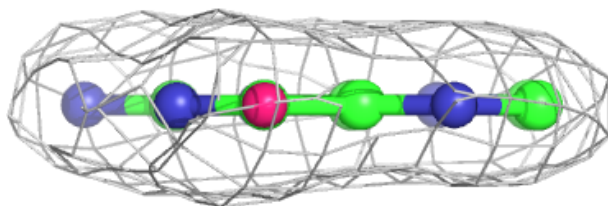
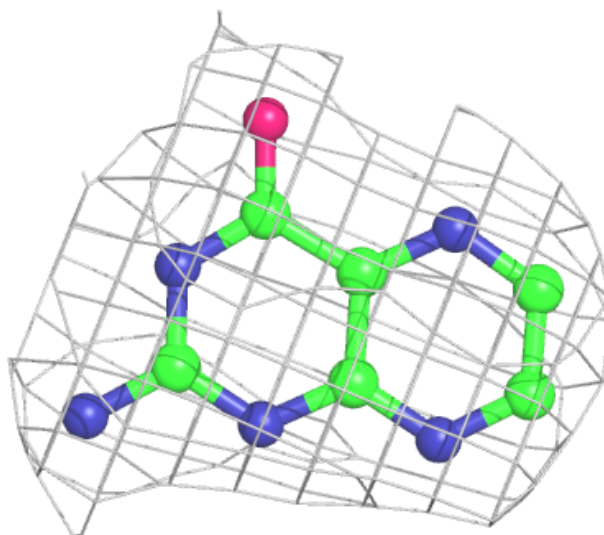
Electron density around APC A 803:

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



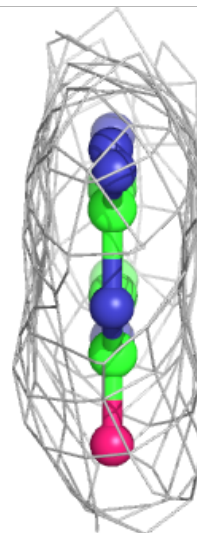
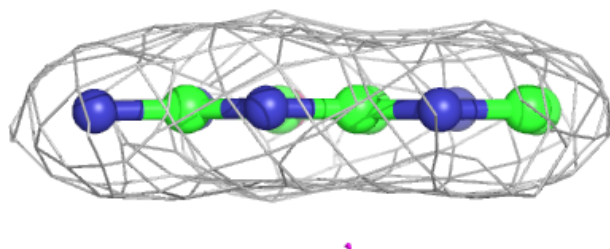
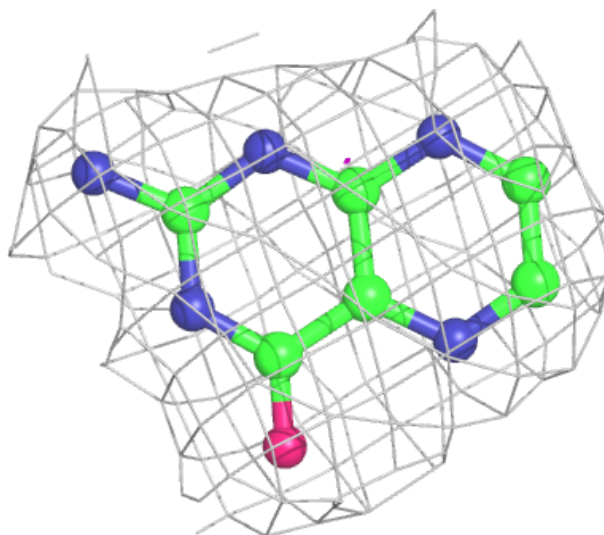
Electron density around PE0 B 801:

$2mF_o-DF_c$ (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.