



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:53 AM UTC

PDB ID : 6KCK / pdb_00006kck
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

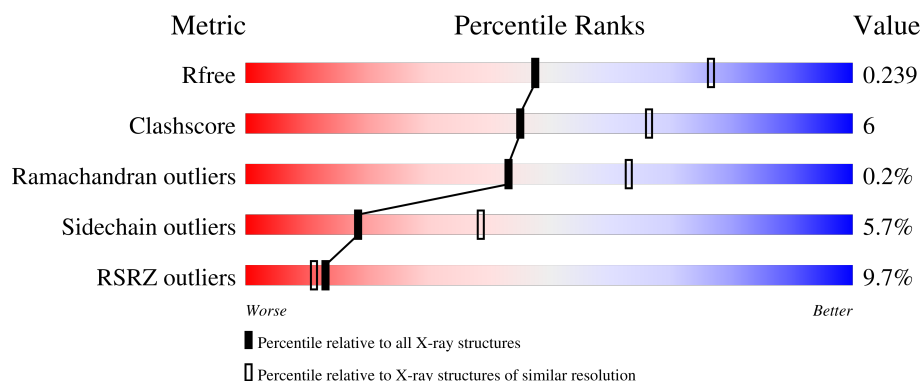
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	5% 65% 10% • 24%
1	B	728	9% 61% 15% • 23%

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:

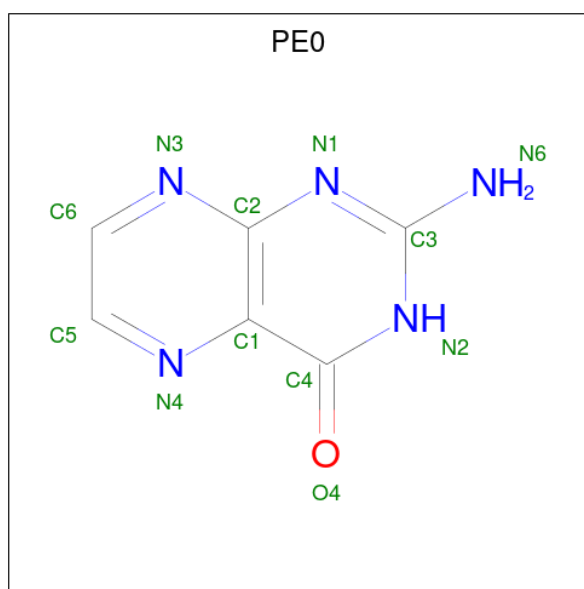
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	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 (CCD ID: PE0) (formula: C₆H₅N₅O) (labeled as "Ligand of Interest" by depositor).



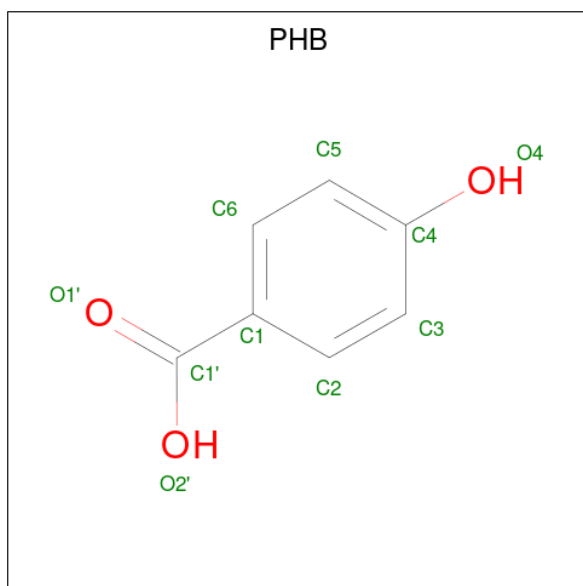
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	5	1		

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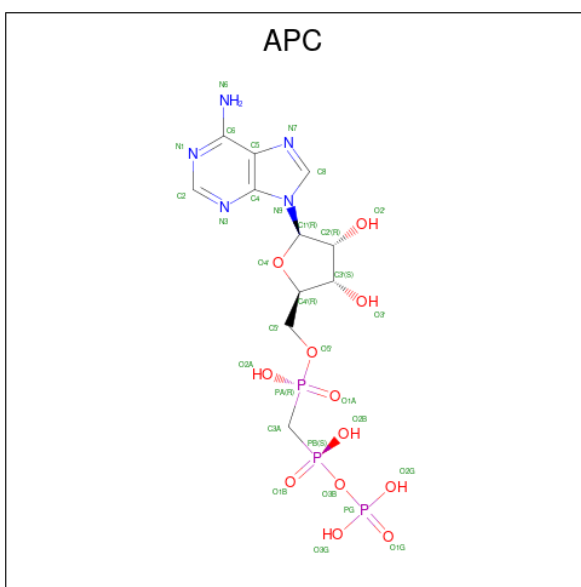
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			12	6	5	1		

- Molecule 3 is P-HYDROXYBENZOIC ACID (CCD ID: 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 (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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		

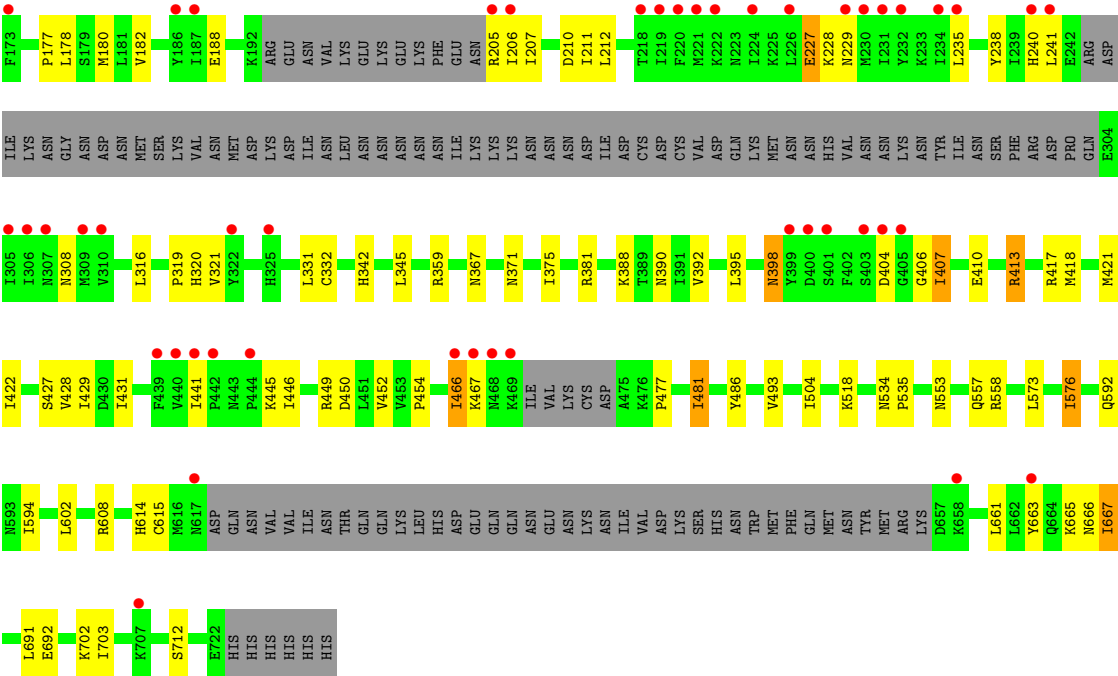
- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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



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 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-2.50) 92.0 (30.00-2.50)	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 (9.22%)	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)	0.32 , 42.4	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	0.94	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, APC, ACT, CA, PE0, PHB, 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	0.79	0/4627	0.93	2/6243 (0.0%)
1	B	0.75	1/4690 (0.0%)	0.95	0/6329
All	All	0.77	1/9317 (0.0%)	0.94	2/12572 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	614	HIS	CG-CD2	5.43	1.41	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	ASP	N-CA-C	5.90	117.79	111.36
1	A	7	LEU	N-CA-C	-5.01	106.94	113.16

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	44	0
1	B	4615	0	4703	68	0
2	A	12	0	5	1	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	0	0
3	B	10	0	4	2	0
4	A	31	0	14	0	0
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	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (111) 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:192:LYS:HE3	1:A:205:ARG:HG3	1.50	0.91
1:A:20:LEU:HD21	1:A:180:MET:HE3	1.52	0.90
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
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:20:LEU:CD2	1:A:180:MET:HE3	2.31	0.57
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:54:LEU:HD12	1:B:166:LEU:HB2	1.88	0.56
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.35	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:21:ASN:C	1:B:22:LEU:HD12	2.31	0.55
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:OE1	1:B:692:GLU:N	2.40	0.53
1:A:18:ALA:CB	1:A:180:MET:HE1	2.36	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: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:O	1:A:471:VAL:HG13	2.12	0.50
1:A:180:MET:HE2	1:A:211:ILE:HD13	1.93	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:N	1:B:407:ILE:CD1	2.77	0.47
1:B:398:ASN:H	1:B:398:ASN:ND2	2.10	0.47
1:B:407:ILE:H	1:B:407:ILE:CD1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:HE3	1:B:429:ILE:HD12	1.96	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:54:LEU:HB3	1:A:375:ILE:HB	1.98	0.45
1:A:464:ASN:OD1	1:A:467:LYS:NZ	2.50	0.45
1:B:132:TYR:OH	1:B:319:PRO:O	2.28	0.45
1:B:576:ILE:H	1:B:576:ILE:HD13	1.82	0.45
1:B:227:GLU:C	1:B:229:ASN:H	2.24	0.45
1:B:388:LYS:NZ	1:B:390:ASN:OD1	2.45	0.45
1:A:680:LYS:HD3	1:A:680:LYS:HA	1.71	0.45
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:180:MET:HE3	1:B:211:ILE:HD13	1.99	0.44
1:B:558:ARG:HA	1:B:558:ARG:HD2	1.67	0.44
1:A:576:ILE:HD13	1:A:576:ILE:H	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:B:449:ARG:HD3	1:B:449:ARG:C	2.43	0.43
1:B:691:LEU:C	1:B:691:LEU:HD23	2.44	0.43
1:A:609:LYS:NZ	2:A:801:PEO:O4	2.51	0.43
1:A:702:LYS:HG2	1:B:615:CYS:SG	2.58	0.43
1:A:20:LEU:HD21	1:A:180:MET:HE1	1.96	0.43
1:B:227:GLU:C	1:B:229:ASN:N	2.77	0.43
1:B:97:TYR:HE1	1:B:238:TYR:HD1	1.66	0.42
1:B:450:ASP:O	1:B:454:PRO:HG2	2.19	0.42
1:A:583:LYS:HB2	1:A:583:LYS:HE2	1.68	0.42
1:B:18:ALA:HB1	1:B:180:MET:HE1	2.01	0.42
1:B:504:ILE:HG12	9:B:959:HOH:O	2.18	0.42
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.50	0.42
1:A:388:LYS:HD3	1:A:390:ASN:OD1	2.20	0.42
1:B:486:TYR:CD1	1:B:486:TYR:C	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ILE:O	1:B:466:ILE:HG23	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:54:LEU:HB3	1:B:375:ILE:HB	2.02	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: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:B:534:ASN:C	1:B:534:ASN:OD1	2.64	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 [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%)	43	63
1	B	548/728 (75%)	519 (95%)	28 (5%)	1 (0%)	43	63
All	All	1085/1456 (74%)	1036 (96%)	47 (4%)	2 (0%)	43	63

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%)	497 (95%)	28 (5%)	20	42
1	B	529/696 (76%)	497 (94%)	32 (6%)	17	36
All	All	1054/1392 (76%)	994 (94%)	60 (6%)	18	39

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	12	GLU
1	A	54	LEU
1	A	82	VAL
1	A	85	ILE
1	A	96	LYS
1	A	111	GLU
1	A	119	VAL
1	A	120	ASP
1	A	123	ILE
1	A	134	LEU
1	A	146	ILE
1	A	180	MET
1	A	193	ARG
1	A	304	GLU
1	A	344	VAL
1	A	347	ASN
1	A	351	CYS
1	A	363	GLN
1	A	370	GLU
1	A	457	GLN
1	A	469	LYS
1	A	493	VAL
1	A	576	ILE
1	A	583	LYS
1	A	662	LEU
1	A	666	ASN

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Mol	Chain	Res	Type
1	A	702	LYS
1	B	14	LYS
1	B	15	THR
1	B	27	ARG
1	B	57	THR
1	B	89	MET
1	B	90	GLN
1	B	119	VAL
1	B	123	ILE
1	B	206	ILE
1	B	207	ILE
1	B	227	GLU
1	B	308	ASN
1	B	359	ARG
1	B	398	ASN
1	B	407	ILE
1	B	413	ARG
1	B	417	ARG
1	B	427	SER
1	B	441	ILE
1	B	445	LYS
1	B	446	ILE
1	B	466	ILE
1	B	467	LYS
1	B	481	ILE
1	B	493	VAL
1	B	518	LYS
1	B	573	LEU
1	B	576	ILE
1	B	663	TYR
1	B	667	ILE
1	B	702	LYS
1	B	712	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	29	ASN
1	A	137	ASN
1	A	138	ASN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	308	ASN
1	A	325	HIS
1	A	343	ASN
1	A	457	GLN
1	A	495	ASN
1	A	660	GLN
1	A	705	GLN
1	B	229	ASN
1	B	398	ASN
1	B	553	ASN
1	B	705	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.40	1 (7%)	15,18,18	1.83	4 (26%)
2	PE0	A	801	-	13,13,13	1.43	1 (7%)	15,18,18	1.58	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	A	806	-	3,3,3	0.92	0	3,3,3	0.23	0
7	ACT	B	807	-	3,3,3	0.92	0	3,3,3	0.69	0
3	PHB	A	802	-	10,10,10	0.87	0	13,13,13	1.02	1 (7%)
8	GOL	B	808	-	5,5,5	0.58	0	5,5,5	1.39	0
4	APC	B	803	5	29,33,33	1.63	6 (20%)	44,52,52	1.86	10 (22%)
3	PHB	B	802	-	10,10,10	0.86	0	13,13,13	1.43	2 (15%)
8	GOL	A	807	-	5,5,5	0.42	0	5,5,5	1.31	1 (20%)
4	APC	A	803	5	29,33,33	1.68	7 (24%)	44,52,52	1.97	9 (20%)

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
2	PE0	A	801	-	-	-	0/2/2/2
3	PHB	A	802	-	-	0/4/4/4	0/1/1/1
8	GOL	B	808	-	-	2/4/4/4	-
4	APC	B	803	5	-	9/19/38/38	0/3/3/3
3	PHB	B	802	-	-	0/4/4/4	0/1/1/1
8	GOL	A	807	-	-	1/4/4/4	-
4	APC	A	803	5	-	5/19/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	APC	C5-C4	5.25	1.48	1.39
4	A	803	APC	C5-C4	5.18	1.48	1.39
2	A	801	PE0	C1-C2	3.72	1.48	1.40
2	B	801	PE0	C1-C2	3.54	1.47	1.40
4	A	803	APC	PB-O3B	3.06	1.61	1.58
4	A	803	APC	C5-C6	3.00	1.49	1.41
4	B	803	APC	PB-O3B	2.96	1.61	1.58
4	B	803	APC	C5-C6	2.76	1.48	1.41
4	A	803	APC	C5-N7	-2.54	1.34	1.39
4	B	803	APC	C8-N7	2.47	1.36	1.31
4	B	803	APC	PA-O2A	2.37	1.62	1.56
4	A	803	APC	C8-N7	2.24	1.36	1.31
4	A	803	APC	PB-O2B	2.13	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	APC	PA-O2A	2.10	1.61	1.56
4	B	803	APC	PB-O2B	2.09	1.61	1.56

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	APC	C5-C4-N3	-6.42	117.88	126.72
4	B	803	APC	C5-C4-N3	-5.89	118.60	126.72
4	A	803	APC	N3-C4-N9	5.08	135.81	127.17
4	B	803	APC	N3-C4-N9	5.02	135.71	127.17
4	A	803	APC	C2-N3-C4	4.28	122.29	111.83
4	A	803	APC	N3-C2-N1	-4.04	122.46	128.58
4	B	803	APC	C2-N3-C4	3.77	121.03	111.83
4	B	803	APC	N3-C2-N1	-3.59	123.14	128.58
2	B	801	PE0	C1-C2-N1	-3.46	118.33	123.19
2	B	801	PE0	C4-C1-N4	3.25	124.08	118.38
4	A	803	APC	O4'-C1'-N9	3.23	114.29	108.09
4	A	803	APC	C4-C5-N7	-3.11	107.03	110.58
3	B	802	PHB	C5-C6-C1	-3.01	117.58	120.80
4	A	803	APC	PB-O3B-PG	-2.82	122.33	132.45
2	A	801	PE0	C1-C2-N1	-2.65	119.47	123.19
4	B	803	APC	C4-C5-N7	-2.64	107.56	110.58
2	A	801	PE0	O4-C4-C1	-2.62	119.12	124.32
3	B	802	PHB	C6-C1-C2	2.49	121.73	118.57
4	A	803	APC	C2-N1-C6	2.43	122.72	118.73
4	B	803	APC	PB-O3B-PG	-2.43	123.75	132.45
2	A	801	PE0	N3-C2-N1	2.33	123.17	116.41
8	A	807	GOL	O1-C1-C2	-2.28	100.12	110.38
4	B	803	APC	C3'-C2'-C1'	2.23	105.68	101.46
4	B	803	APC	C4-N9-C8	2.21	108.06	105.74
4	B	803	APC	C2'-C3'-C4'	2.19	106.84	102.61
2	B	801	PE0	C2-C1-N4	-2.17	118.84	122.95
4	A	803	APC	C5-N7-C8	2.10	106.75	103.45
2	B	801	PE0	C1-C4-N2	2.06	118.00	114.07
3	A	802	PHB	C6-C1-C2	2.05	121.17	118.57
2	A	801	PE0	O4-C4-N2	2.04	123.04	120.62
4	B	803	APC	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

All (17) 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	B	803	APC	PA-C3A-PB-O1B
4	B	803	APC	PA-C3A-PB-O2B
8	B	808	GOL	C1-C2-C3-O3
4	A	803	APC	O4'-C4'-C5'-O5'
4	A	803	APC	C3'-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
4	B	803	APC	C2'-C1'-N9-C4
8	A	807	GOL	O1-C1-C2-O2
4	B	803	APC	C2'-C1'-N9-C8
4	B	803	APC	PA-C3A-PB-O3B
4	B	803	APC	O4'-C1'-N9-C8

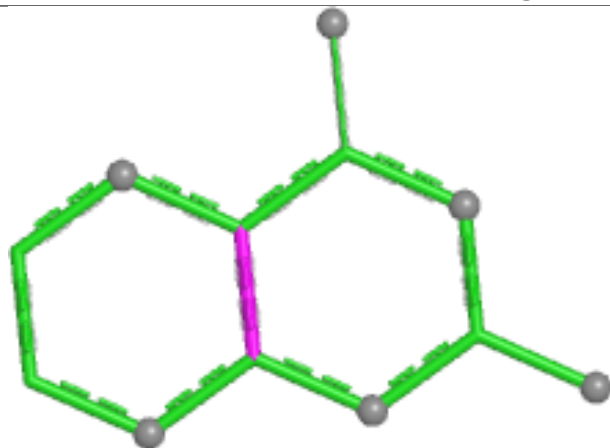
There are no ring outliers.

3 monomers are involved in 3 short contacts:

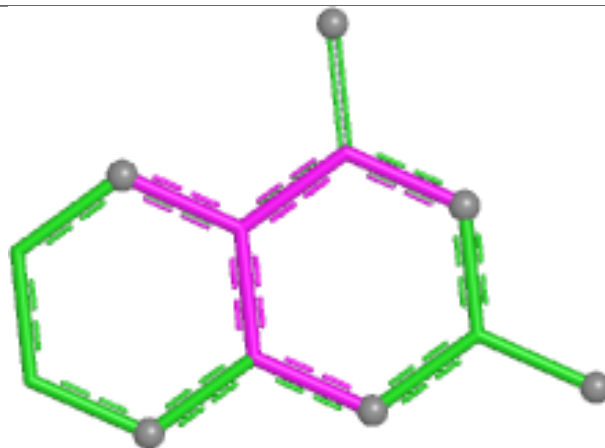
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PE0	1	0
8	B	808	GOL	2	0
3	B	802	PHB	2	0

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 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.

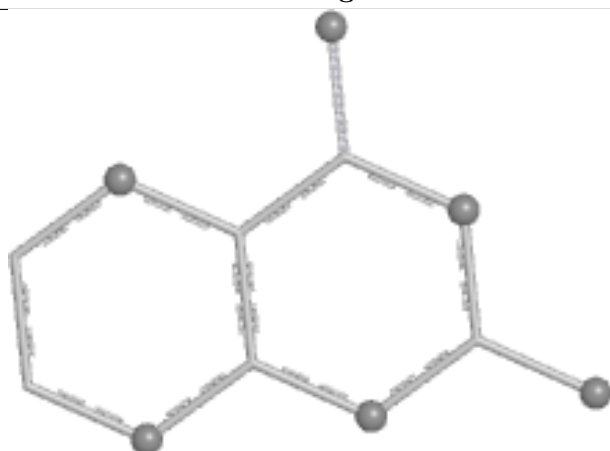
Ligand PE0 B 801



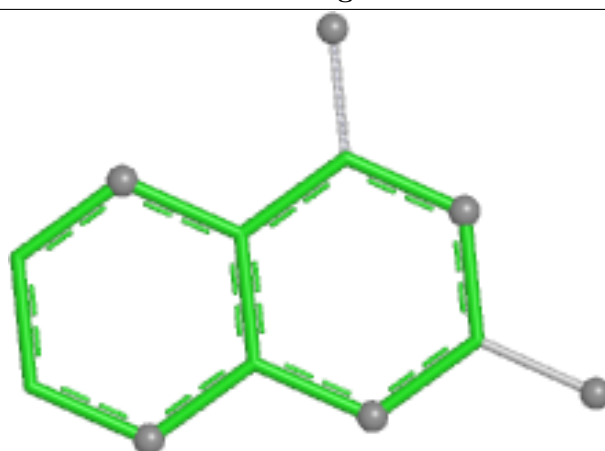
Bond lengths



Bond angles

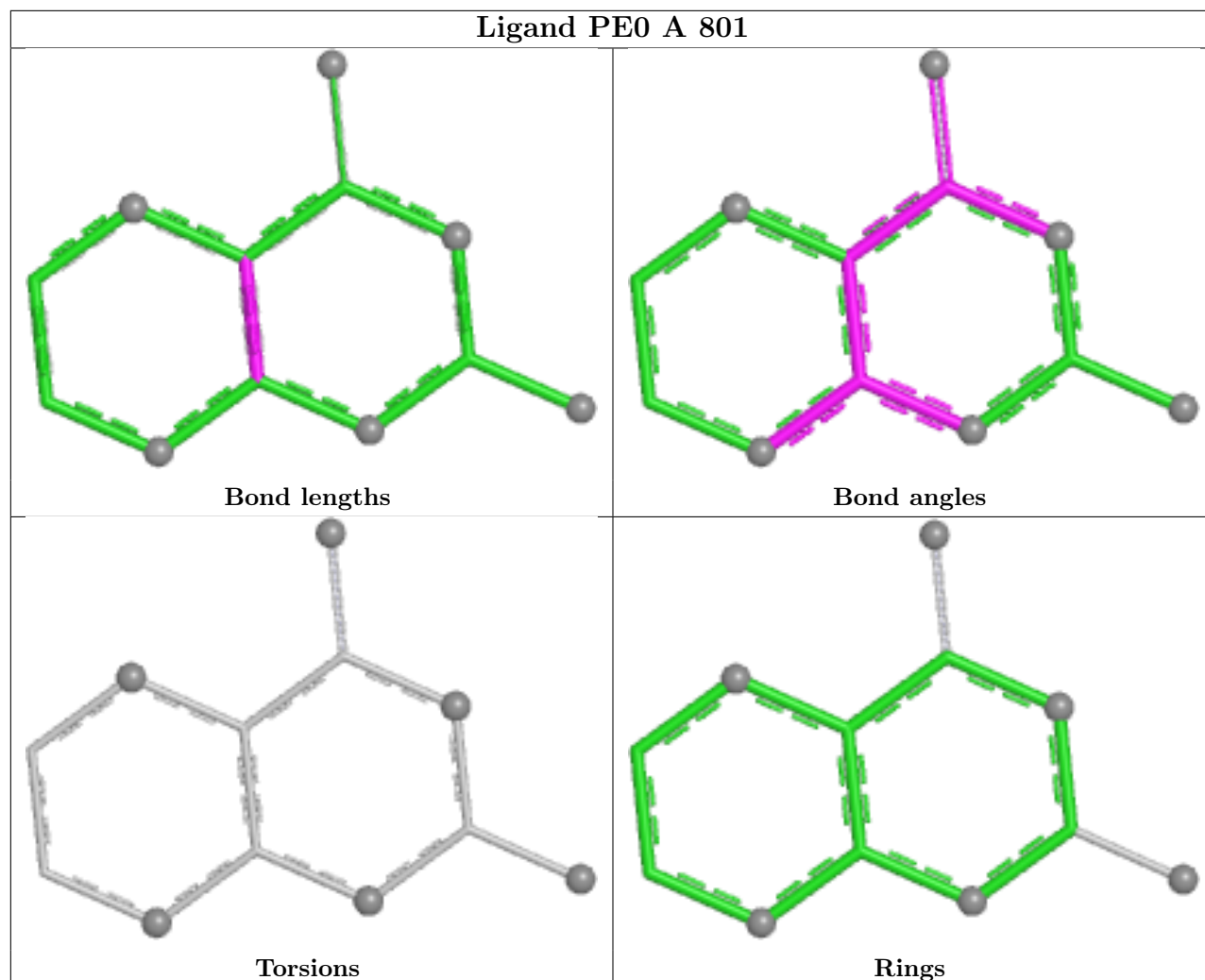


Torsions

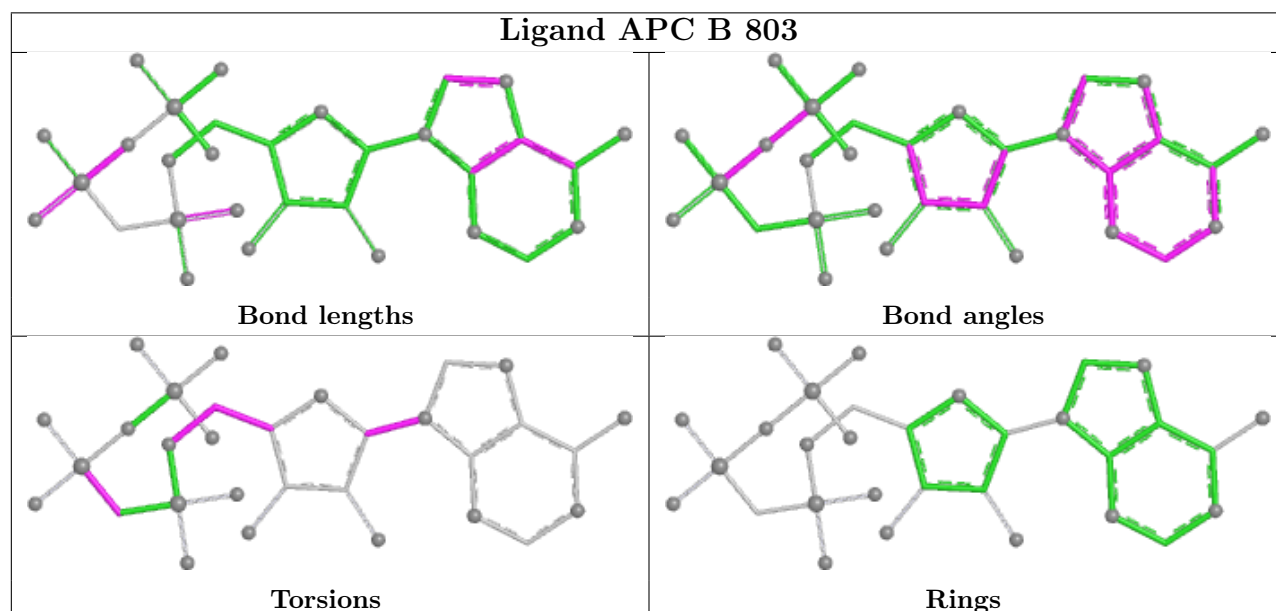


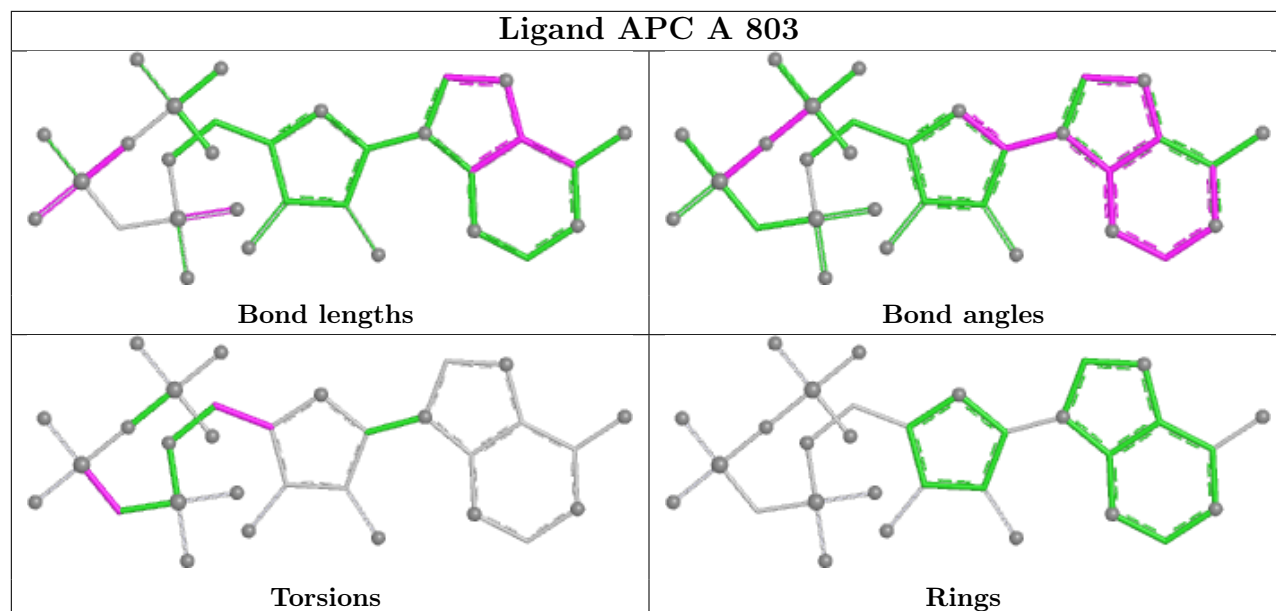
Rings

Ligand PE0 A 801



Ligand APC B 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%)	0.03	39 (7%) 22 19	10, 31, 96, 120	0
1	B	562/728 (77%)	0.56	69 (12%) 8 7	9, 44, 106, 120	0
All	All	1113/1456 (76%)	0.30	108 (9%) 13 11	9, 37, 103, 120	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	6.2
1	B	82	VAL	6.2
1	A	471	VAL	6.1
1	B	9	LEU	5.7
1	A	84	TYR	5.3
1	A	146	ILE	5.2
1	B	123	ILE	5.0
1	B	469	LYS	4.9
1	A	7	LEU	4.3
1	A	302	PRO	4.2
1	B	305	ILE	4.1
1	B	442	PRO	4.0
1	A	470	ILE	3.9
1	B	405	GLY	3.8
1	B	466	ILE	3.8
1	B	468	ASN	3.7
1	A	408	PHE	3.6
1	A	473	CYS	3.5
1	B	148	LYS	3.5
1	A	364	TYR	3.5
1	B	231	ILE	3.5
1	A	162	TYR	3.5
1	A	444	PRO	3.5
1	B	663	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	58	VAL	3.4
1	A	205	ARG	3.4
1	B	404	ASP	3.3
1	A	442	PRO	3.3
1	B	444	PRO	3.3
1	B	309	MET	3.3
1	B	235	LEU	3.2
1	A	305	ILE	3.2
1	B	146	ILE	3.2
1	B	230	MET	3.2
1	B	232	TYR	3.2
1	B	134	LEU	3.1
1	B	205	ARG	3.1
1	B	147	MET	3.0
1	B	220	PHE	3.0
1	B	14	LYS	2.9
1	B	310	VAL	2.9
1	B	658	LYS	2.9
1	B	127	VAL	2.9
1	A	472	LYS	2.9
1	B	84	TYR	2.9
1	A	5	GLN	2.8
1	B	163	PHE	2.8
1	B	10	SER	2.7
1	A	474	ASP	2.7
1	B	226	LEU	2.7
1	B	441	ILE	2.7
1	B	136	CYS	2.6
1	B	440	VAL	2.6
1	B	219	ILE	2.6
1	B	241	LEU	2.6
1	B	224	ILE	2.6
1	A	193	ARG	2.5
1	A	618	ASP	2.5
1	B	221	MET	2.5
1	B	399	TYR	2.5
1	A	366	ILE	2.5
1	A	468	ASN	2.5
1	A	225	LYS	2.5
1	A	58	VAL	2.5
1	B	59	PRO	2.4
1	B	206	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	467	LYS	2.4
1	B	15	THR	2.4
1	A	59	PRO	2.4
1	B	140	ILE	2.4
1	B	187	ILE	2.4
1	A	365	ASN	2.4
1	B	13	ASN	2.4
1	B	92	LEU	2.4
1	B	401	SER	2.3
1	B	218	THR	2.3
1	A	161	SER	2.3
1	A	311	ASP	2.3
1	A	658	LYS	2.3
1	B	97	TYR	2.3
1	B	707	LYS	2.2
1	B	234	ILE	2.2
1	A	94	GLU	2.2
1	B	186	TYR	2.2
1	B	400	ASP	2.2
1	A	303	GLN	2.1
1	A	304	GLU	2.1
1	A	708	ASP	2.1
1	B	403	SER	2.1
1	A	439	PHE	2.1
1	B	617	ASN	2.1
1	B	306	ILE	2.1
1	B	322	TYR	2.1
1	B	240	HIS	2.1
1	A	409	VAL	2.1
1	A	28	ARG	2.1
1	A	306	ILE	2.1
1	B	139	ILE	2.1
1	B	222	LYS	2.1
1	B	124	LEU	2.1
1	B	439	PHE	2.0
1	A	443	ASN	2.0
1	B	325	HIS	2.0
1	B	173	PHE	2.0
1	B	145	GLU	2.0
1	B	229	ASN	2.0
1	B	307	ASN	2.0
1	A	663	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

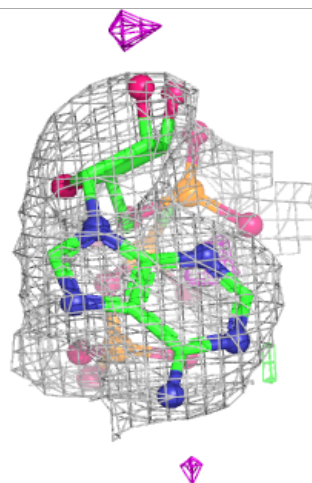
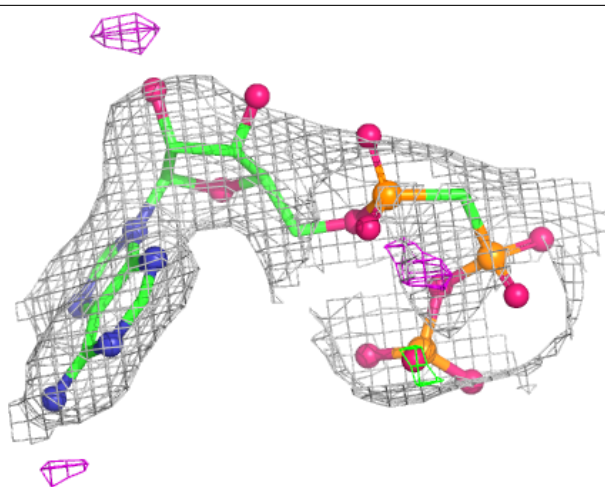
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	APC	B	803	31/31	0.80	0.12	42,73,100,105	0
8	GOL	B	808	6/6	0.83	0.13	28,32,35,39	0
4	APC	A	803	31/31	0.88	0.11	36,56,101,104	0
8	GOL	A	807	6/6	0.90	0.10	21,23,24,25	0
5	MG	B	804	1/1	0.91	0.17	61,61,61,61	0
5	MG	B	805	1/1	0.93	0.08	50,50,50,50	0
7	ACT	A	806	4/4	0.93	0.12	24,25,27,29	0
6	CA	B	806	1/1	0.94	0.07	67,67,67,67	0
3	PHB	A	802	10/10	0.96	0.07	18,19,21,24	0
3	PHB	B	802	10/10	0.97	0.06	20,21,23,25	0
5	MG	A	804	1/1	0.97	0.04	32,32,32,32	0
2	PE0	B	801	12/12	0.98	0.06	14,15,16,16	0
6	CA	A	805	1/1	0.98	0.04	34,34,34,34	0
2	PE0	A	801	12/12	0.99	0.04	12,13,13,13	0
7	ACT	B	807	4/4	0.99	0.05	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.

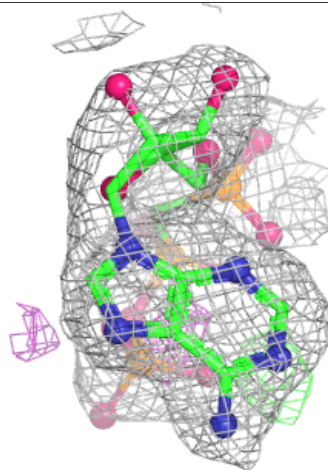
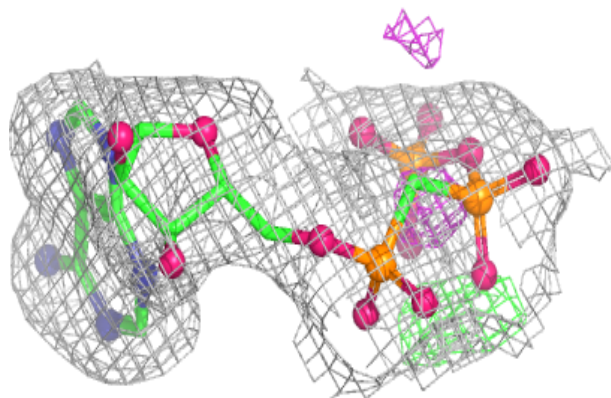
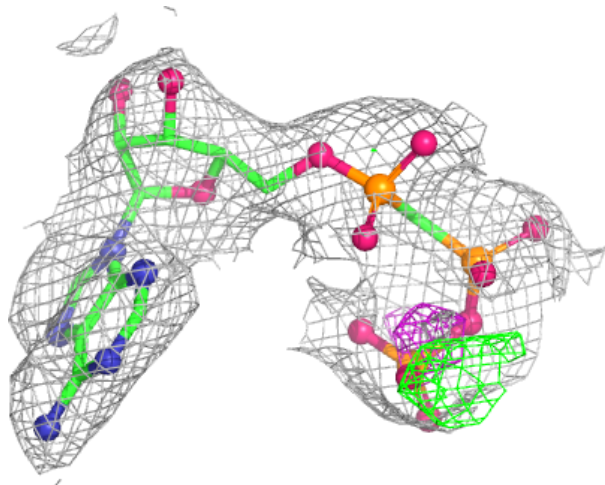
Electron density around APC B 803:

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



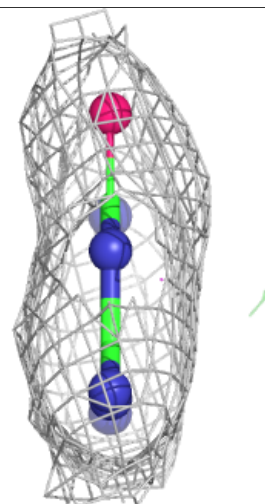
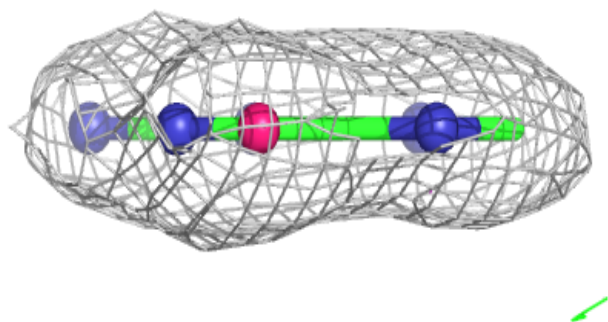
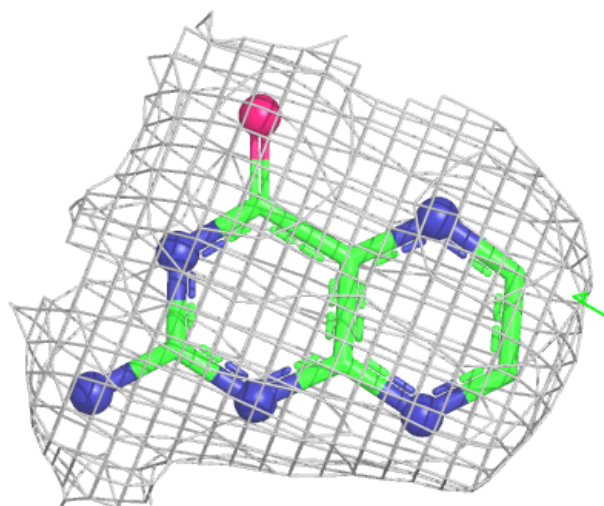
Electron density around APC A 803:

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



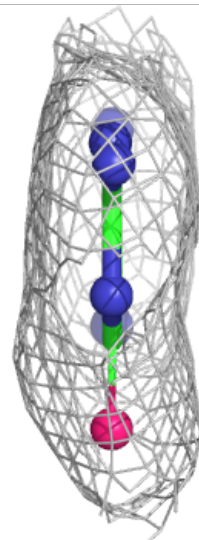
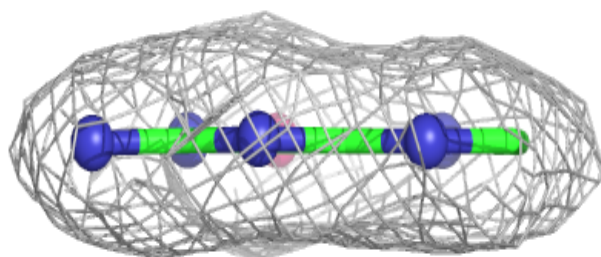
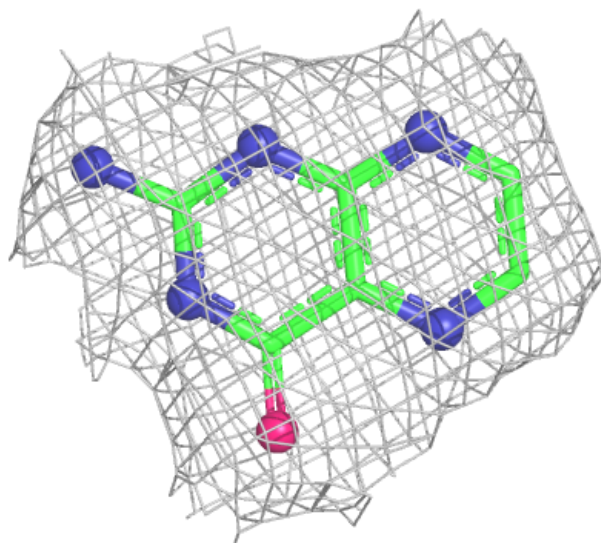
Electron density around PE0 B 801:

$2mF_o-DF_c$ (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.