Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:24 PM EDT

PDB ID	:	3B62
Title	:	EmrE multidrug transporter in complex with P4P, P21 crystal form
Authors	:	Chang, G.; Chen, Y.J.
Deposited on	:	2007-10-26
Resolution	:	4.40 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 (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:

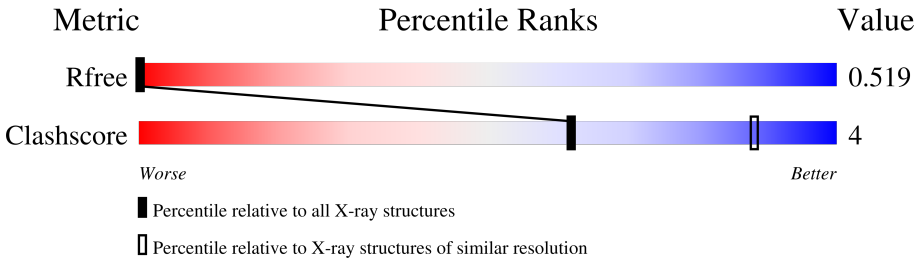
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	110	86% 14%
1	B	110	79% 21%
1	C	110	86% 14%
1	D	110	79% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P4P	A	350	-	X	-	-
2	P4P	C	750	-	X	-	-

2 Entry composition

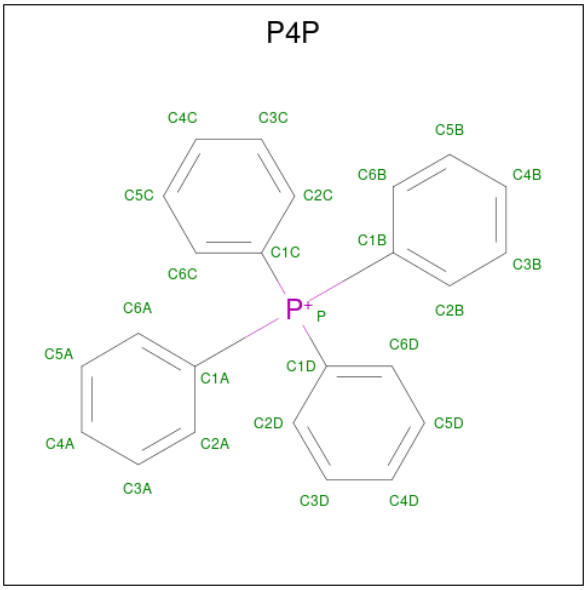
There are 2 unique types of molecules in this entry. The entry contains 414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug transporter emrE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	95	Total C 95 95	0	0	95
1	B	87	Total C 87 87	0	0	87
1	C	95	Total C 95 95	0	0	95
1	D	87	Total C 87 87	0	0	87

- Molecule 2 is TETRAPHENYLPHOSPHONIUM (three-letter code: P4P) (formula: $C_{24}H_{20}P$).



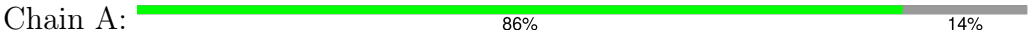
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C P 25 24 1	0	0
2	C	1	Total C P 25 24 1	0	0

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. 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. 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.

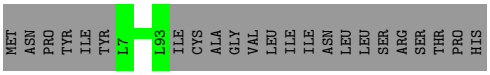
• Molecule 1: Multidrug transporter emrE

Chain A:



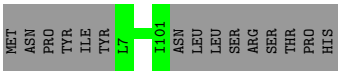
• Molecule 1: Multidrug transporter emrE

Chain B:



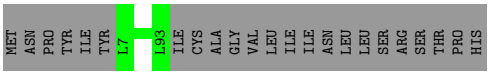
• Molecule 1: Multidrug transporter emrE

Chain C:



• Molecule 1: Multidrug transporter emrE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.50Å 42.70Å 115.40Å 90.00° 109.10° 90.00°	Depositor
Resolution (Å)	19.80 – 4.40 19.79 – 4.40	Depositor EDS
% Data completeness (in resolution range)	72.9 (19.80-4.40) 72.9 (19.79-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	12.61 (at 4.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.343 , 0.364 0.516 , 0.519	Depositor DCC
R_{free} test set	345 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	153.5	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.07 , 269.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	414	wwPDB-VP
Average B, all atoms (Å^2)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 94.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2685e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4P

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	95	0	0	0	0
1	B	87	0	0	0	0
1	C	95	0	0	0	0
1	D	87	0	0	0	0
2	A	25	0	20	1	0
2	C	25	0	20	1	0
All	All	414	0	40	2	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 4.

All (2) 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)
2:A:350:P4P:H2C	2:A:350:P4P:C6D	2.49	0.43
2:C:750:P4P:H2C	2:C:750:P4P:C6D	2.49	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	P4P	A	350	-	28,28,28	4.11	23 (82%)	38,38,38	2.21	15 (39%)
2	P4P	C	750	-	28,28,28	4.07	23 (82%)	38,38,38	2.22	16 (42%)

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	P4P	A	350	-	-	0/24/24/24	0/4/4/4
2	P4P	C	750	-	-	0/24/24/24	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	P4P	C6D-C1D	7.10	1.50	1.39
2	A	350	P4P	C5A-C6A	6.99	1.50	1.38
2	C	750	P4P	C6D-C1D	6.98	1.50	1.39
2	C	750	P4P	C5A-C6A	6.91	1.50	1.38
2	A	350	P4P	C2D-C1D	6.22	1.49	1.39
2	C	750	P4P	C2D-C1D	6.16	1.49	1.39
2	A	350	P4P	C5D-C6D	5.67	1.48	1.38
2	C	750	P4P	C2B-C1B	5.63	1.48	1.39
2	C	750	P4P	C3B-C2B	5.54	1.48	1.38
2	A	350	P4P	C2B-C1B	5.53	1.48	1.39
2	C	750	P4P	C5D-C6D	5.47	1.48	1.38
2	A	350	P4P	C3B-C2B	5.46	1.48	1.38
2	A	350	P4P	C2C-C1C	5.37	1.47	1.39
2	C	750	P4P	C2C-C1C	5.33	1.47	1.39
2	C	750	P4P	P-C1B	5.32	1.89	1.79
2	C	750	P4P	P-C1D	5.01	1.88	1.79
2	A	350	P4P	P-C1B	4.90	1.88	1.79
2	A	350	P4P	P-C1D	4.70	1.88	1.79
2	A	350	P4P	C6C-C1C	4.60	1.46	1.39
2	C	750	P4P	C6C-C1C	4.37	1.46	1.39
2	A	350	P4P	P-C1A	4.33	1.87	1.79
2	A	350	P4P	C3C-C4C	4.15	1.47	1.38
2	C	750	P4P	C3C-C4C	4.04	1.47	1.38
2	C	750	P4P	P-C1A	3.93	1.86	1.79
2	A	350	P4P	C3A-C2A	3.89	1.45	1.38
2	C	750	P4P	C3A-C2A	3.81	1.45	1.38
2	A	350	P4P	C4C-C5C	3.67	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	750	P4P	C4C-C5C	3.60	1.46	1.38
2	C	750	P4P	C5A-C4A	3.48	1.45	1.38
2	A	350	P4P	P-C1C	3.47	1.85	1.79
2	A	350	P4P	C5A-C4A	3.46	1.45	1.38
2	C	750	P4P	P-C1C	3.32	1.85	1.79
2	A	350	P4P	C4D-C5D	3.27	1.45	1.38
2	C	750	P4P	C4D-C5D	3.13	1.45	1.38
2	A	350	P4P	C2A-C1A	2.96	1.44	1.39
2	C	750	P4P	C2A-C1A	2.76	1.43	1.39
2	C	750	P4P	C5B-C6B	2.66	1.43	1.38
2	A	350	P4P	C5B-C6B	2.64	1.43	1.38
2	A	350	P4P	C3D-C4D	2.43	1.43	1.38
2	C	750	P4P	C6B-C1B	2.42	1.43	1.39
2	A	350	P4P	C6B-C1B	2.35	1.43	1.39
2	C	750	P4P	C3D-C4D	2.32	1.43	1.38
2	A	350	P4P	C3D-C2D	2.32	1.42	1.38
2	C	750	P4P	C3B-C4B	2.31	1.43	1.38
2	A	350	P4P	C3B-C4B	2.30	1.43	1.38
2	C	750	P4P	C3D-C2D	2.20	1.42	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	750	P4P	C6A-C1A-C2A	4.56	124.61	118.93
2	A	350	P4P	C6A-C1A-C2A	4.37	124.38	118.93
2	C	750	P4P	C4A-C5A-C6A	-3.83	115.51	120.24
2	C	750	P4P	P-C1C-C2C	-3.80	113.31	120.05
2	A	350	P4P	P-C1C-C2C	-3.80	113.32	120.05
2	A	350	P4P	P-C1C-C6C	3.79	126.74	120.05
2	C	750	P4P	P-C1C-C6C	3.76	126.70	120.05
2	C	750	P4P	C3A-C2A-C1A	-3.75	116.00	120.29
2	A	350	P4P	C4A-C5A-C6A	-3.73	115.64	120.24
2	A	350	P4P	C3A-C2A-C1A	-3.67	116.08	120.29
2	A	350	P4P	C1D-P-C1C	3.57	116.62	109.43
2	C	750	P4P	C1D-P-C1C	3.57	116.62	109.43
2	A	350	P4P	C3B-C2B-C1B	-3.51	116.27	120.29
2	C	750	P4P	C3B-C2B-C1B	-3.50	116.28	120.29
2	A	350	P4P	P-C1B-C2B	-3.27	114.25	120.05
2	C	750	P4P	C5A-C4A-C3A	3.24	124.30	119.87
2	C	750	P4P	P-C1B-C2B	-3.23	114.33	120.05
2	A	350	P4P	C5A-C4A-C3A	3.19	124.24	119.87
2	A	350	P4P	C3D-C4D-C5D	2.94	123.89	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	750	P4P	C3D-C4D-C5D	2.91	123.86	119.87
2	C	750	P4P	P-C1A-C6A	-2.74	115.19	120.05
2	A	350	P4P	P-C1A-C6A	-2.61	115.44	120.05
2	A	350	P4P	C1C-P-C1A	-2.40	104.59	109.43
2	C	750	P4P	P-C1B-C6B	2.32	124.15	120.05
2	A	350	P4P	P-C1B-C6B	2.31	124.13	120.05
2	A	350	P4P	C2B-C1B-C6B	2.16	121.62	118.93
2	C	750	P4P	C1C-P-C1A	-2.13	105.13	109.43
2	C	750	P4P	C1B-P-C1D	-2.12	105.15	109.43
2	C	750	P4P	C2B-C1B-C6B	2.08	121.52	118.93
2	C	750	P4P	C5A-C6A-C1A	-2.04	117.95	120.29
2	A	350	P4P	C5A-C6A-C1A	-2.01	117.98	120.29

There are no chirality outliers.

There are no torsion outliers.

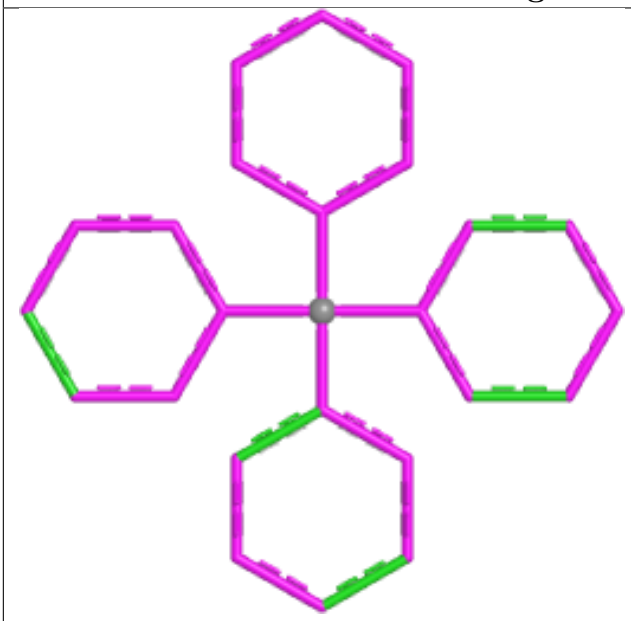
There are no ring outliers.

2 monomers are involved in 2 short contacts:

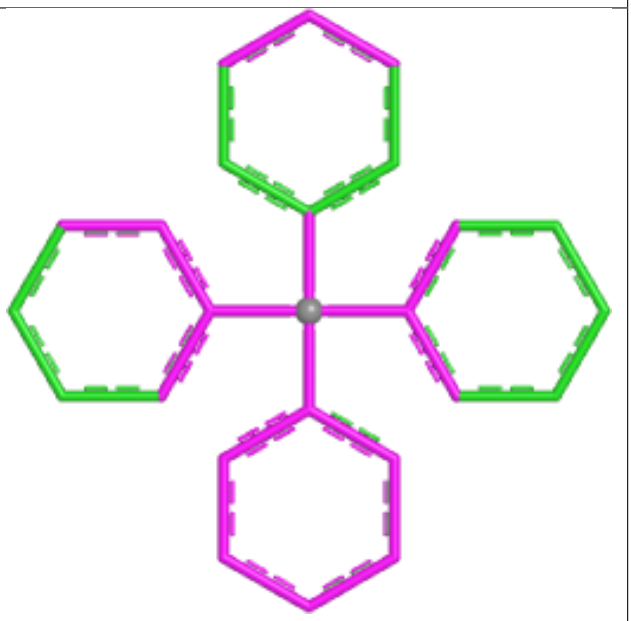
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	P4P	1	0
2	C	750	P4P	1	0

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 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.

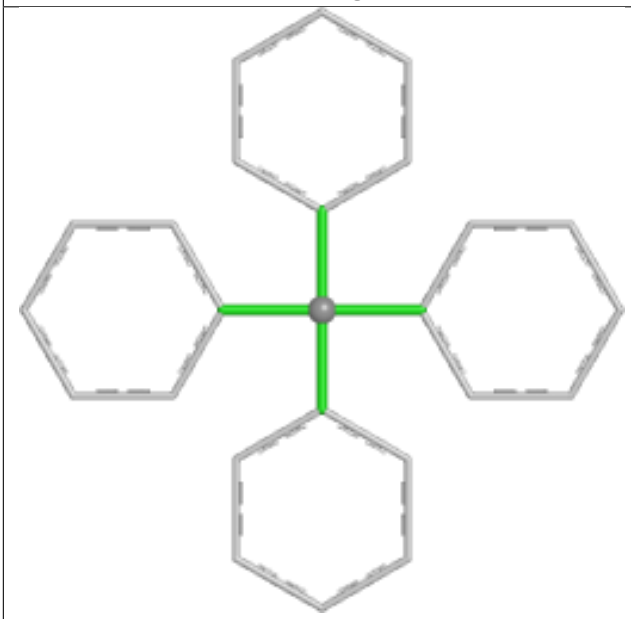
Ligand P4P A 350



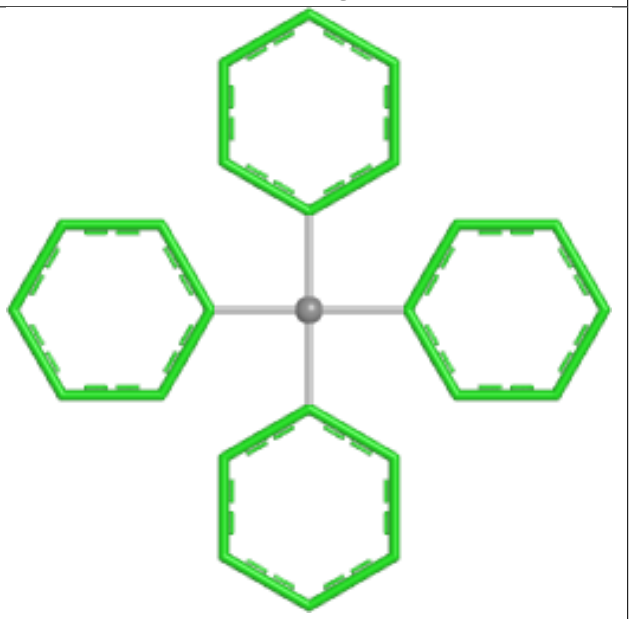
Bond lengths



Bond angles

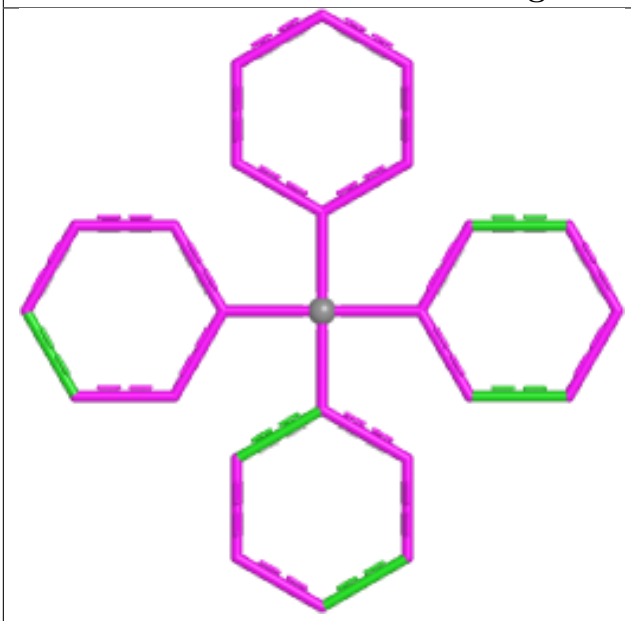


Torsions

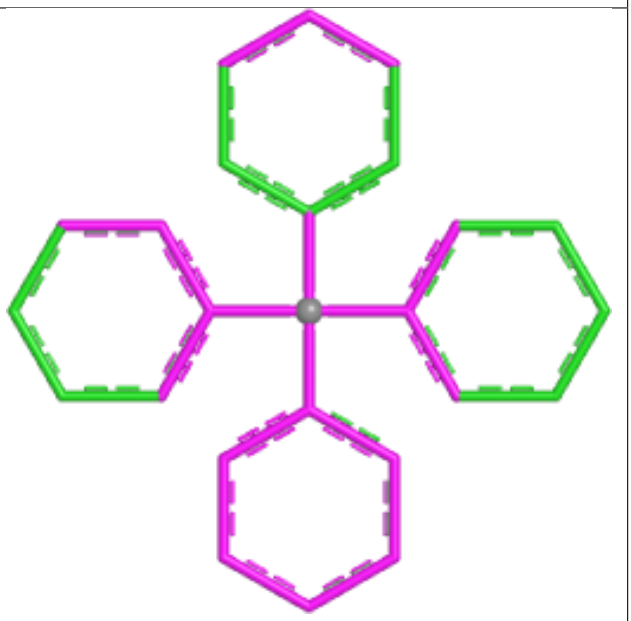


Rings

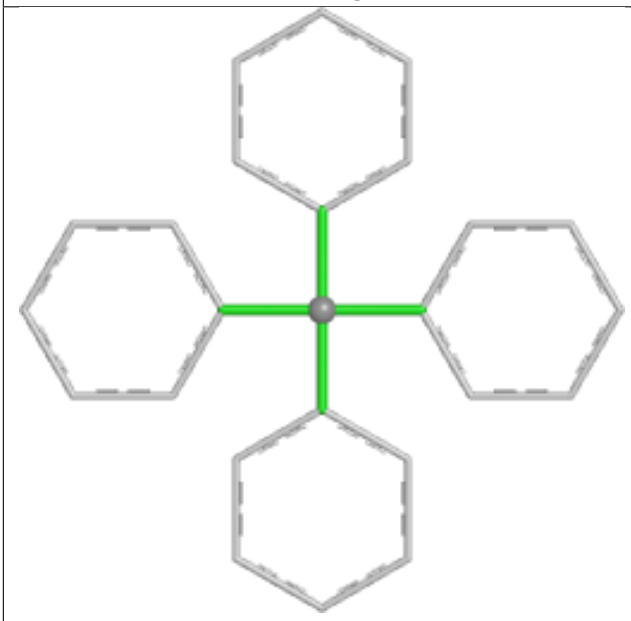
Ligand P4P C 750



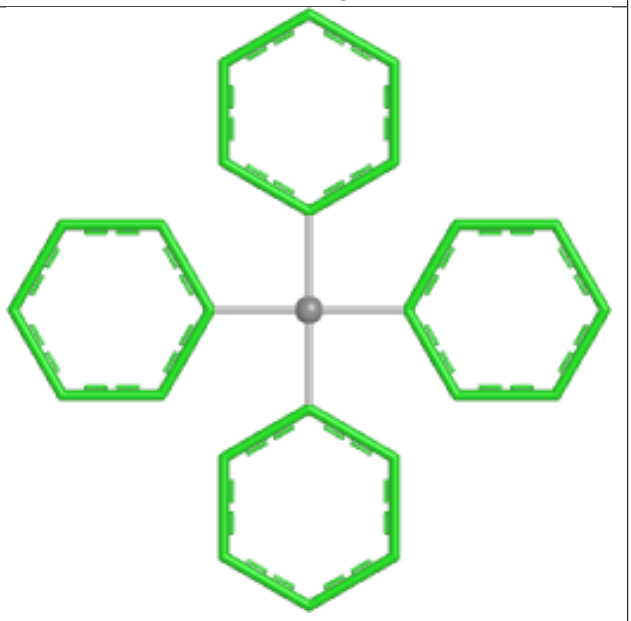
Bond lengths



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

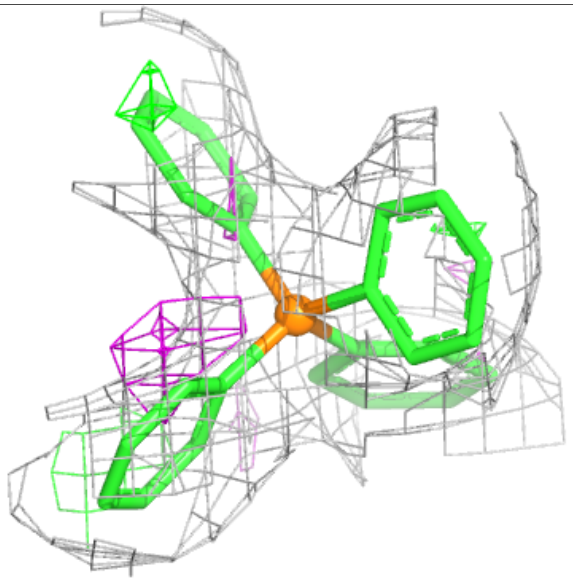
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P4P A 350:

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

Electron density around P4P C 750:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.