



wwPDB EM Validation Summary Report ⓘ

Feb 23, 2025 – 12:47 AM JST

PDB ID : 9IK4
EMDB ID : EMD-60648
Title : Cryo-EM structure of Arabidopsis thaliana phosphate transporter PHO1;H1
Authors : Fang, S.; Zhang, X.; Zhang, P.
Deposited on : 2024-06-26
Resolution : 3.34 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.41.2

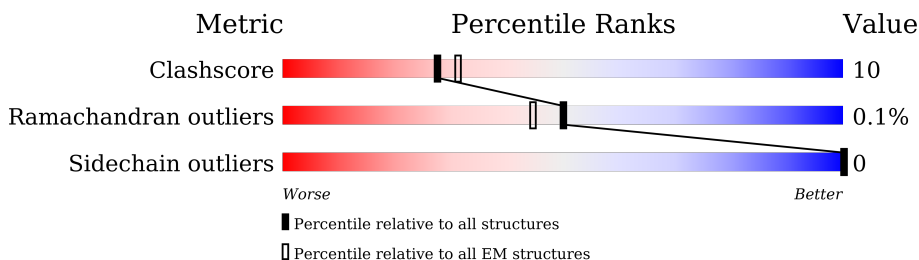
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	772	
1	B	772	

2 Entry composition [i](#)

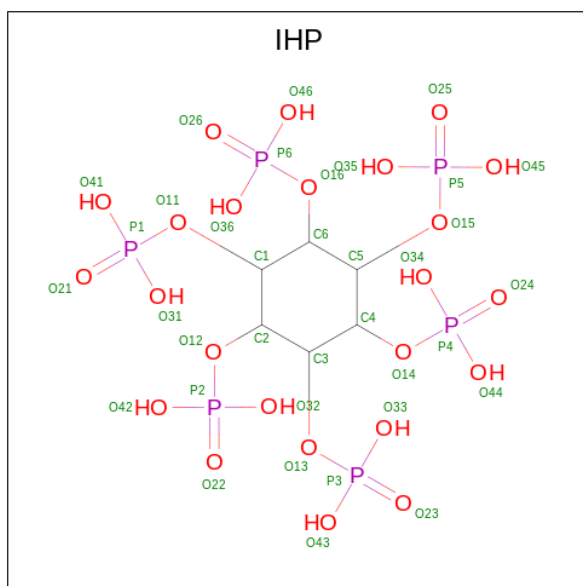
There are 3 unique types of molecules in this entry. The entry contains 10114 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Phosphate transporter PHO1 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	607	Total	C	N	O	S	0	0
			5016	3289	834	861	32		
1	B	607	Total	C	N	O	S	0	0
			5016	3289	834	861	32		

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			36	6	24	6	
2	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

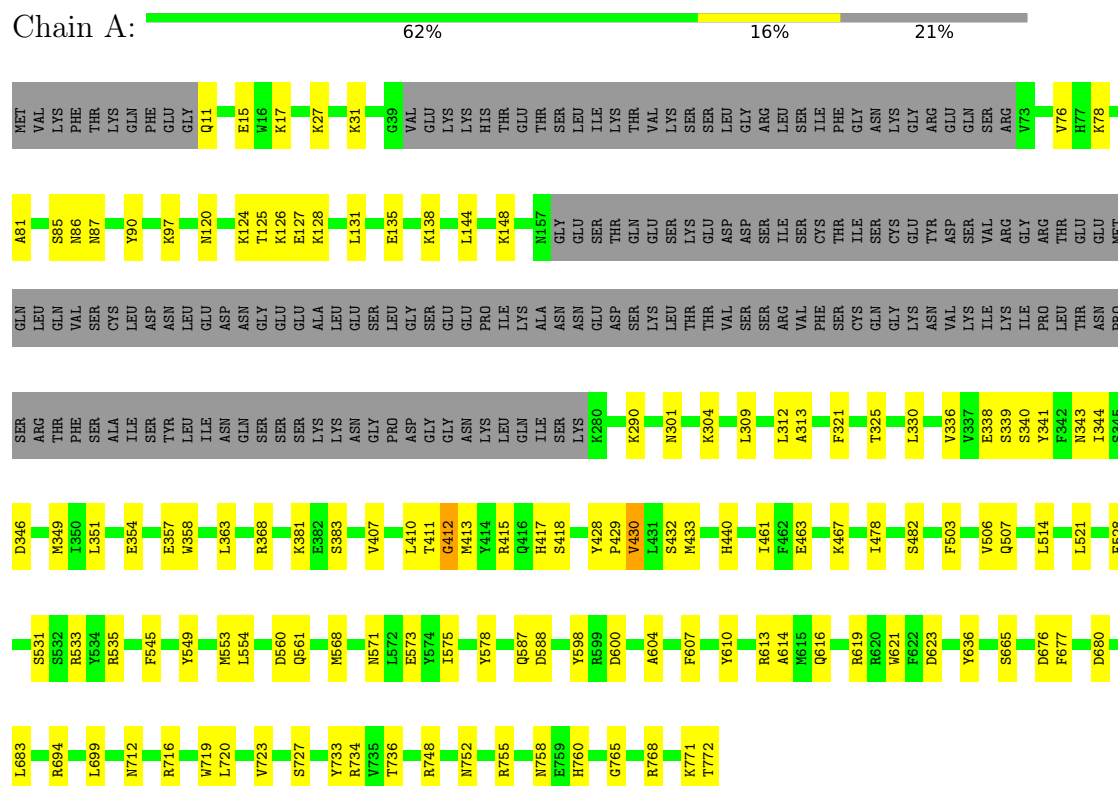


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	O	P	0
			5	4	1	
3	B	1	Total	O	P	0
			5	4	1	

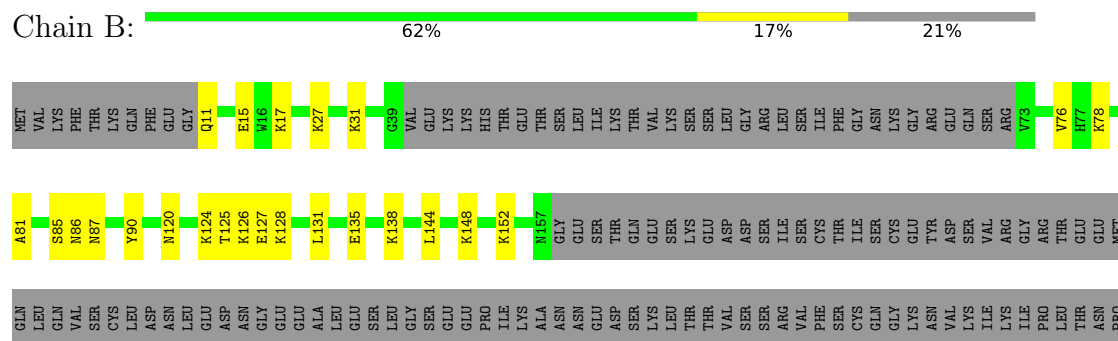
3 Residue-property plots

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. 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: Phosphate transporter PHO1 homolog 1



• Molecule 1: Phosphate transporter PHO1 homolog 1



R694	S531	D346	SER
L699	S532	M349	ARG
I704	R533	I350	THR
N712	F545	L351	PHE
R716	Y549	E354	SER
W719	M553	E357	TYR
L720	L554	W358	LEU
V723	D560	L363	ILE
S727	Q561	R368	ASN
Y733	M568	K373	GLN
R734	N571	K381	SER
W735	L572	E382	SER
T736	E573	S383	LYS
L740	Y574	V407	ASN
L743	I575	L410	GLY
R748	Y578	T411	GLY
N752	Q587	G412	ASN
R755	D588	M413	LYS
N758	Y598	Y414	LEU
E759	R599	R415	GLN
H760	D600	Q416	ILE
G765	A604	H417	SER
K771	F607	S418	LYS
T772	Y610	Y428	K280
	R613	P429	K290
	A614	V430	N301
	M615	L431	K304
	Q616	S432	L309
	R619	M433	L312
	R620	H440	A313
	W621	I461	F321
	F622	K467	T325
	D623	I478	L330
	Y636	S482	V336
	S665	F503	V337
	D676	V506	E338
	F677	Q507	S339
	D680	L514	S340
	L683	L521	Y341
		F528	F342
			N343
			I344
			S345

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	375307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IHP

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	0.41	0/5138	0.66	6/6927 (0.1%)
1	B	0.41	0/5138	0.66	5/6927 (0.1%)
All	All	0.41	0/10276	0.66	11/13854 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	GLY	N-CA-C	9.87	137.78	113.10
1	B	412	GLY	N-CA-C	9.85	137.73	113.10
1	B	410	LEU	CA-CB-CG	6.94	131.26	115.30
1	A	410	LEU	CA-CB-CG	6.93	131.24	115.30
1	B	699	LEU	CA-CB-CG	5.40	127.72	115.30

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	5016	0	5086	96	0
1	B	5016	0	5086	100	0
2	A	36	0	6	4	0
2	B	36	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	B	5	0	0	1	0
All	All	10114	0	10184	193	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 10.

The worst 5 of 193 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:B:733:TYR:CD2	1:B:736:THR:CG2	1.88	1.53
1:A:733:TYR:CD2	1:A:736:THR:CG2	1.88	1.52
1:A:733:TYR:CE2	1:A:736:THR:CG2	1.98	1.45
1:B:733:TYR:CE2	1:B:736:THR:CG2	1.98	1.45
1:B:733:TYR:CD2	1:B:736:THR:HG21	1.52	1.37

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 PDB entries followed by that with respect to all EM entries.

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	601/772 (78%)	515 (86%)	86 (14%)	0	100	100
1	B	601/772 (78%)	517 (86%)	83 (14%)	1 (0%)	44	72
All	All	1202/1544 (78%)	1032 (86%)	169 (14%)	1 (0%)	50	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	TYR

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 PDB entries followed by that with respect to all EM entries.

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	540/690 (78%)	540 (100%)	0	100	100
1	B	540/690 (78%)	540 (100%)	0	100	100
All	All	1080/1380 (78%)	1080 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	507	GLN
1	B	457	ASN
1	B	120	ASN
1	B	417	HIS
1	A	571	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	PO4	A	802	-	4,4,4	0.92	0	6,6,6	0.75	0
3	PO4	B	1001	-	4,4,4	0.91	0	6,6,6	0.75	0
2	IHP	A	801	-	36,36,36	0.77	1 (2%)	54,60,60	1.93	17 (31%)
2	IHP	B	1002	-	36,36,36	0.77	1 (2%)	54,60,60	1.93	17 (31%)

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	IHP	A	801	-	-	5/30/54/54	0/1/1/1
2	IHP	B	1002	-	-	5/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IHP	P3-O13	2.05	1.63	1.59
2	B	1002	IHP	P3-O13	2.03	1.63	1.59

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	IHP	C5-C6-C1	5.27	121.94	110.41
2	A	801	IHP	C5-C6-C1	5.26	121.92	110.41
2	B	1002	IHP	O16-C6-C5	-4.93	97.07	108.69
2	A	801	IHP	O16-C6-C5	-4.93	97.07	108.69
2	A	801	IHP	O14-C4-C5	-3.72	99.92	108.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

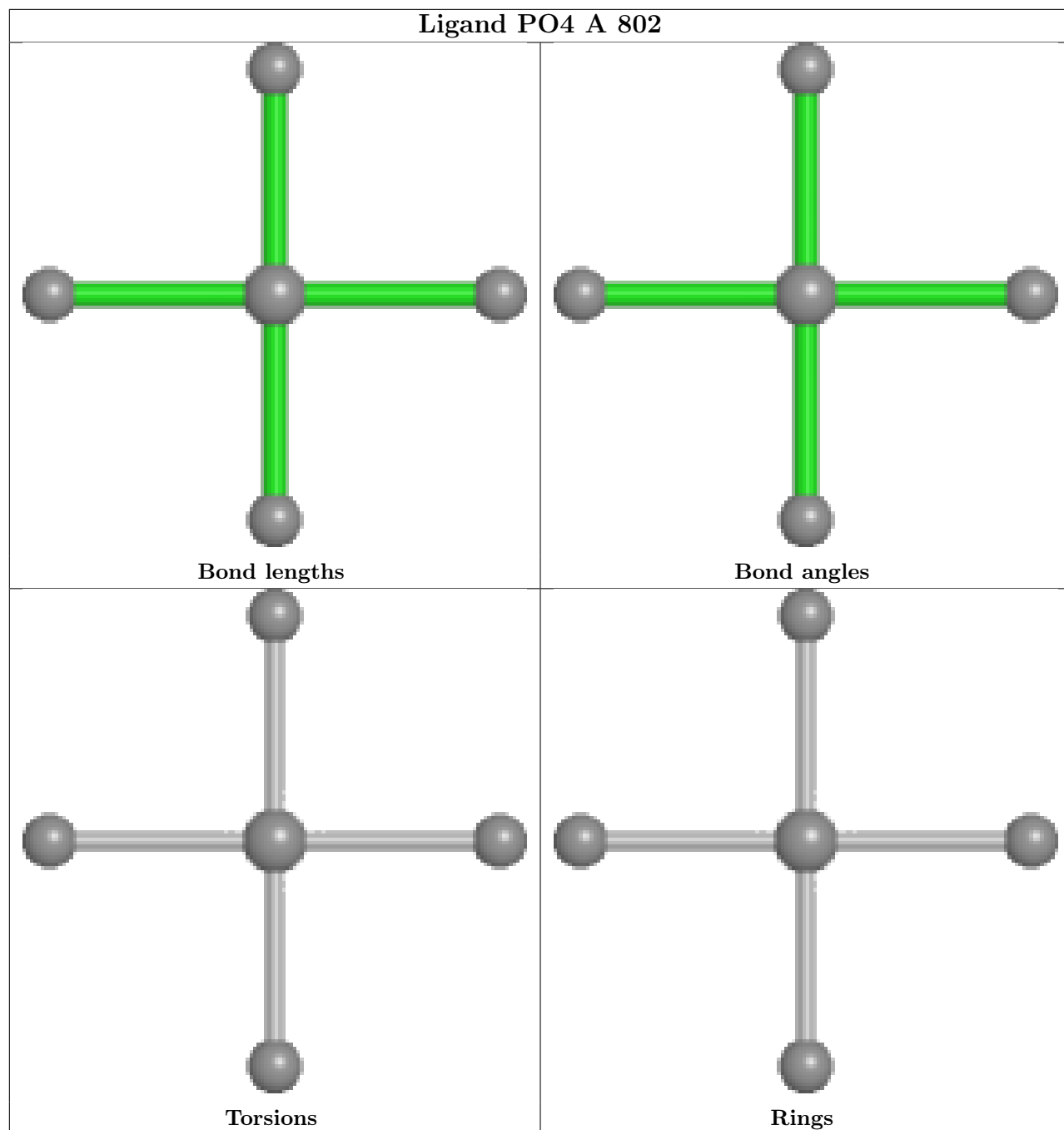
Mol	Chain	Res	Type	Atoms
2	A	801	IHP	C2-O12-P2-O22
2	A	801	IHP	C4-O14-P4-O44
2	B	1002	IHP	C2-O12-P2-O22
2	B	1002	IHP	C4-O14-P4-O44
2	A	801	IHP	C4-O14-P4-O24

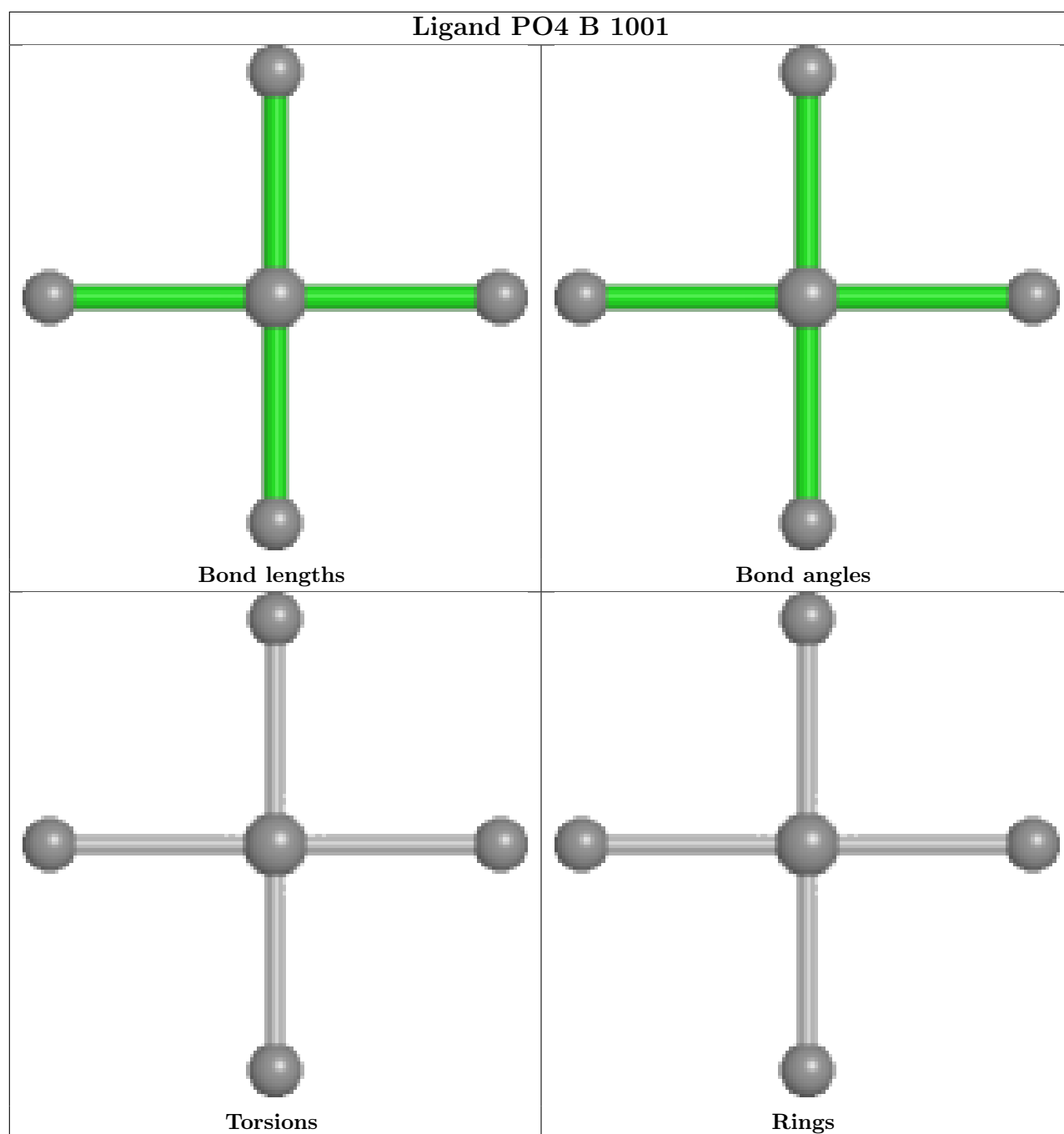
There are no ring outliers.

4 monomers are involved in 10 short contacts:

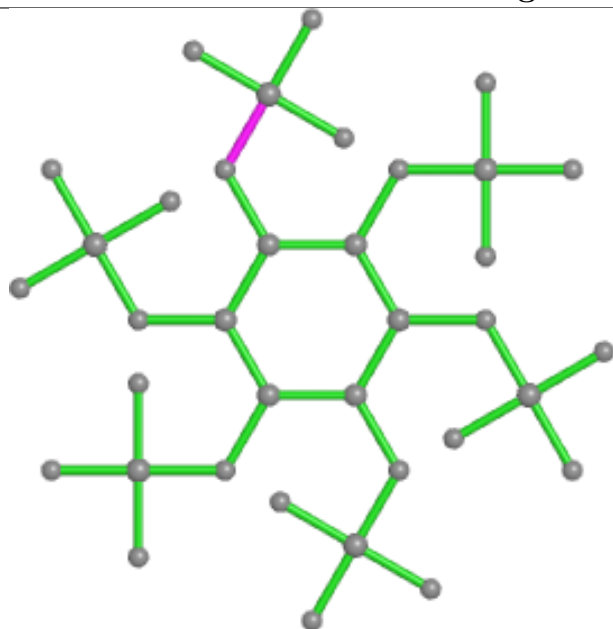
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PO4	1	0
3	B	1001	PO4	1	0
2	A	801	IHP	4	0
2	B	1002	IHP	4	0

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.

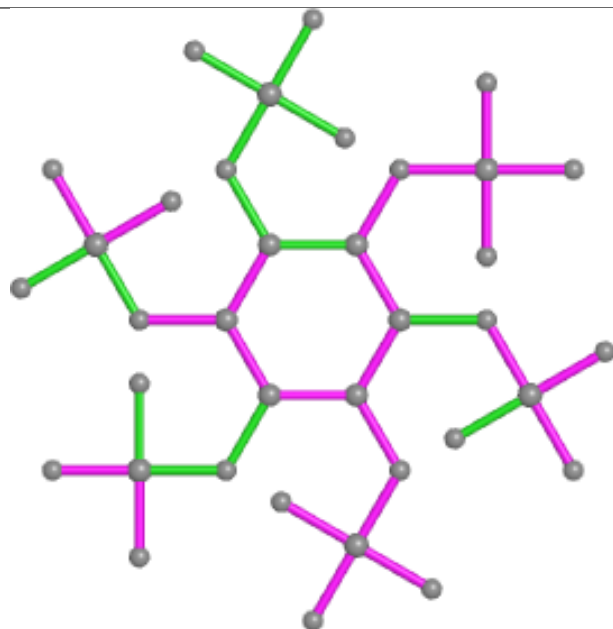




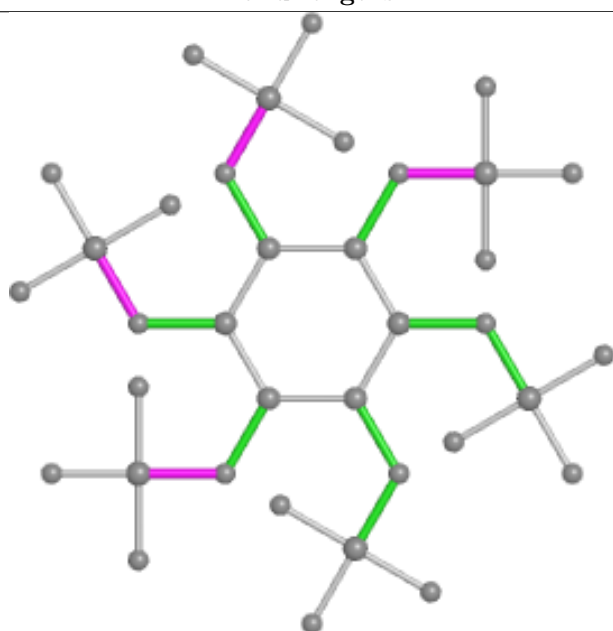
Ligand IHP A 801



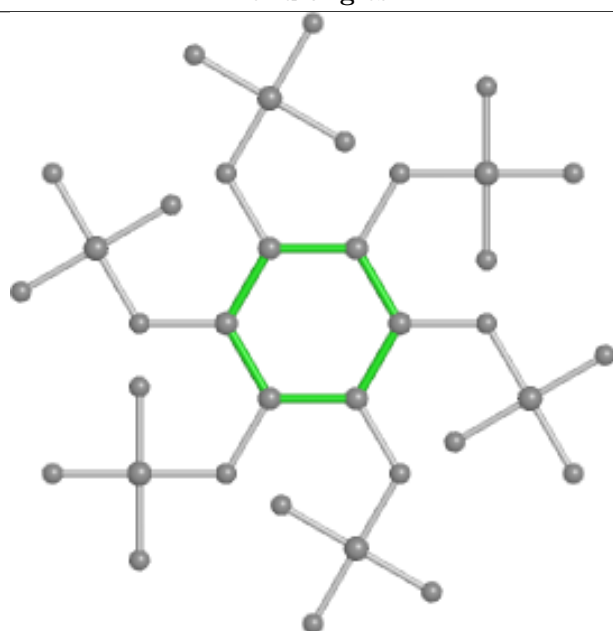
Bond lengths



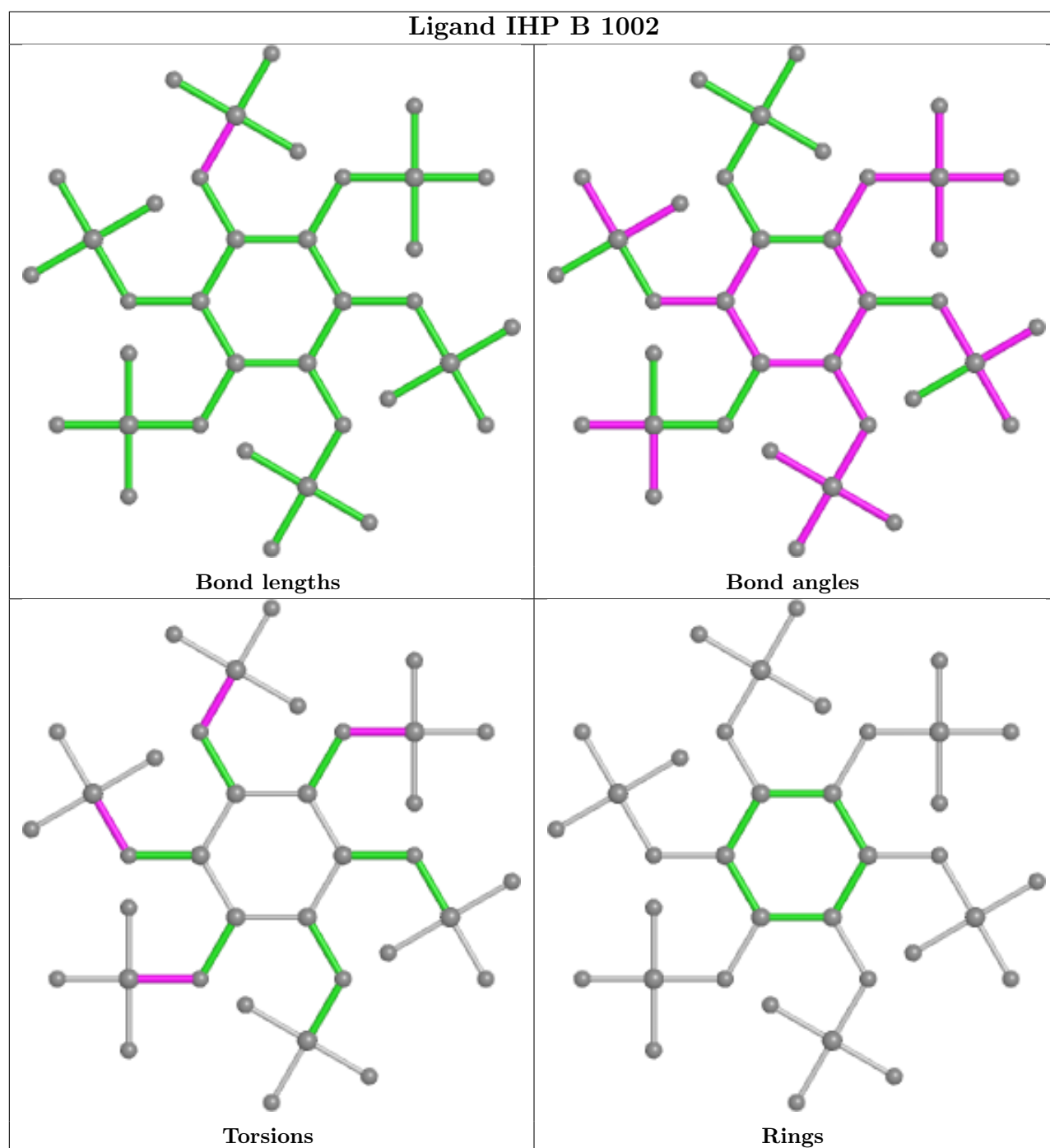
Bond angles



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.