



## wwPDB EM Validation Summary Report ⓘ

Apr 6, 2025 – 01:44 AM JST

PDB ID : 9J97 / pdb\_00009j97  
EMDB ID : EMD-61254  
Title : Closed structure of human XPR1  
Authors : Wang, Y.; Wang, Y.; Yang, H.; Shen, H.  
Deposited on : 2024-08-22  
Resolution : 3.30 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](mailto: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>.

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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) : 2.42

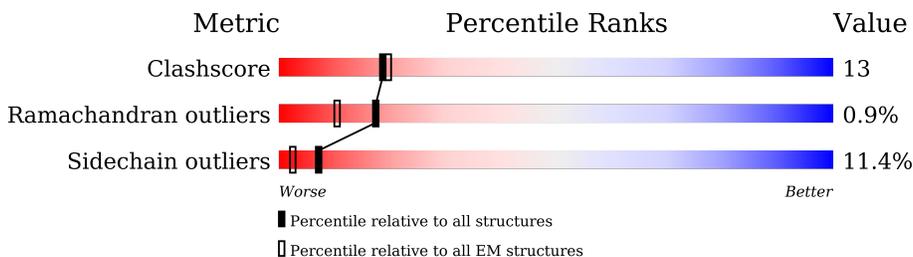
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 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	969	 30% 8% • 59%
1	B	969	 30% 8% • 59%

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
4	PO4	A	1003	-	X	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6704 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 Solute carrier family 53 member 1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	393	3272	2198	526	532	16	0	0
1	B	393	3272	2198	526	532	16	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLY	-	linker	UNP Q9UBH6
A	698	GLY	-	linker	UNP Q9UBH6
A	699	ARG	-	linker	UNP Q9UBH6
A	700	LEU	-	linker	UNP Q9UBH6
A	701	GLU	-	linker	UNP Q9UBH6
A	702	VAL	-	linker	UNP Q9UBH6
A	703	LEU	-	linker	UNP Q9UBH6
A	704	PHE	-	linker	UNP Q9UBH6
A	705	GLN	-	linker	UNP Q9UBH6
A	706	GLY	-	linker	UNP Q9UBH6
A	707	PRO	-	linker	UNP Q9UBH6
A	708	ALA	-	linker	UNP Q9UBH6
A	709	ALA	-	linker	UNP Q9UBH6
A	710	ALA	-	linker	UNP Q9UBH6
A	711	ALA	-	linker	UNP Q9UBH6
A	712	VAL	-	linker	UNP Q9UBH6
A	775	LEU	PHE	conflict	UNP P42212
A	776	THR	SER	conflict	UNP P42212
A	818	THR	LYS	conflict	UNP P42212
A	917	LYS	ALA	conflict	UNP P42212
A	942	LEU	HIS	conflict	UNP P42212
A	950	SER	-	expression tag	UNP P42212
A	951	GLY	-	expression tag	UNP P42212
A	952	LEU	-	expression tag	UNP P42212
A	953	ARG	-	expression tag	UNP P42212
A	954	SER	-	expression tag	UNP P42212

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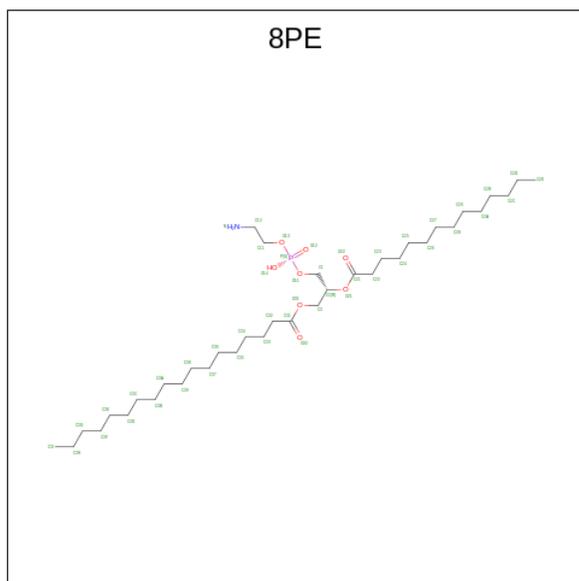
Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ASP	-	expression tag	UNP P42212
A	956	TYR	-	expression tag	UNP P42212
A	957	LYS	-	expression tag	UNP P42212
A	958	ASP	-	expression tag	UNP P42212
A	959	HIS	-	expression tag	UNP P42212
A	960	ASP	-	expression tag	UNP P42212
A	961	ILE	-	expression tag	UNP P42212
A	962	ASP	-	expression tag	UNP P42212
A	963	TYR	-	expression tag	UNP P42212
A	964	LYS	-	expression tag	UNP P42212
A	965	ASP	-	expression tag	UNP P42212
A	966	ASP	-	expression tag	UNP P42212
A	967	ASP	-	expression tag	UNP P42212
A	968	ASP	-	expression tag	UNP P42212
A	969	LYS	-	expression tag	UNP P42212
B	697	GLY	-	linker	UNP Q9UBH6
B	698	GLY	-	linker	UNP Q9UBH6
B	699	ARG	-	linker	UNP Q9UBH6
B	700	LEU	-	linker	UNP Q9UBH6
B	701	GLU	-	linker	UNP Q9UBH6
B	702	VAL	-	linker	UNP Q9UBH6
B	703	LEU	-	linker	UNP Q9UBH6
B	704	PHE	-	linker	UNP Q9UBH6
B	705	GLN	-	linker	UNP Q9UBH6
B	706	GLY	-	linker	UNP Q9UBH6
B	707	PRO	-	linker	UNP Q9UBH6
B	708	ALA	-	linker	UNP Q9UBH6
B	709	ALA	-	linker	UNP Q9UBH6
B	710	ALA	-	linker	UNP Q9UBH6
B	711	ALA	-	linker	UNP Q9UBH6
B	712	VAL	-	linker	UNP Q9UBH6
B	775	LEU	PHE	conflict	UNP P42212
B	776	THR	SER	conflict	UNP P42212
B	818	THR	LYS	conflict	UNP P42212
B	917	LYS	ALA	conflict	UNP P42212
B	942	LEU	HIS	conflict	UNP P42212
B	950	SER	-	expression tag	UNP P42212
B	951	GLY	-	expression tag	UNP P42212
B	952	LEU	-	expression tag	UNP P42212
B	953	ARG	-	expression tag	UNP P42212
B	954	SER	-	expression tag	UNP P42212
B	955	ASP	-	expression tag	UNP P42212

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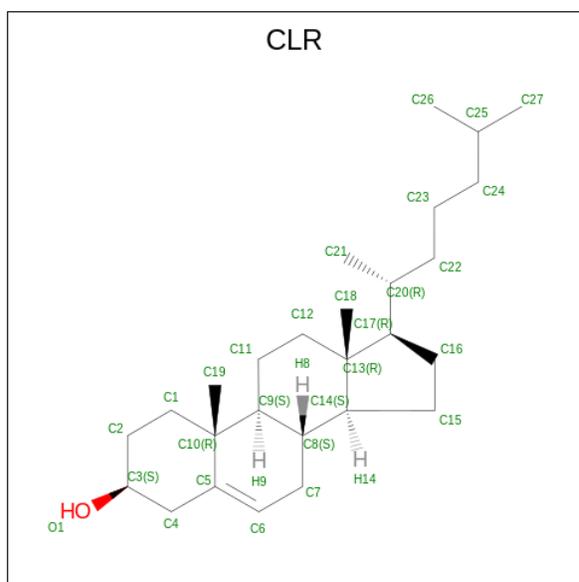
Chain	Residue	Modelled	Actual	Comment	Reference
B	956	TYR	-	expression tag	UNP P42212
B	957	LYS	-	expression tag	UNP P42212
B	958	ASP	-	expression tag	UNP P42212
B	959	HIS	-	expression tag	UNP P42212
B	960	ASP	-	expression tag	UNP P42212
B	961	ILE	-	expression tag	UNP P42212
B	962	ASP	-	expression tag	UNP P42212
B	963	TYR	-	expression tag	UNP P42212
B	964	LYS	-	expression tag	UNP P42212
B	965	ASP	-	expression tag	UNP P42212
B	966	ASP	-	expression tag	UNP P42212
B	967	ASP	-	expression tag	UNP P42212
B	968	ASP	-	expression tag	UNP P42212
B	969	LYS	-	expression tag	UNP P42212

- Molecule 2 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



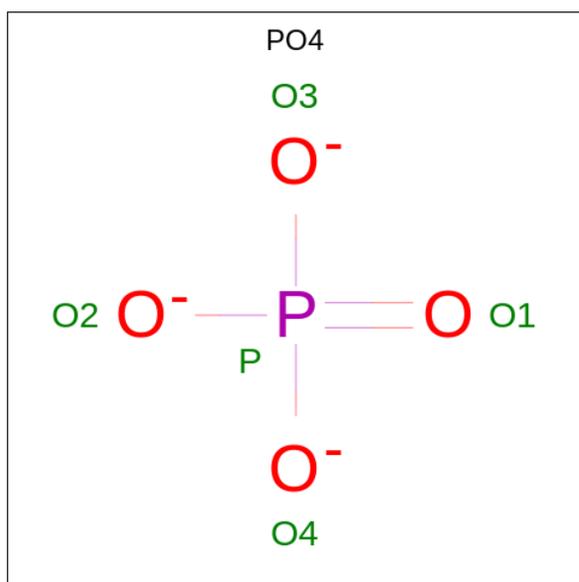
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	47	37	1	8	1	0
2	B	1	47	37	1	8	1	0

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ) (labeled as "Ligand of Interest" by depositor).



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

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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150104	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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: CLR, 8PE, PO4

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	0.66	7/3381 (0.2%)	0.73	10/4598 (0.2%)
1	B	0.63	6/3381 (0.2%)	0.72	9/4598 (0.2%)
All	All	0.65	13/6762 (0.2%)	0.72	19/9196 (0.2%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	GLY	C-O	-8.35	1.10	1.23
1	B	621	GLY	C-O	-8.33	1.10	1.23
1	B	454	ILE	C-N	8.26	1.50	1.34
1	A	454	ILE	C-N	8.18	1.49	1.34
1	B	522	SER	CA-CB	-7.65	1.41	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	624	ARG	CB-CG-CD	-8.71	88.96	111.60
1	B	620	CYS	CA-CB-SG	-7.19	101.05	114.00
1	A	620	CYS	CA-CB-SG	-7.14	101.15	114.00
1	B	624	ARG	CB-CA-C	-6.78	96.85	110.40
1	B	518	TYR	CB-CA-C	6.67	123.74	110.40

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	3272	0	3258	75	0
1	B	3272	0	3258	77	0
2	A	47	0	73	8	0
2	B	47	0	73	8	0
3	A	28	0	46	5	0
3	B	28	0	46	4	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
All	All	6704	0	6754	171	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 13.

The worst 5 of 171 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:572:ALA:HA	1:B:575:ILE:HG13	1.49	0.95
1:A:453:CYS:O	1:A:453:CYS:SG	2.25	0.95
1:B:489:MET:CE	1:B:574:THR:OG1	2.15	0.94
1:A:572:ALA:HA	1:A:575:ILE:HG13	1.49	0.93
1:B:453:CYS:SG	1:B:453:CYS:O	2.25	0.92

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	387/969 (40%)	356 (92%)	27 (7%)	4 (1%)	13	42
1	B	387/969 (40%)	358 (92%)	26 (7%)	3 (1%)	16	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	774/1938 (40%)	714 (92%)	53 (7%)	7 (1%)	17	44

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	PRO
1	A	622	GLU
1	B	586	PRO
1	B	622	GLU
1	A	445	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	347/857 (40%)	307 (88%)	40 (12%)	4	18
1	B	347/857 (40%)	308 (89%)	39 (11%)	5	19
All	All	694/1714 (40%)	615 (89%)	79 (11%)	7	18

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	454	ILE
1	B	576	GLN
1	B	477	LEU
1	B	521	SER
1	B	587	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	614	ASN
1	B	310	ASN

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Mol	Chain	Res	Type
1	B	614	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](#)

6 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	8PE	A	1001	-	46,46,46	1.04	3 (6%)	49,51,51	1.39	5 (10%)
2	8PE	B	1001	-	46,46,46	1.04	3 (6%)	49,51,51	1.39	5 (10%)
4	PO4	B	1003	-	4,4,4	1.47	1 (25%)	6,6,6	0.99	0
4	PO4	A	1003	-	4,4,4	2.96	4 (100%)	6,6,6	0.43	0
3	CLR	A	1002	-	31,31,31	0.96	0	48,48,48	1.86	12 (25%)
3	CLR	B	1002	-	31,31,31	0.96	0	48,48,48	1.85	12 (25%)

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
3	CLR	A	1002	-	-	4/10/68/68	0/4/4/4
2	8PE	A	1001	-	-	22/50/50/50	-
3	CLR	B	1002	-	-	4/10/68/68	0/4/4/4
2	8PE	B	1001	-	-	22/50/50/50	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	PO4	P-O1	4.51	1.61	1.50
2	B	1001	8PE	O32-C31	-3.21	1.13	1.22
2	A	1001	8PE	O32-C31	-3.17	1.13	1.22
4	B	1003	PO4	P-O3	-2.33	1.47	1.54
4	A	1003	PO4	P-O3	2.29	1.61	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	CLR	C19-C10-C1	-6.32	99.45	109.43
3	B	1002	CLR	C19-C10-C1	-6.28	99.51	109.43
2	A	1001	8PE	O21-C21-C22	5.70	123.79	111.50
2	B	1001	8PE	O21-C21-C22	5.69	123.76	111.50
2	B	1001	8PE	O13-P-O12	-4.39	91.92	109.07

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	O22-C21-O21-C2
2	A	1001	8PE	C22-C21-O21-C2
2	B	1001	8PE	O22-C21-O21-C2
2	B	1001	8PE	C22-C21-O21-C2
3	A	1002	CLR	C21-C20-C22-C23

There are no ring outliers.

5 monomers are involved in 26 short contacts:

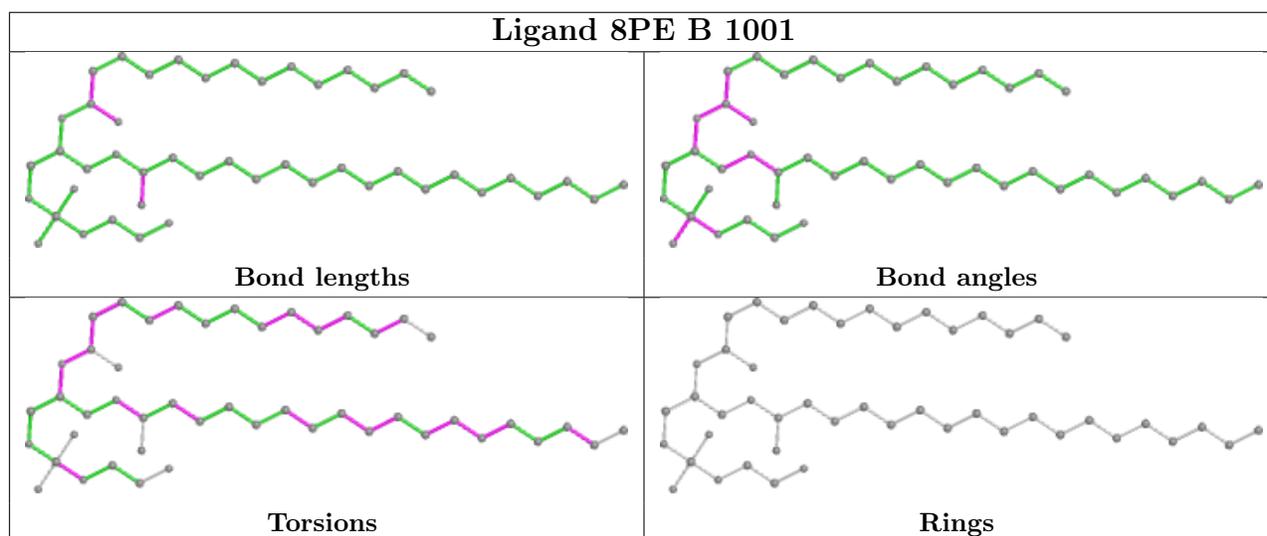
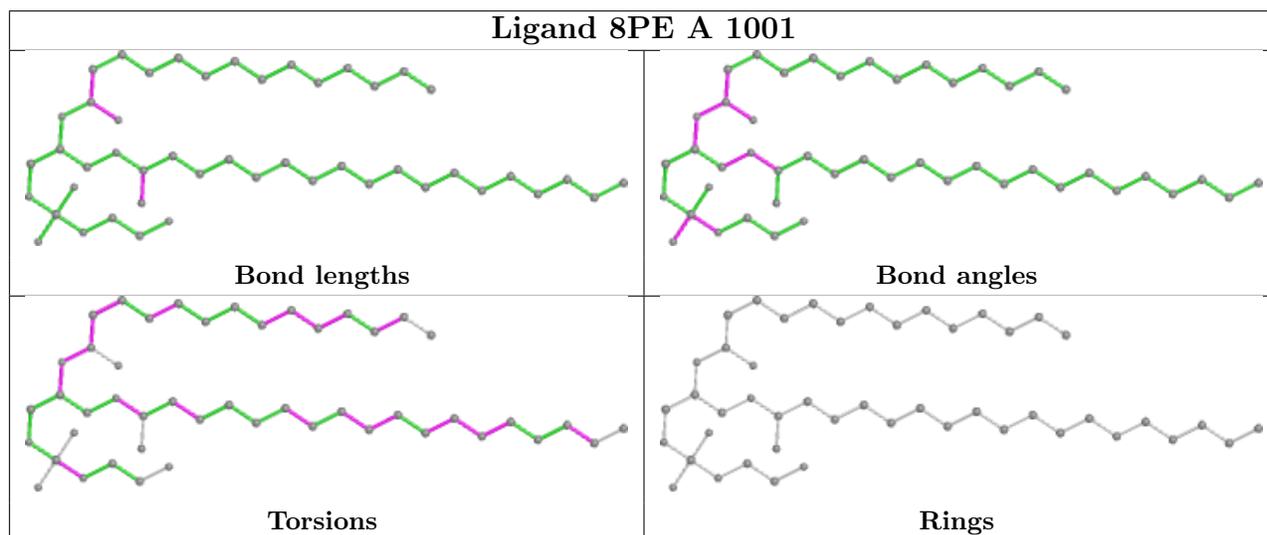
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	8PE	8	0
2	B	1001	8PE	8	0
4	B	1003	PO4	1	0
3	A	1002	CLR	5	0

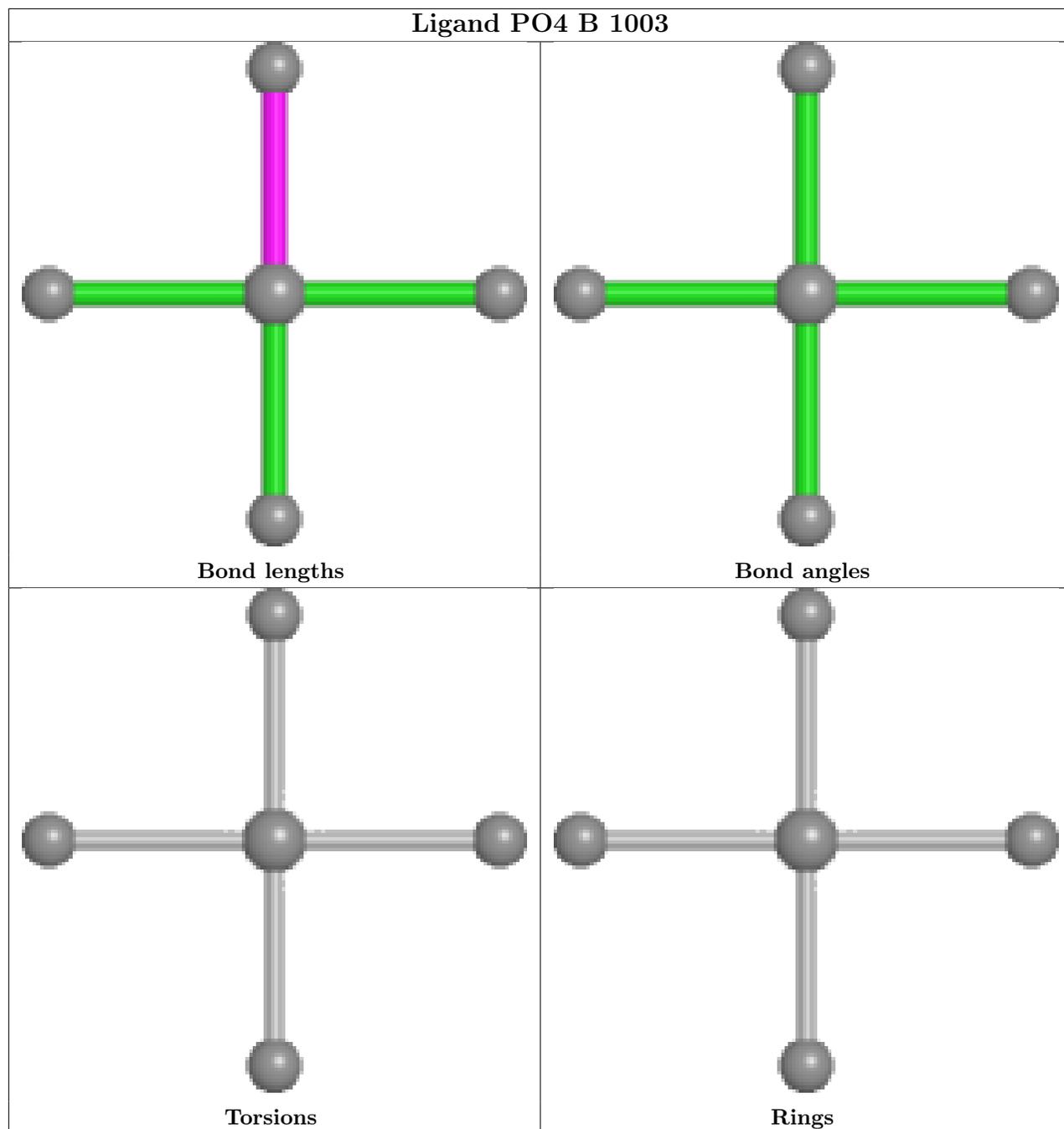
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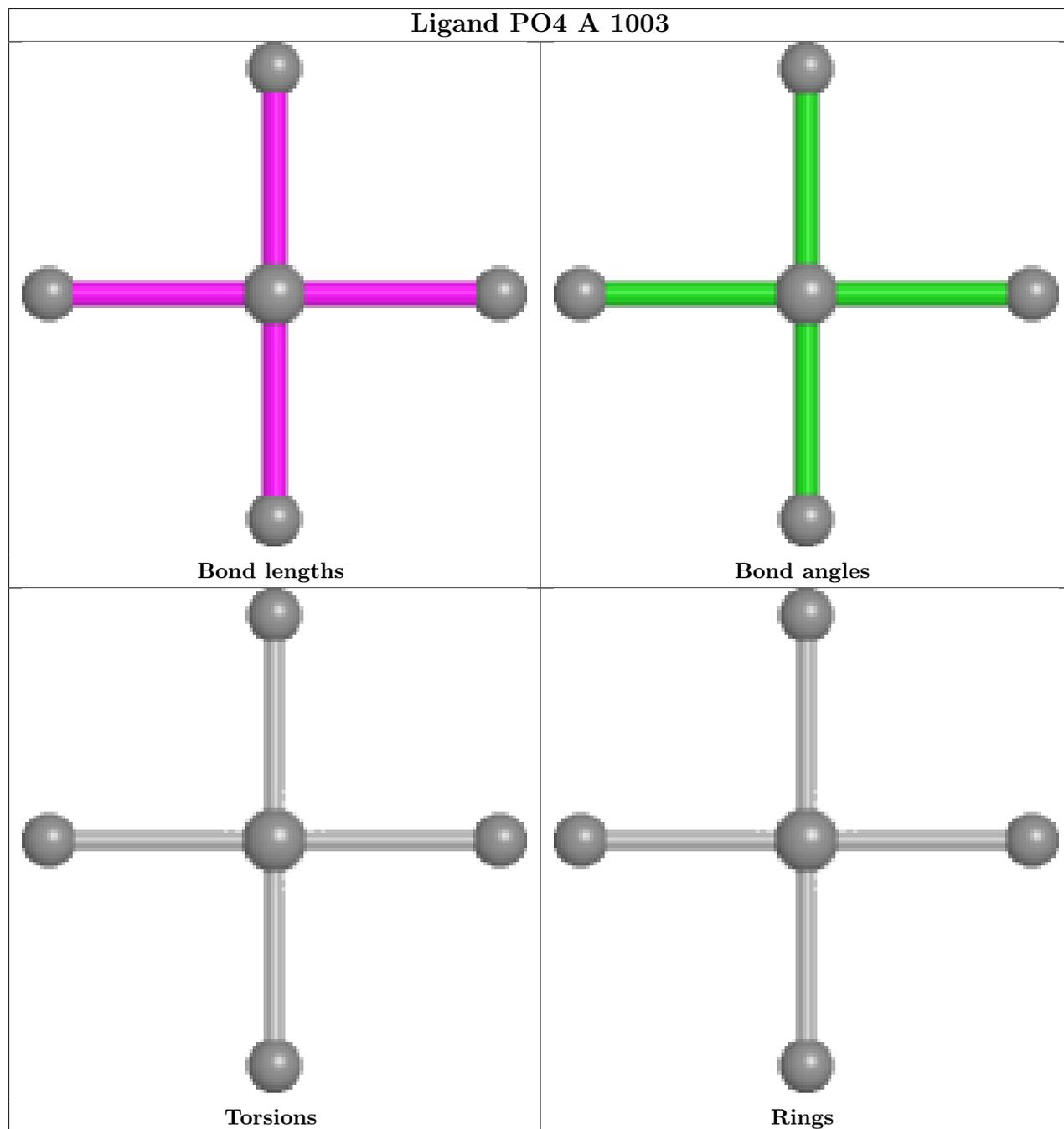
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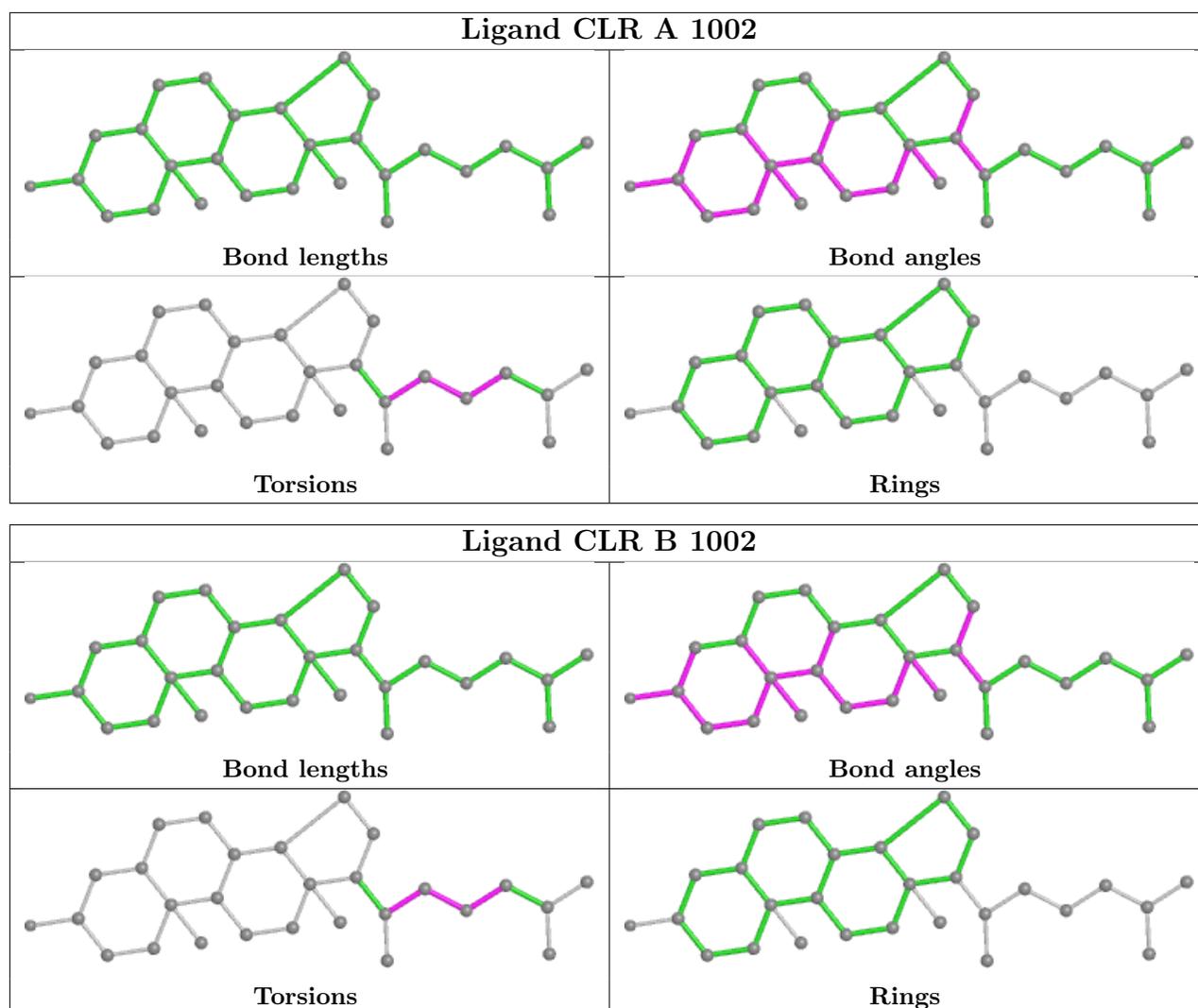
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	CLR	4	0

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.









## 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.