



## 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	: <b>FAILED</b>
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	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.42

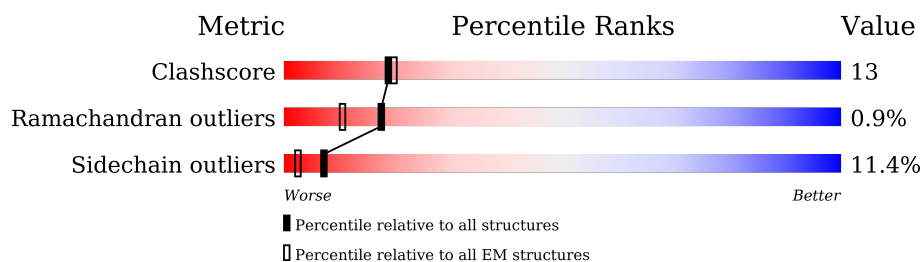
# 1 Overall quality at a glance

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	
1	B	969	

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

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
1	A	393	Total	C	N	O	S	0	0
			3272	2198	526	532	16		
1	B	393	Total	C	N	O	S	0	0
			3272	2198	526	532	16		

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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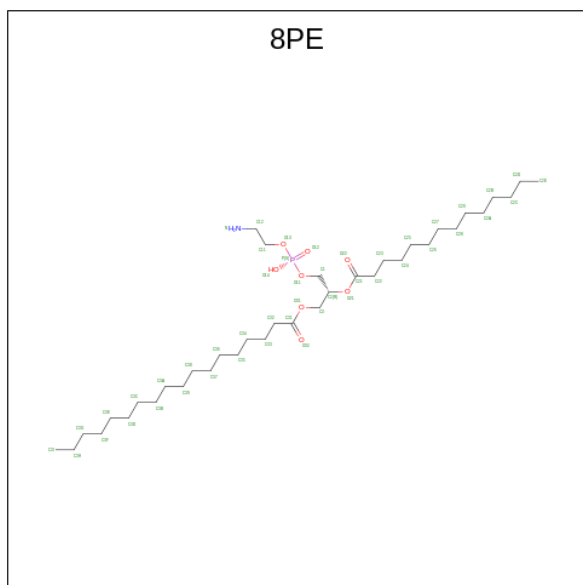
Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ASP	-	expression tag	UNP P42212
A	956	TYR	-	expression tag	UNP P42212
A	957	LYS	-	expression tag	UNP P42212
A	958	ASP	-	expression tag	UNP P42212
A	959	HIS	-	expression tag	UNP P42212
A	960	ASP	-	expression tag	UNP P42212
A	961	ILE	-	expression tag	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).



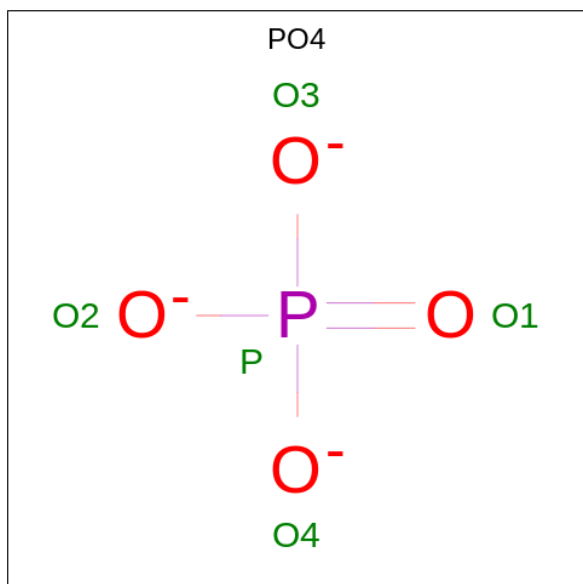
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

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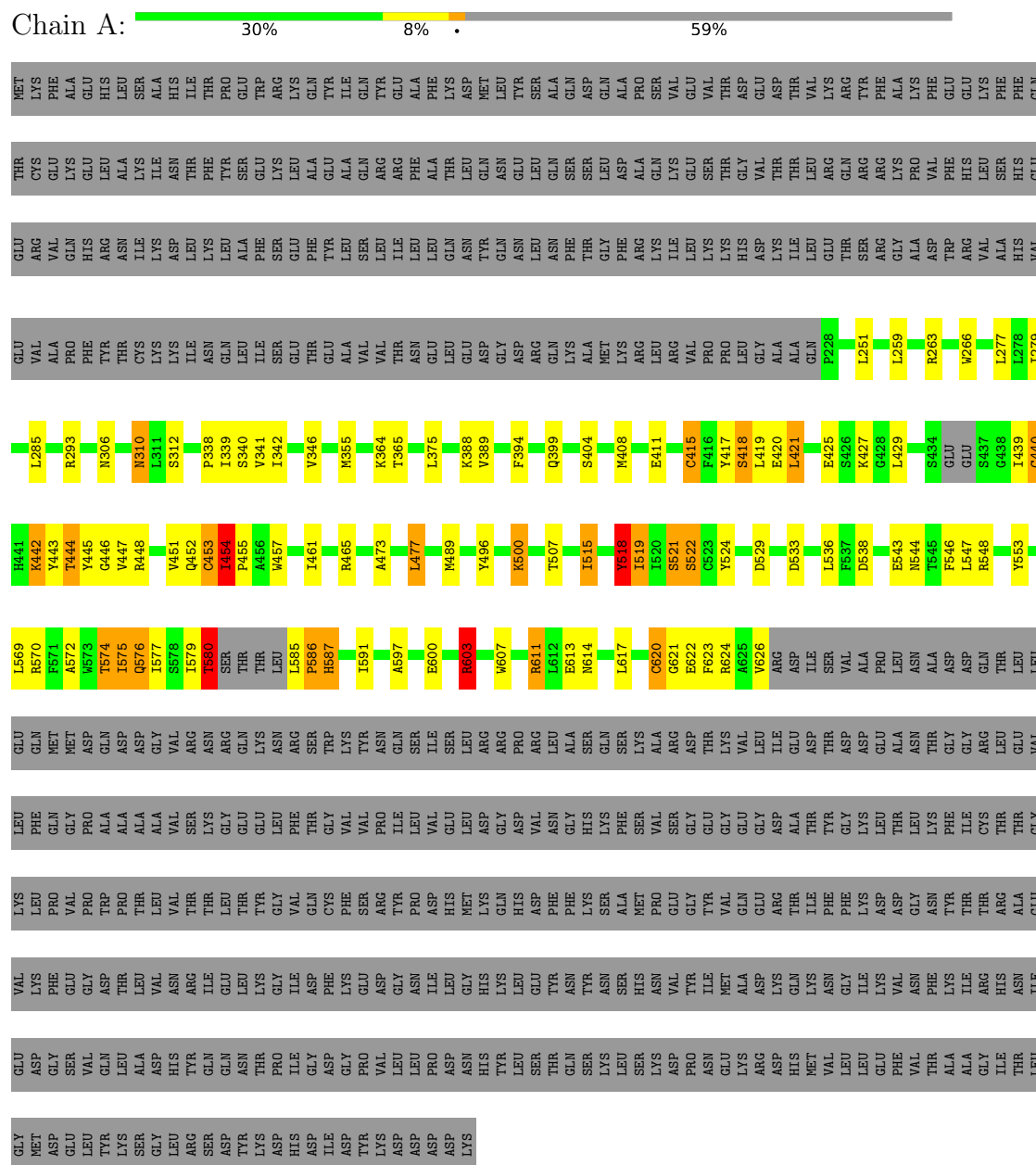
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Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
4	B	1	5	4	1	0

### 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. 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: Solute carrier family 53 member 1, Green fluorescent protein



- Molecule 1: Solute carrier family 53 member 1, Green fluorescent protein



Chain B:  30% 8% 59%

MET	THR	GLU	GLU	GLU	VAL	VAL	R293	Y443	A572	MET	GLY	SER	GLU	SER	GLU	LEU
LYS	CYS	ARG	VAL	GLN	ALA	ALA	R293	T444	W573	ASP	PRO	VAL	GLY	VAL	THR	TYR
PHE	GLU	VAL	PRO	LYS	PHE	ALA	N306	Y445	T574	GLN	ALA	GLN	ASP	LEU	ILE	LEU
ALA	LYS	HIS	ARG	LEU	THR	THR	N310	G446	I575	ASP	ALA	ASP	ALA	ALA	THR	LYS
GLU	LEU	ARG	TYR	ASN	THR	CYS	I311	V447	Q576	ASP	ALA	GLY	VAL	VAL	VAL	ASN
LEU	ALA	ASN	THR	ILE	THR	LYS	S312	R448	I577	VAL	VAL	ARG	VAL	VAL	ARG	THR
SER	LYS	ILE	CYS	LYS	THR	LYS	L332	V451	I579	ARG	SER	THR	VAL	THR	THR	ASN
ALA	ASN	THR	LYS	ILE	THR	ILE	L332	Q452	T580	GLN	GLY	THR	GLY	GLY	GLY	GLY
ILE	THR	THR	ASP	LEU	THR	THR	P338	C453	I484	GLN	GLY	THR	GLY	GLY	GLY	LEU
THR	PHE	LYS	ASN	LEU	THR	GLN	I339	P455	A456	LYS	LEU	ASN	GLY	GLY	GLY	LEU
PRO	TYR	LEU	LEU	ALA	LEU	LEU	S340	A457	A456	ARG	PHE	ARG	LEU	VAL	VAL	ASN
GLU	SER	PHE	ALA	ILE	ILE	ILE	V341	V457	L585	THR	LEU	THR	GLY	VAL	VAL	GLY
TRP	LYS	GLU	SER	SER	SER	SER	I342	I461	P586	TRP	GLY	TRP	THR	GLY	GLY	GLY
LYS	LEU	LEU	GLU	THR	THR	THR	V346	L464	H587	LYS	VAL	LYS	GLY	VAL	VAL	VAL
GLN	ALA	TYR	GLY	THR	ALA	ALA	M355	R465	I591	ASN	PRO	ASN	ASN	ARG	ARG	ASN
ILE	ALA	TYR	LEU	SER	VAL	VAL	K364	A473	A597	GLN	ILE	GLN	ILE	ILE	ILE	GLN
TYR	GLN	SER	LEU	ILE	THR	THR	T365	L477	E600	SER	VAL	ILE	VAL	VAL	VAL	VAL
ALA	PHE	ILE	LEU	ARG	THR	THR	K388	M489	R611	LEU	GLY	GLY	GLY	GLY	GLY	GLY
PHE	ALA	LEU	LEU	GLN	ASN	ASN	V389	M489	E612	ASP	GLY	ASP	GLY	GLY	GLY	GLY
LYS	THR	GLN	ASN	LEU	GLY	GLY	F394	L495	L612	PRO	GLY	ARG	GLY	GLY	GLY	GLY
ASP	LEU	TYR	TYR	GLU	ASP	ASP	Q399	Y496	E613	VAL	VAL	ASP	VAL	VAL	VAL	VAL
LEU	GLN	ASN	ASN	ASN	GLY	GLY	S404	K500	E614	LEU	GLY	ALA	GLY	GLY	GLY	GLY
ALA	ASN	ASN	ASN	ASN	ARG	GLN	M408	T507	N614	GLN	GLY	SER	ILE	ILE	ILE	ILE
ALA	LYS	PHE	LYS	LYS	GLN	LYS	E411	I515	L617	LYS	VAL	ALA	ASP	ASP	ASP	ASP
PRO	ASP	GLY	LYS	ARG	THR	THR	C415	I518	G620	ASP	GLY	ARG	GLY	GLY	GLY	GLY
SER	GLN	ILE	LEU	ARG	THR	THR	F416	I519	G621	THR	GLY	ASP	GLY	GLY	GLY	GLY
VAL	LYS	ILE	GLY	ARG	THR	THR	Y417	T520	E622	THR	GLY	THR	THR	THR	THR	THR
GLU	GLY	ILE	ARG	LEU	LEU	LEU	S418	S521	F623	LYS	GLY	LYS	VAL	VAL	VAL	VAL
THR	THR	LYS	PRO	PRO	PRO	PRO	L419	S522	R624	VAL	GLY	VAL	VAL	VAL	VAL	VAL
ASP	GLY	HIS	LEU	LEU	LEU	LEU	E420	C523	V626	LEU	ASP	ILE	ILE	ILE	ILE	ILE
GLU	VAL	ASP	GLY	GLY	GLY	GLY	L421	Y524	ARG	ILE	ASP	GLY	GLY	GLY	GLY	GLY
ASP	THR	LYS	ASP	ASP	ASP	ASP	E425	D529	ILE	THR	ILE	THR	THR	THR	THR	THR
THR	THR	ILE	ILE	ILE	ILE	ILE	S426	D533	SER	THR	THR	THR	THR	THR	THR	THR
LYS	ARG	GLU	GLU	GLU	GLU	GLU	K427	L536	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	G428	F537	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY
TYR	ARG	SER	SER	SER	SER	SER	L429	D538	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
PHE	LYS	ARG	ARG	ARG	ARG	ARG	S434	E543	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLU	N544	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
LYS	PRO	ALA	ALA	ALA	ALA	ALA	W266	T545	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
PHE	VAL	VAL	VAL	VAL	VAL	VAL	S437	F546	THR	THR	THR	THR	THR	THR	THR	THR
GLU	TRP	TRP	TRP	TRP	TRP	TRP	G438	L547	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
LYS	ARG	ARG	ARG	ARG	ARG	ARG	I439	R548	THR	THR	THR	THR	THR	THR	THR	THR
PHE	LEU	HIS	HIS	HIS	HIS	HIS	C440	L548	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLN	HIS	LEU	ALA	ALA	ALA	ALA	H441	R548	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
							K442	Y553	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
									MET	MET	MET	MET	MET	MET	MET	MET

## 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 ⓘ

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:

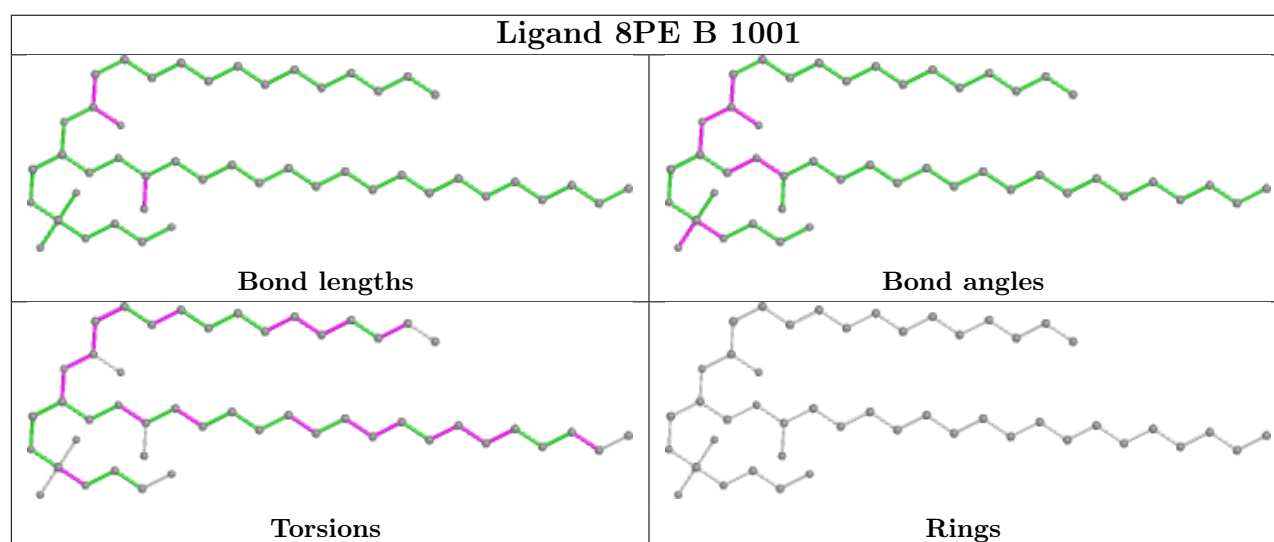
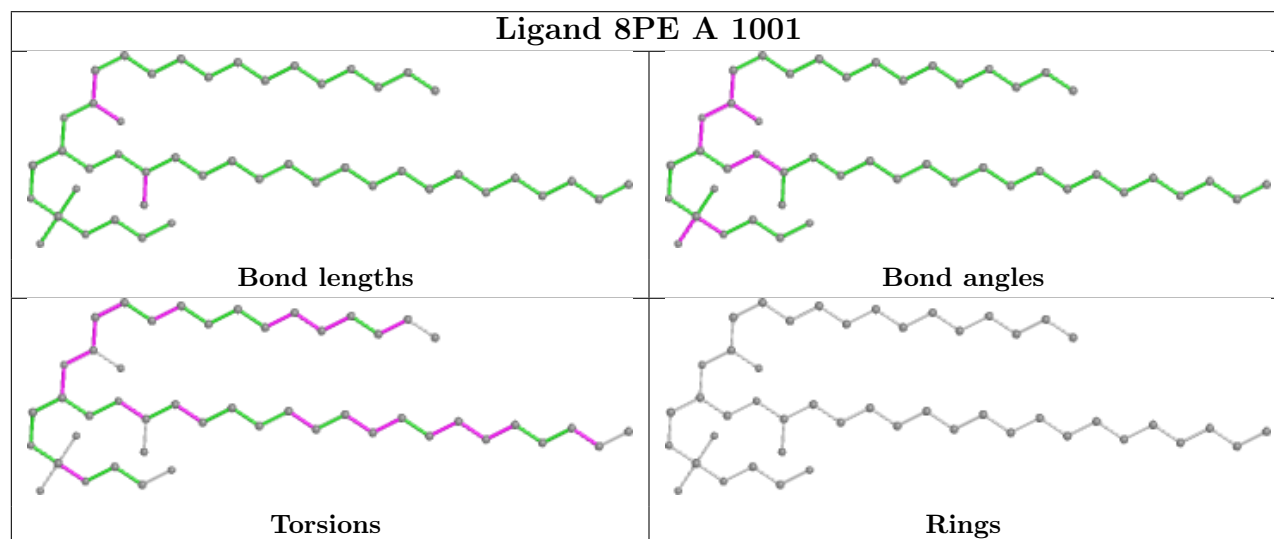
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	8PE	8	0
2	B	1001	8PE	8	0
4	B	1003	PO4	1	0
3	A	1002	CLR	5	0

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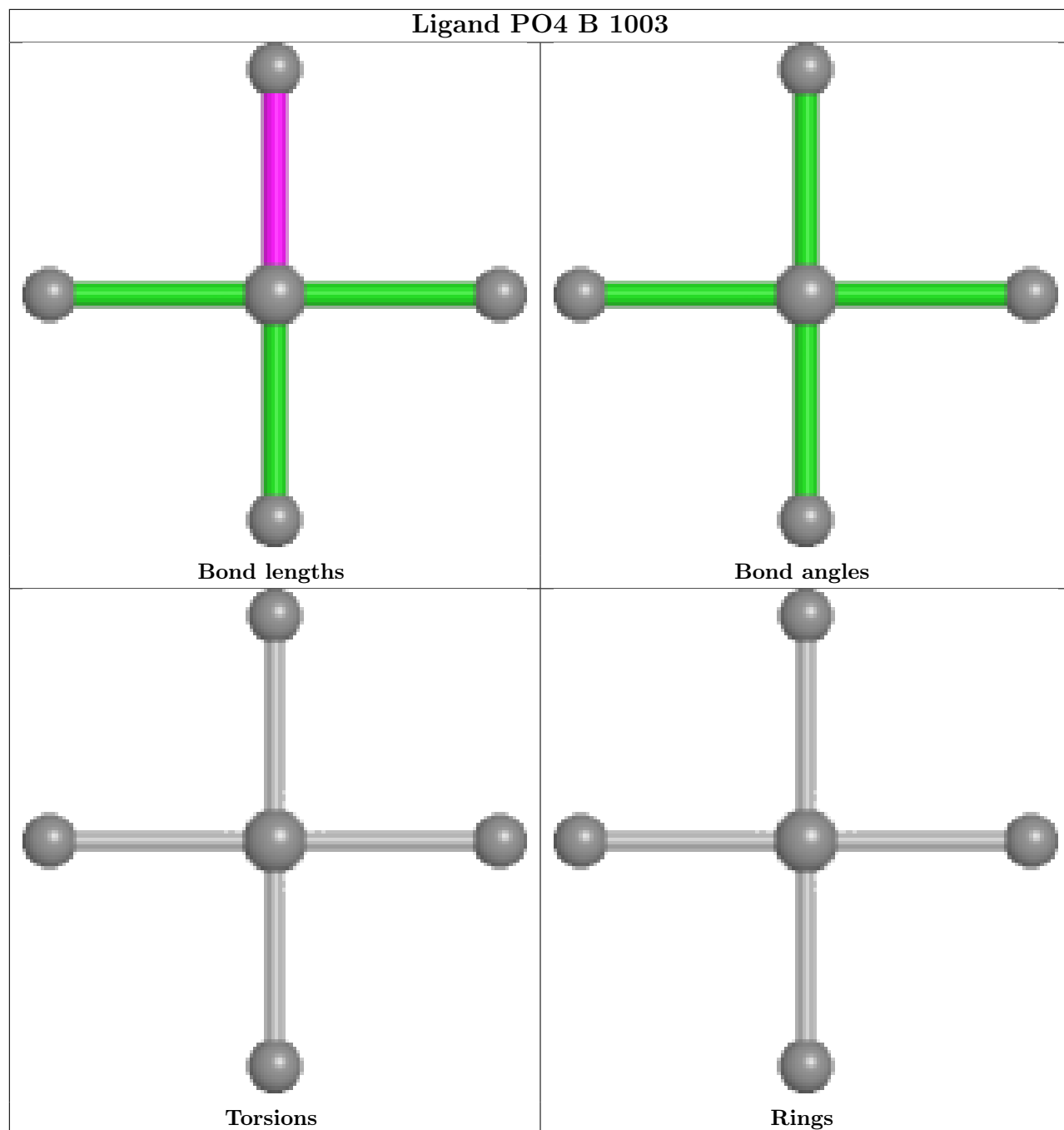
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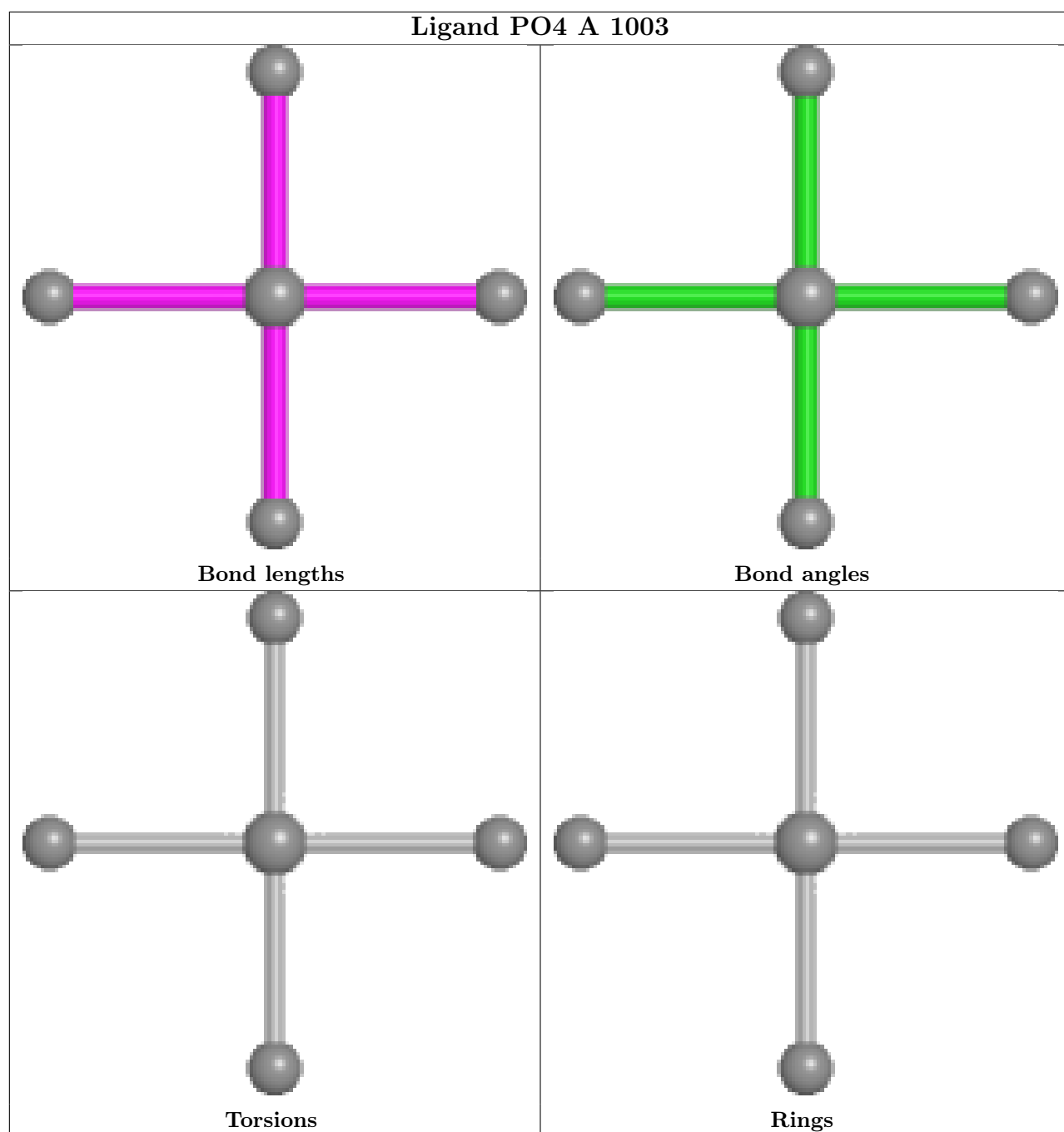
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	CLR	4	0

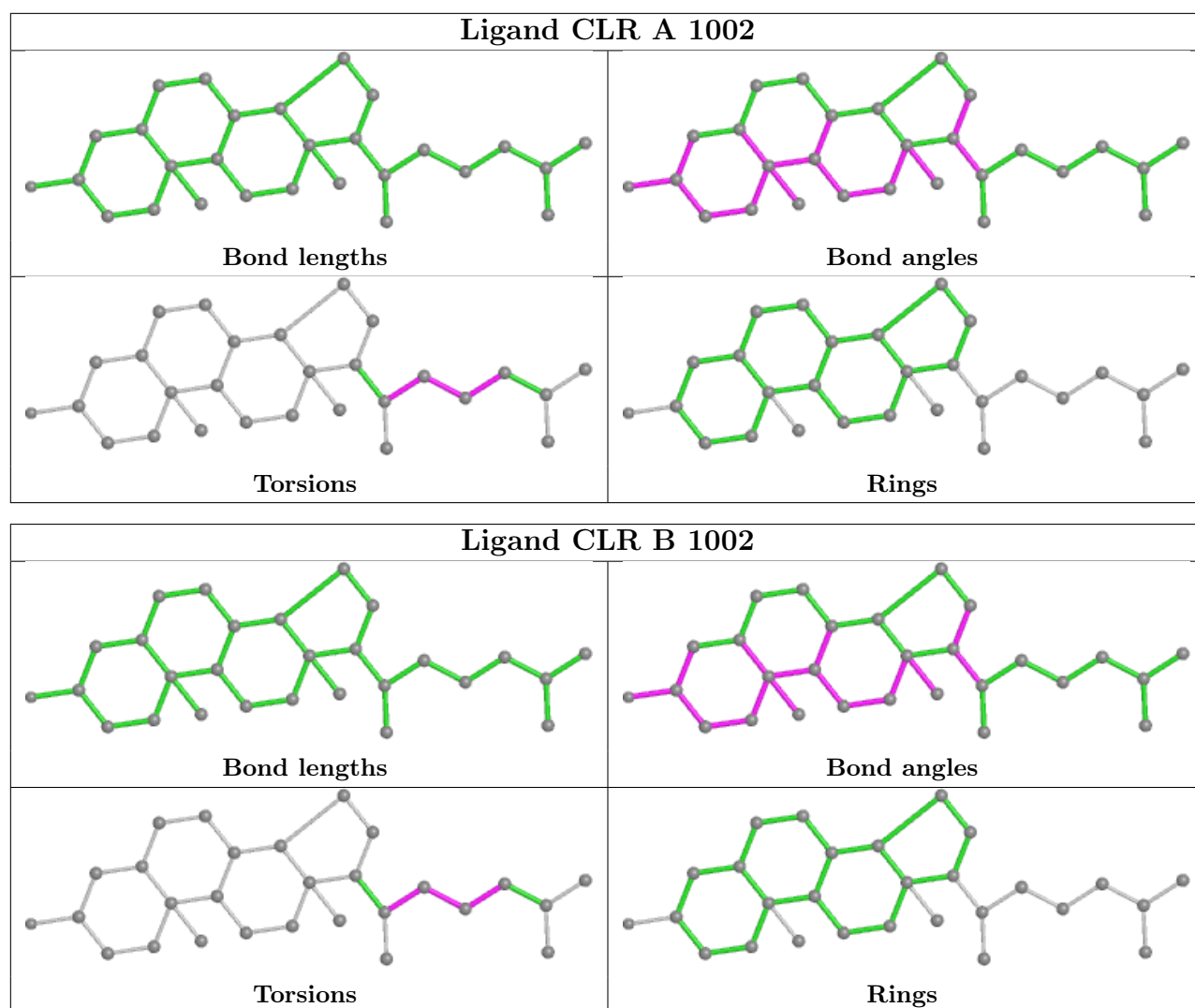
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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