



wwPDB EM Validation Summary Report ⓘ

Jul 16, 2025 – 12:51 AM JST

PDB ID : 8ISK / pdb_00008isk
EMDB ID : EMD-35693
Title : Pr conformer of Zea mays phytochrome A1 - ZmphyA1-Pr
Authors : Zhang, Y.; Ma, C.; Zhao, J.; Gao, N.; Wang, J.
Deposited on : 2023-03-20
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

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	: 4-5-2 with Phenix2.0rc1
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)	: 2.44

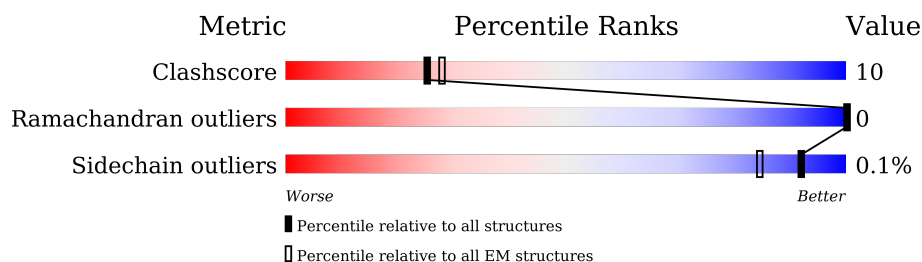
1 Overall quality at a glance

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

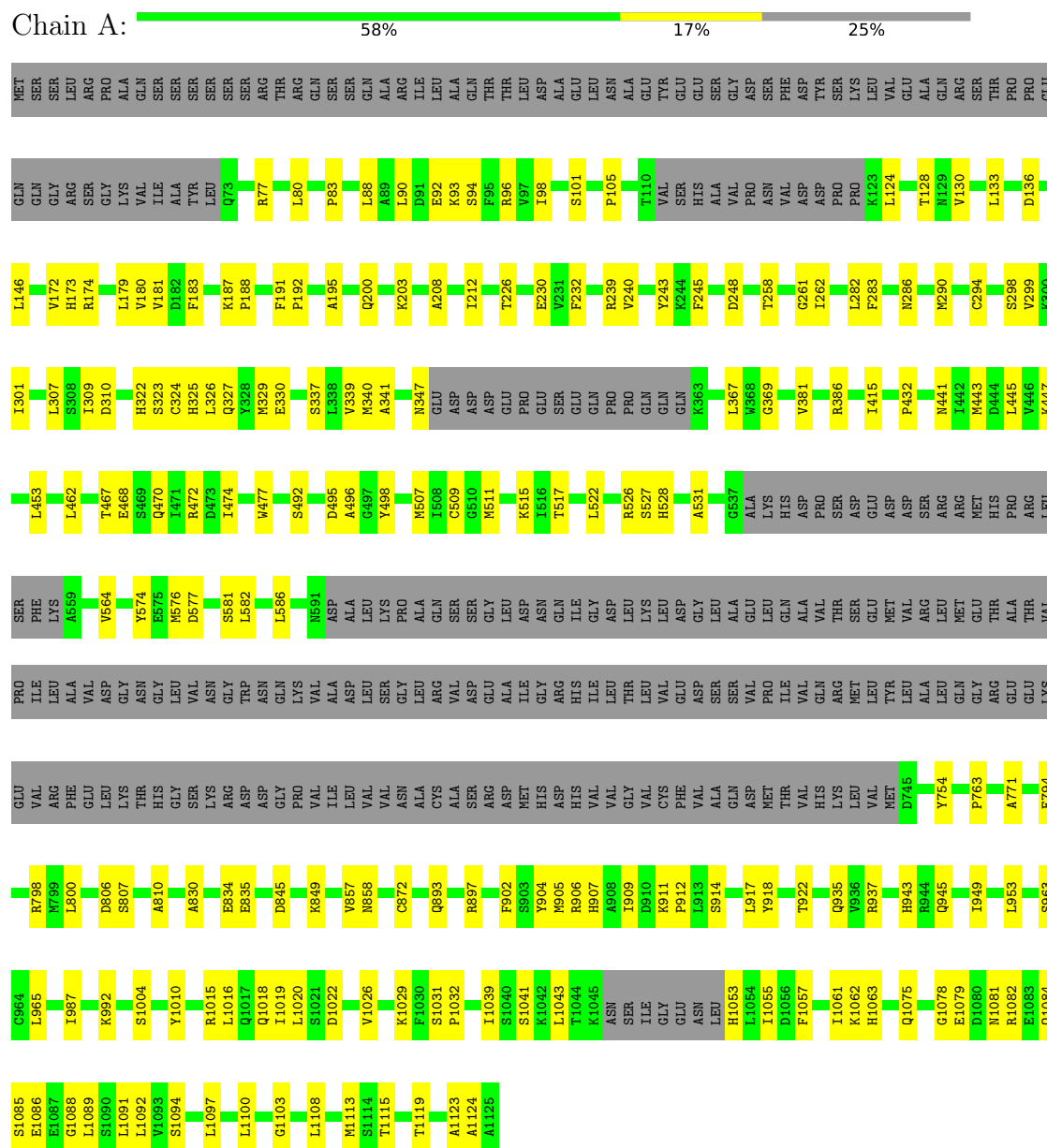
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	1125	
1	B	1125	

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: Phytochrome



• Molecule 1: Phytochrome

Chain B:

57%

19%

25%

GLN	GLN	R174	V344	F476	D573	LEU	GLY	R222	D960	L1059
GLN	GLY	A175	N345	F476	H580	VAL	SER	R223	S963	R1060
ARG	ARG	C178	E346	E480	S581	ASN	LYS	L823	K1061	T1081
SER	SER	L179	N347	T486	L582	TRP	ASP	C824	C964	K1062
GLY	GLY	V180	GLU	G487	R587	ASN	ASP	N828	L965	H1063
LYS	LYS	V181	ASP	L488	N591	GLN	GLY	N829	D966	Q1064
VAL	VAL	E190	ASP	L493	N591	LYS	PRO	E837	L967	Q1071
ILE	ILE	A193	ASP	L493	N591	ALA	VAL	P840	D968	T1072
ALA	ALA	T194	PRO	Y498	N591	LEU	LEU	C853	Q975	Q1075
SER	SER	T194	GLU	P499	N591	SER	VAL	C853	V978	G1078
SER	SER	A195	SER	P499	N591	GLY	ASN	S856	V979	G1078
SER	SER	A196	GLU	P499	N591	LEU	ALA	S856	S980	N1081
ARG	ARG	G197	GLN	M507	N591	ALA	ALA	I874	Q984	R1082
THR	THR	L80	PRO	I508	N591	VAL	CYS	H875	V985	E1083
ARG	ARG	A89	PRO	I508	N591	ASP	ALA	V876	L986	Q1084
GLN	GLN	L90	GLN	M511	N591	GLY	SER	L885	L987	S1085
SER	SER	S201	GLN	A512	N591	LEU	ASP	L885	R987	E1086
SER	SER	Y202	GLN	A514	N591	ILE	ASP	Q889	R995	L1089
SER	SER	K203	GLN	A514	N591	ASP	HIS	A890	L1000	L1092
GLN	GLN	L204	GLN	I516	N591	GLY	ASP	Q893	S1004	L1098
ALA	ALA	I98	GLN	S518	N591	ILE	VAL	L896	M1005	R1099
ALA	ALA	S101	ILE	S518	N591	ILE	VAL	L899	Y1010	L1100
LEU	LEU	E102	LEU	K519	N591	LEU	VAL	R906	D1012	M1101
ALA	ALA	N103	LEU	D520	N591	THR	GLY	H907	L1016	D1104
GLN	GLN	A104	LEU	I521	N591	LEU	VAL	P912	Q1017	T1105
THR	THR	P105	LEU	L522	N591	LEU	VAL	L913	Q1018	G1112
THR	THR	E106	LEU	F523	N591	VAL	CYS	S914	I1019	M1113
LEU	LEU	M107	LEU	F523	N591	ASP	PHE	G915	L1020	S1114
ASP	ASP	L108	LEU	R526	N591	SER	VAL	M916	S1036	T1115
ALA	ALA	T109	LEU	R526	N591	ASP	ALA	L917	V1037	F1116
GLU	GLU	T110	LEU	R526	N591	SER	GLN	Y918	D1038	T1117
LEU	LEU	VAL	LEU	G536	N591	LEU	ASP	S919	S1041	A1123
ASN	ASN	HIS	LEU	G537	N591	VAL	MET	N941	K1042	A1124
ALA	ALA	ALA	LEU	L436	N591	ILE	THR	K746	L1043	A1125
GLU	GLU	VAL	LEU	M443	N591	GLN	THR	T748	T1044	
TYR	TYR	PRO	LEU	L445	N591	VAL	LEU	R749	K1045	
GLU	GLU	ASN	VAL	A452	N591	ARG	GLY	N762	ASN	
GLY	GLY	ASP	LEU	A455	N591	LYS	ASP	P763	SER	
SER	SER	PRO	GLU	Y455	N591	VAL	ASP	L764	ILE	
PHE	PHE	PRO	ASP	K458	N591	ALA	ASP	P767	GLY	
ASP	ASP	ASP	ASP	R461	N591	THR	THR	D952	GLU	
ASP	ASP	ASP	ASP	L462	N591	ALA	ALA	A771	ASN	
ASP	ASP	ASP	ASP	Q463	N591	THR	THR	L953	LEU	
ASP	ASP	ASP	ASP	T464	N591	VAL	VAL	D954	HIS	
ASP	ASP	ASP	ASP	A465	N591	ILE	ILE	Q955	LEU	
ASP	ASP	ASP	ASP	P466	N591	LEU	LEU	D956	GLY	
ASP	ASP	ASP	ASP	T467	N591	ALA	ALA	Q955	ILE	
ASP	ASP	ASP	ASP	E468	N591	VAL	VAL	D957	GLY	
ASP	ASP	ASP	ASP	S469	N591	ASP	ASP	L958	GLY	
ASP	ASP	ASP	ASP	Q470	N591	GLY	GLY	S811	LEU	
ASP	ASP	ASP	ASP	I471	N591	ASN	ASN		ASP	
ASP	ASP	ASP	ASP	S572	N591	GLY	GLY		ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: O6E

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	0.18	0/6704	0.38	0/9051
1	B	0.19	0/6728	0.39	0/9083
All	All	0.19	0/13432	0.38	0/18134

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1082	ARG	Sidechain
1	B	1082	ARG	Sidechain

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	6581	0	6617	138	0
1	B	6606	0	6649	141	0
2	A	43	0	0	1	0
2	B	43	0	0	0	0
All	All	13273	0	13266	270	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 270 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:1075:GLN:HA	1:A:1081:ASN:ND2	1.44	1.28
1:A:1084:GLN:HB3	1:A:1089:LEU:CD2	1.71	1.19
1:B:1064:GLN:HG2	1:B:1113:MET:SD	1.87	1.14
1:A:1084:GLN:CB	1:A:1089:LEU:HD21	1.78	1.13
1:B:1081:ASN:O	1:B:1084:GLN:HG2	1.48	1.11

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	833/1125 (74%)	799 (96%)	34 (4%)	0	100	100
1	B	836/1125 (74%)	802 (96%)	34 (4%)	0	100	100
All	All	1669/2250 (74%)	1601 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	718/962 (75%)	717 (100%)	1 (0%)	92	96
1	B	722/962 (75%)	721 (100%)	1 (0%)	92	96
All	All	1440/1924 (75%)	1438 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	B	1083	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	883	HIS
1	B	957	ASN
1	B	1084	GLN
1	B	1007	GLN
1	B	947	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

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	O6E	B	1201	1	42,46,46	0.97	3 (7%)	50,67,67	1.33	2 (4%)
2	O6E	A	1201	1	42,46,46	0.99	3 (7%)	50,67,67	1.13	5 (10%)

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	O6E	B	1201	1	-	4/25/74/74	0/4/4/4
2	O6E	A	1201	1	-	7/25/74/74	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	O6E	CAO-CAV	3.15	1.37	1.35
2	A	1201	O6E	CAB-CBI	-2.93	1.39	1.47
2	B	1201	O6E	CAB-CBI	-2.87	1.39	1.47
2	B	1201	O6E	CAO-CAV	2.87	1.37	1.35
2	B	1201	O6E	CBI-CBC	2.13	1.41	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	O6E	CBO-CAO-CAV	6.39	136.44	128.81
2	A	1201	O6E	CBM-CBI-CBC	-3.31	103.68	107.92
2	A	1201	O6E	CBO-CAO-CAV	3.29	132.73	128.81
2	B	1201	O6E	CAW-CAP-CBL	3.01	135.44	128.08
2	A	1201	O6E	CAW-CAP-CBL	2.53	134.27	128.08

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

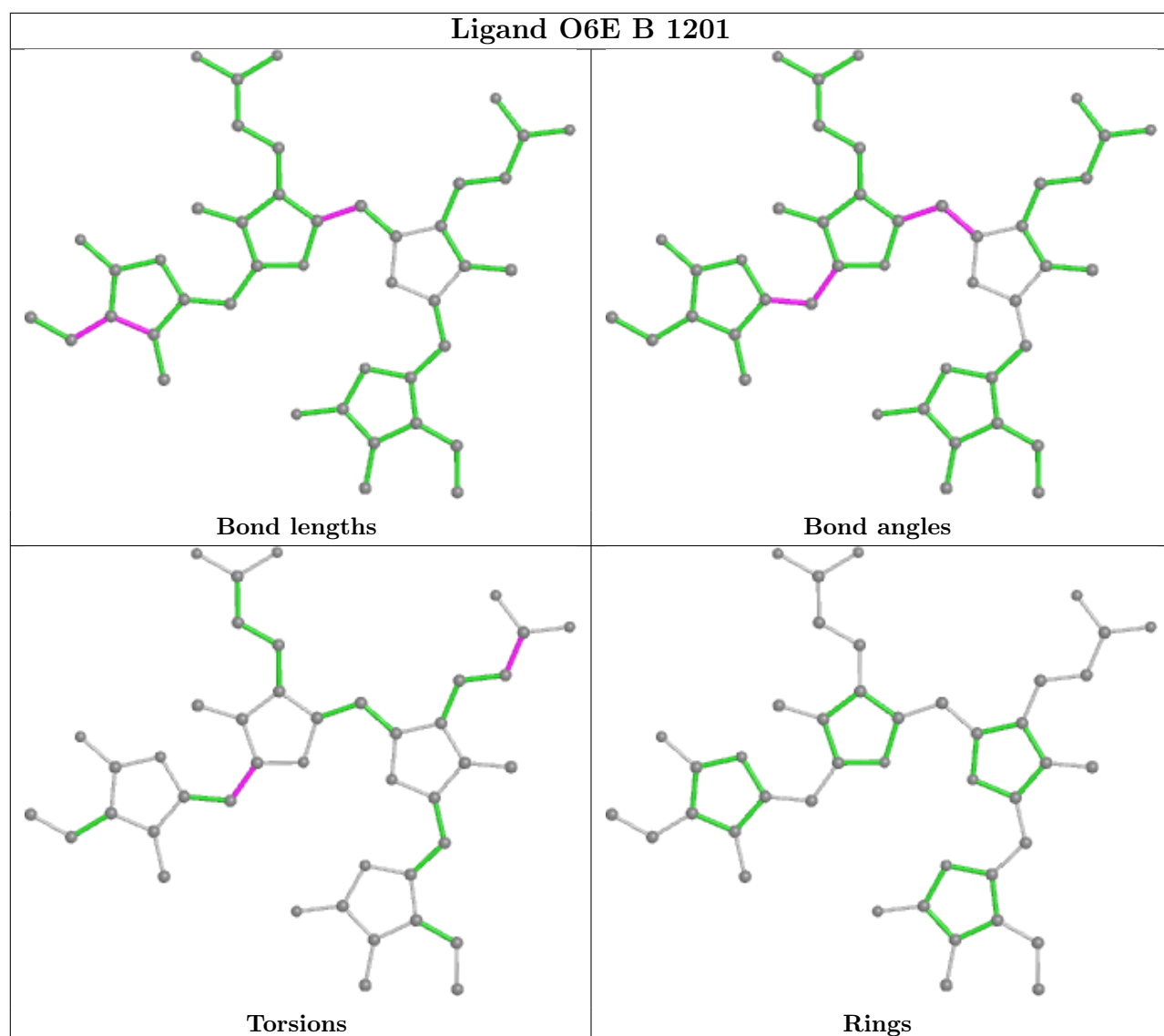
Mol	Chain	Res	Type	Atoms
2	A	1201	O6E	CAW-CAP-CBL-NAE
2	B	1201	O6E	CAW-CAP-CBL-NAE
2	A	1201	O6E	CAW-CAP-CBL-CBH
2	B	1201	O6E	CAW-CAP-CBL-CBH
2	A	1201	O6E	CAH-CAC-CBJ-CBN

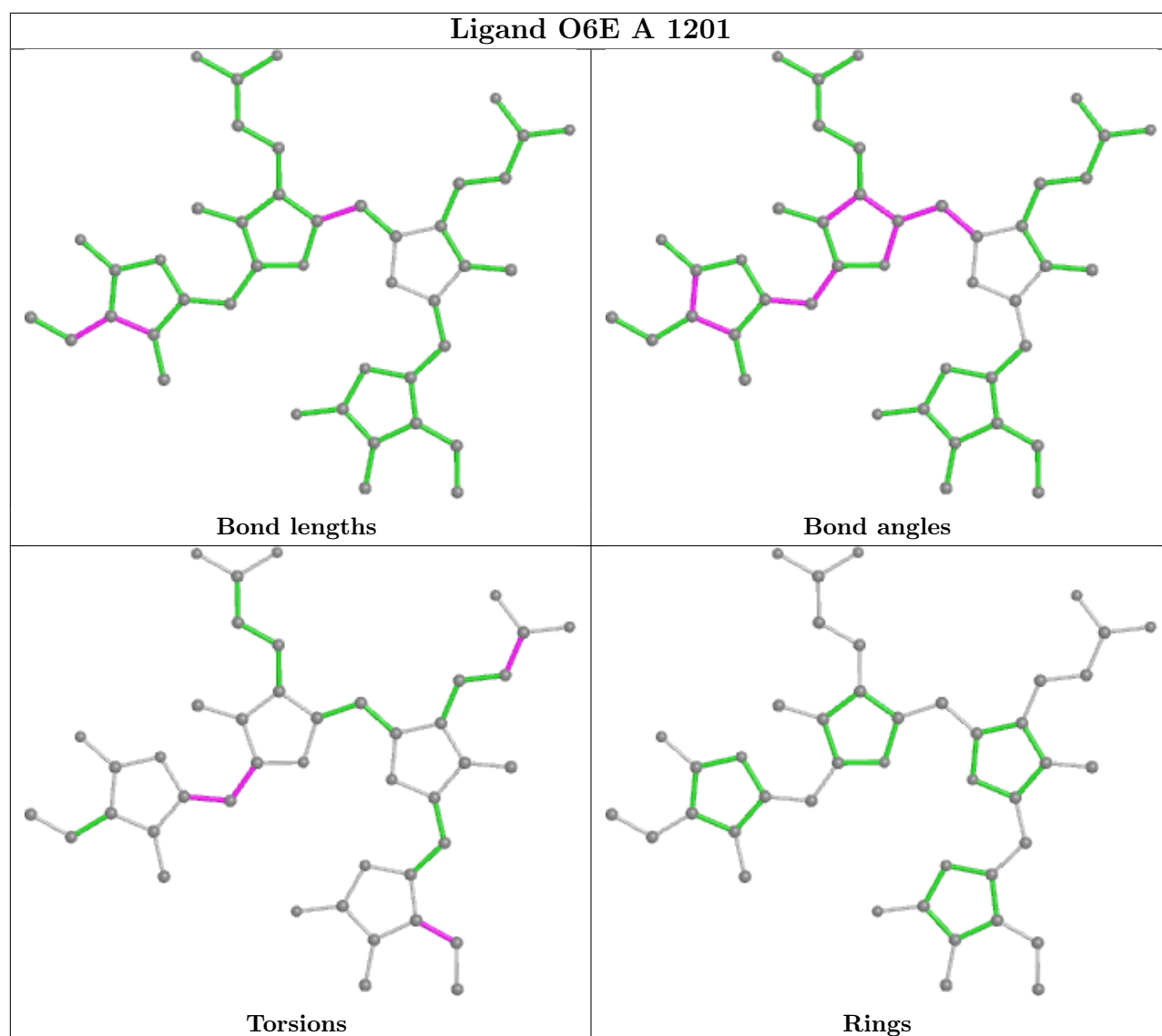
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	O6E	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 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.