



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:16 pm BST

PDB ID : 2VLF
Title : Quinonoid intermediate of Citrobacter freundii tyrosine phenol-lyase formed with alanine
Authors : Milic, D.; Demidkina, T.V.; Matkovic-Calogovic, D.; Antson, A.A.
Deposited on : 2008-01-14
Resolution : 1.89 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

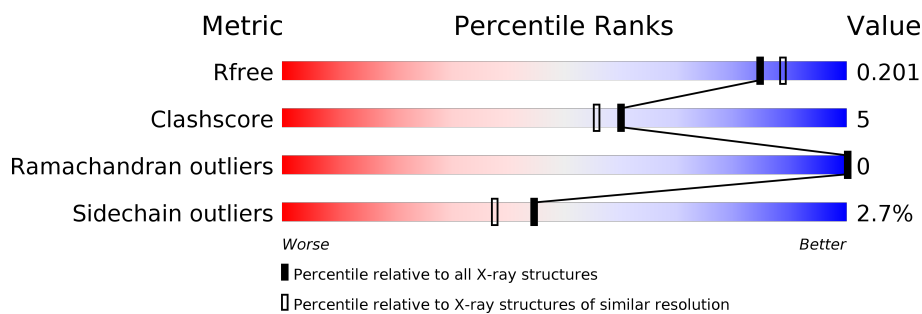
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	

2 Entry composition [i](#)

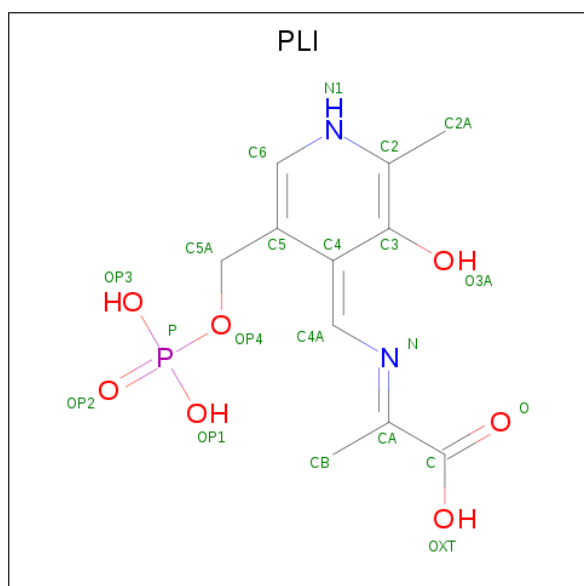
There are 6 unique types of molecules in this entry. The entry contains 8361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE PHENOL-LYASE.

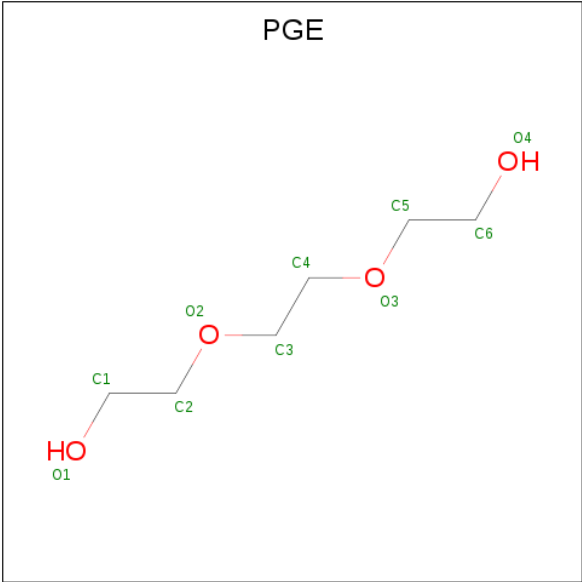
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	4	0
			3635	2300	628	681	26			
1	B	456	Total	C	N	O	S	0	11	1
			3684	2331	635	690	28			

- Molecule 2 is (2E)-2-[(Z)-{3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4(1H)-YLIDENE}METHYL]IMINO}PROPANOIC ACID (three-letter code: PLI) (formula: C₁₁H₁₅N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

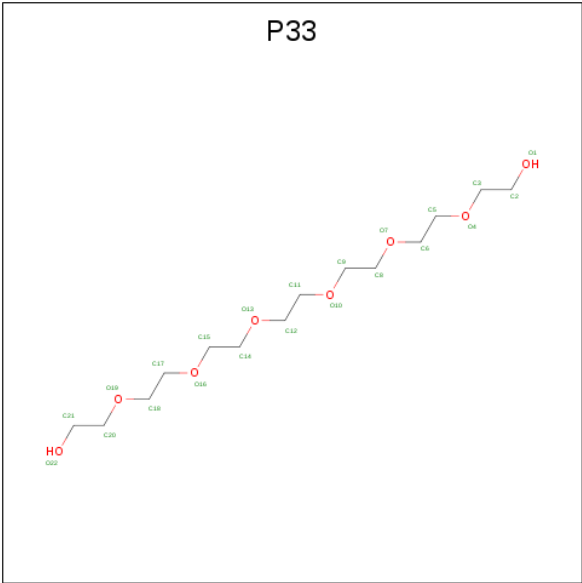


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	K	0	0
			2	2		

- Molecule 5 is 3,6,9,12,15,18-HEXAIOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			22	14	8		

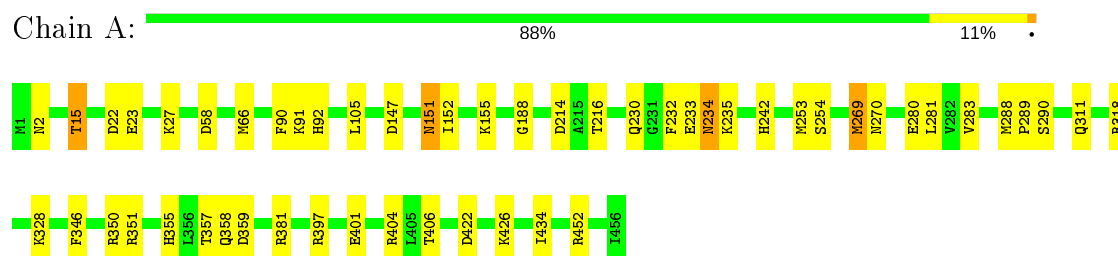
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	451	Total	O	0	0
			451	451		
6	B	515	Total	O	0	0
			515	515		

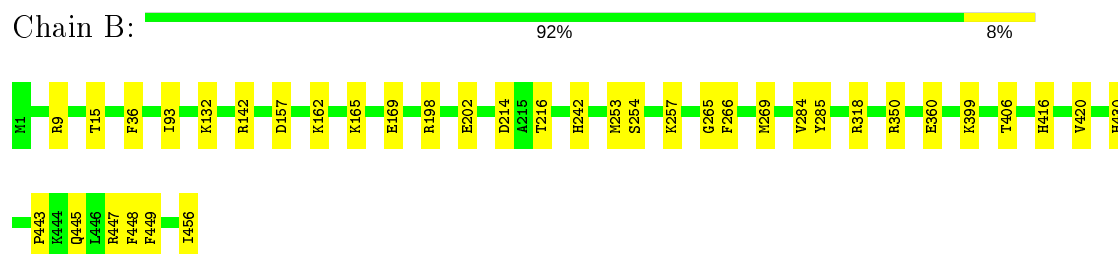
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: TYROSINE PHENOL-LYASE



• Molecule 1: TYROSINE PHENOL-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.85Å 143.69Å 59.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.89 19.86 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-1.89) 96.8 (19.86-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.157 , 0.198 0.159 , 0.201	Depositor DCC
R_{free} test set	1065 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: P33, K, PGE, PLI

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	0.75	0/3710	0.71	3/4997 (0.1%)
1	B	0.74	0/3767	0.71	0/5072
All	All	0.75	0/7477	0.71	3/10069 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	351	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	58	ASP	CB-CG-OD1	5.16	122.94	118.30

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	3635	0	3577	47	0
1	B	3684	0	3616	22	0
2	A	21	0	11	0	0
2	B	21	0	11	1	0
3	A	10	0	14	0	0
4	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	22	0	30	0	0
6	A	451	0	0	11	1
6	B	515	0	0	4	1
All	All	8361	0	7259	68	1

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 5.

The worst 5 of 68 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:422[A]:ASP:OD1	6:A:2409:HOH:O	1.78	0.99
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.27	0.98
1:A:92:HIS:HB2	1:A:269:MET:HE3	1.46	0.96
1:A:92:HIS:HB2	1:A:269:MET:CE	1.96	0.94
1:A:234:ASN:HD22	1:A:234:ASN:H	1.23	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2022:HOH:O	6:B:2009:HOH:O[2_665]	2.14	0.06

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 X-ray entries followed by that with respect to entries of similar resolution.

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	458/456 (100%)	449 (98%)	9 (2%)	0	100	100
1	B	465/456 (102%)	456 (98%)	9 (2%)	0	100	100
All	All	923/912 (101%)	905 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	381/379 (100%)	369 (97%)	12 (3%)	40	32
1	B	388/379 (102%)	380 (98%)	8 (2%)	53	48
All	All	769/758 (102%)	749 (97%)	20 (3%)	44	39

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	MET
1	A	318	ARG
1	B	269	MET
1	A	234	ASN
1	A	253	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	311	GLN
1	B	130	GLN
1	A	242	HIS
1	A	396	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	PLI	A	1457	-	17,21,21	2.65	3 (17%)	21,30,30	1.85	6 (28%)
2	PLI	B	1459	-	17,21,21	2.61	3 (17%)	21,30,30	1.81	6 (28%)
3	PGE	A	1458	-	9,9,9	0.50	0	8,8,8	0.30	0
5	P33	B	1460	-	21,21,21	0.57	0	20,20,20	0.35	0

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	PLI	A	1457	-	-	0/8/15/15	0/1/1/1
2	PLI	B	1459	-	-	0/8/15/15	0/1/1/1
3	PGE	A	1458	-	-	4/7/7/7	-
5	P33	B	1460	-	-	11/19/19/19	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1459	PLI	C3-C2	9.07	1.49	1.40
2	A	1457	PLI	C3-C2	8.53	1.49	1.40
2	A	1457	PLI	C-CA	-4.90	1.44	1.52
2	A	1457	PLI	CA-N	3.53	1.35	1.28
2	B	1459	PLI	CA-N	3.51	1.35	1.28

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1457	PLI	CB-CA-C	4.34	122.73	117.92
2	B	1459	PLI	C4-C3-C2	-4.14	117.63	120.19
2	A	1457	PLI	C4-C3-C2	-3.77	117.86	120.19
2	A	1457	PLI	C6-N1-C2	3.48	125.61	119.17
2	B	1459	PLI	CB-CA-C	3.40	121.69	117.92

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

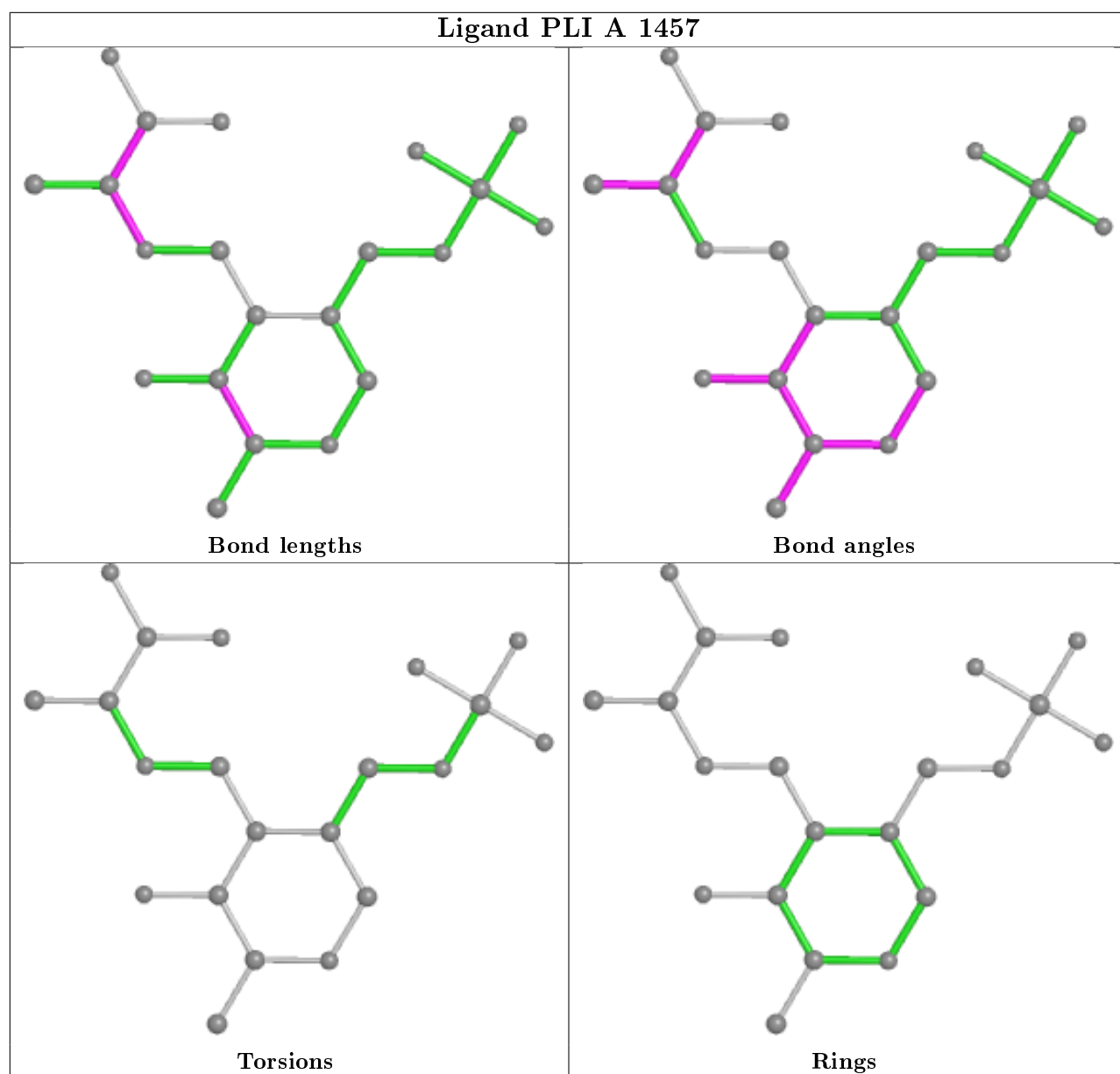
Mol	Chain	Res	Type	Atoms
5	B	1460	P33	O1-C2-C3-O4
5	B	1460	P33	O10-C11-C12-O13
5	B	1460	P33	O13-C14-C15-O16
5	B	1460	P33	O7-C8-C9-O10
3	A	1458	PGE	O1-C1-C2-O2

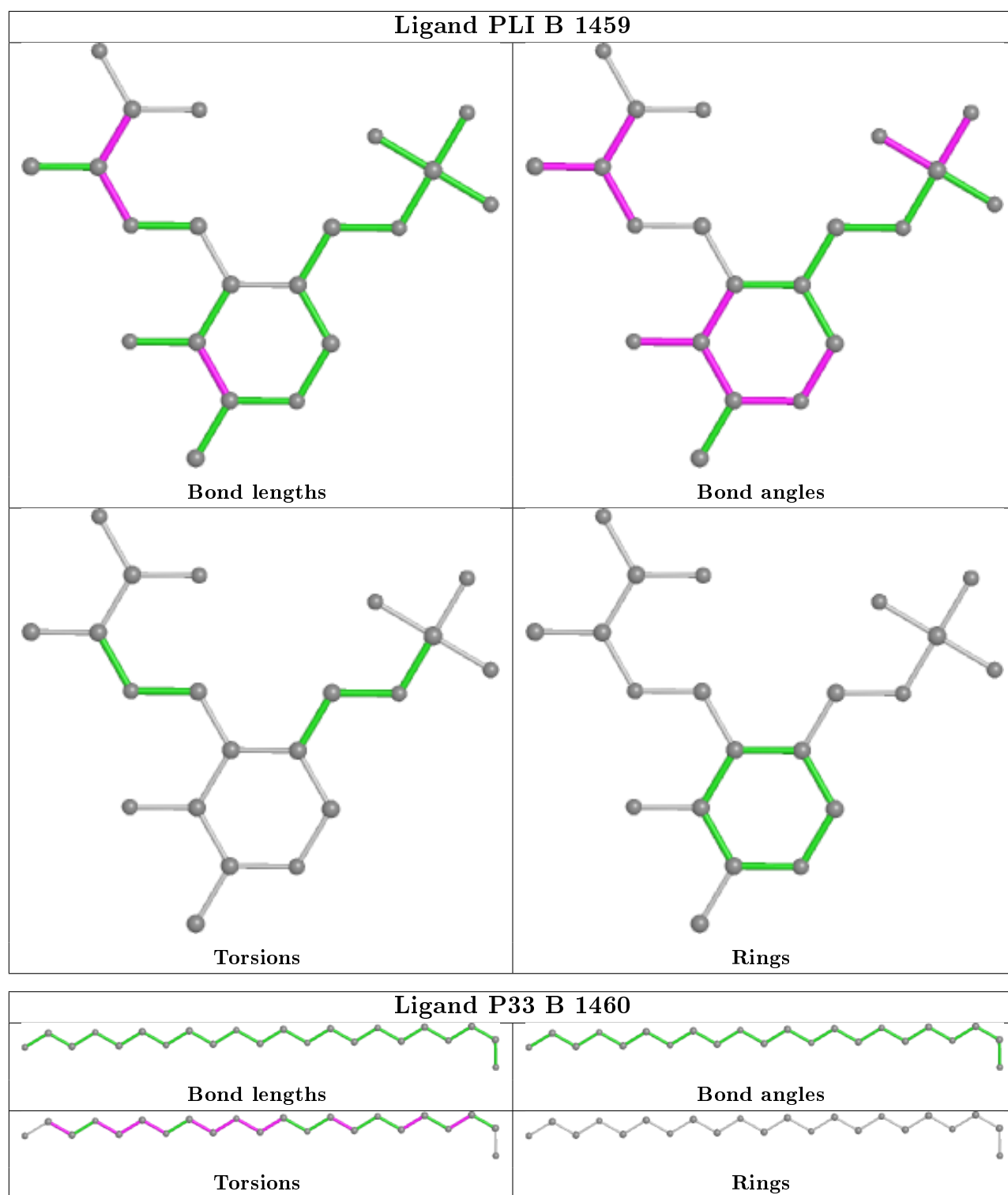
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1459	PLI	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 ⓘ

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.

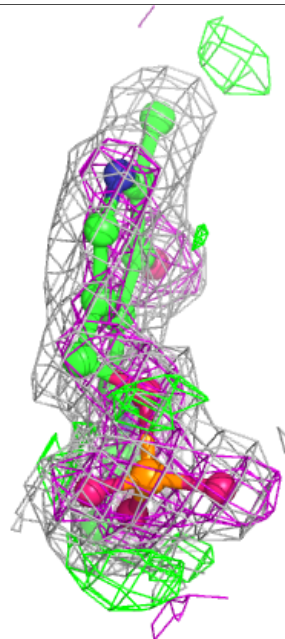
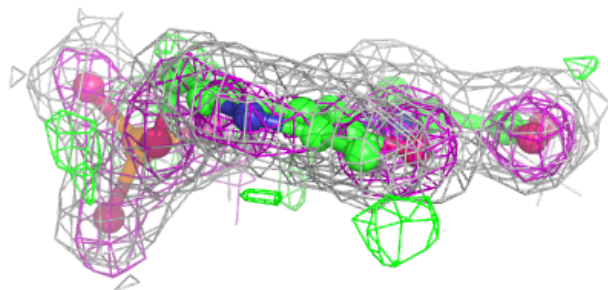
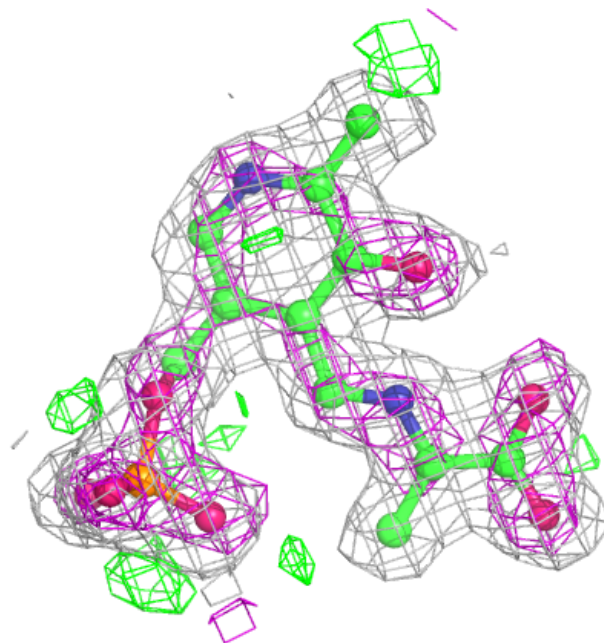
6.4 Ligands ⓘ

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.

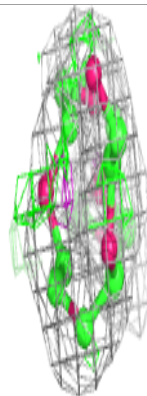
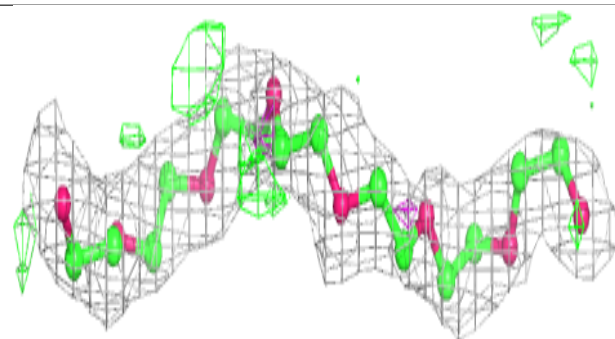
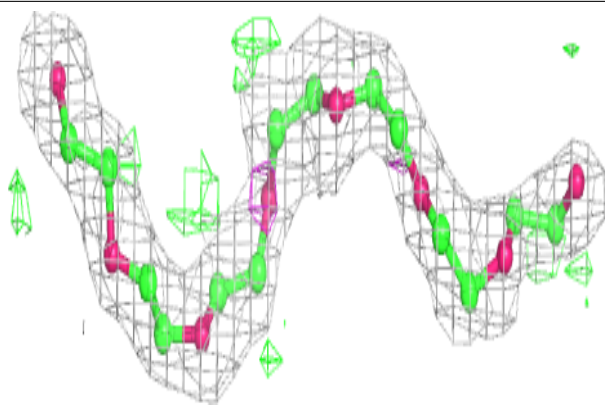
Electron density around PLI A 1457:

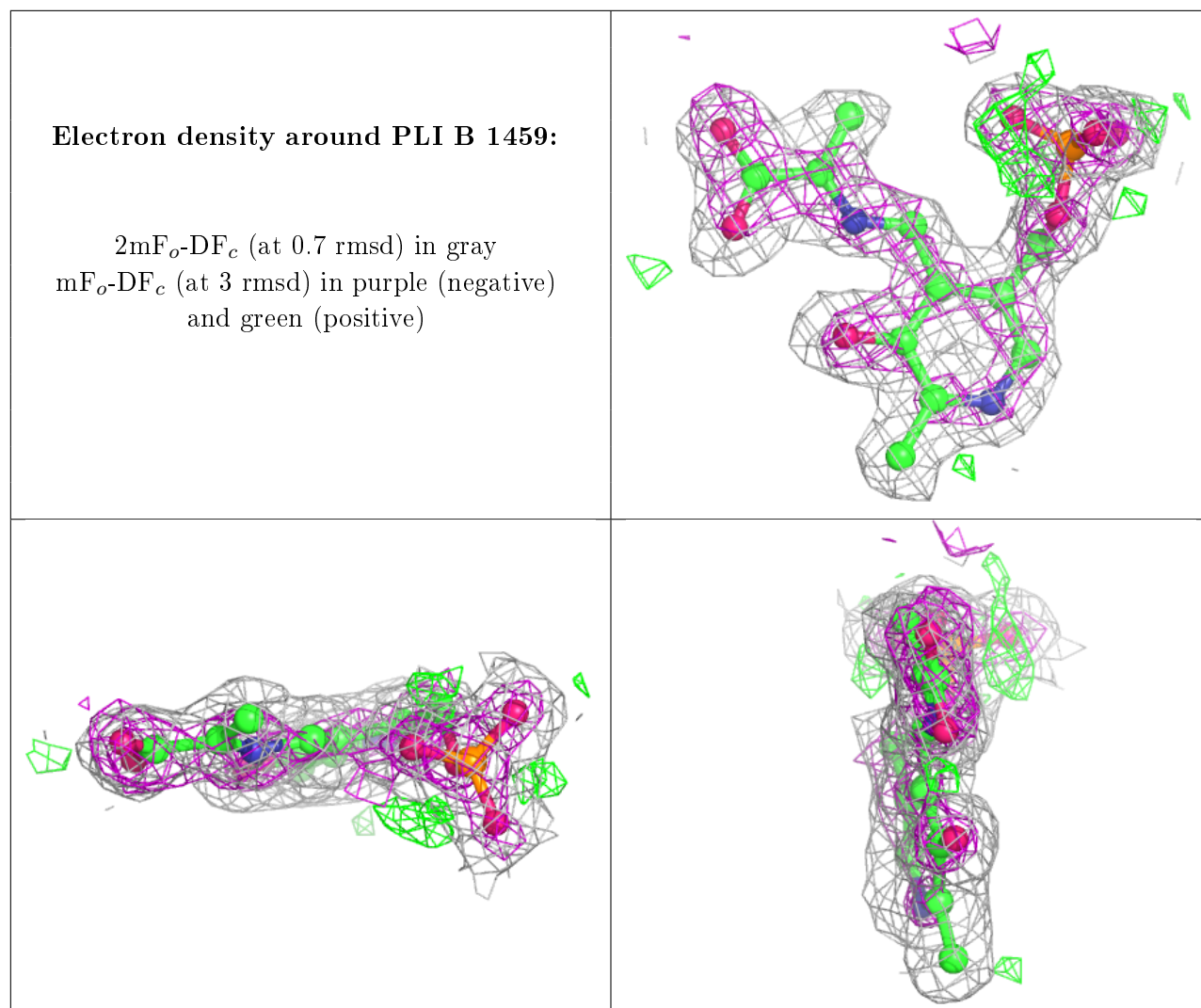
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P33 B 1460:

$2mF_o-DF_c$ (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 depositor's R factor - this section is therefore empty.