



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 04:50 pm BST

PDB ID : 1B12
Title : CRYSTAL STRUCTURE OF TYPE 1 SIGNAL PEPTIDASE FROM ES-
CHERICHIA COLI IN COMPLEX WITH A BETA-LACTAM INHIBITOR
Authors : Paetzel, M.; Dalbey, R.; Strynadka, N.C.J.
Deposited on : 1999-11-24
Resolution : 1.95 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

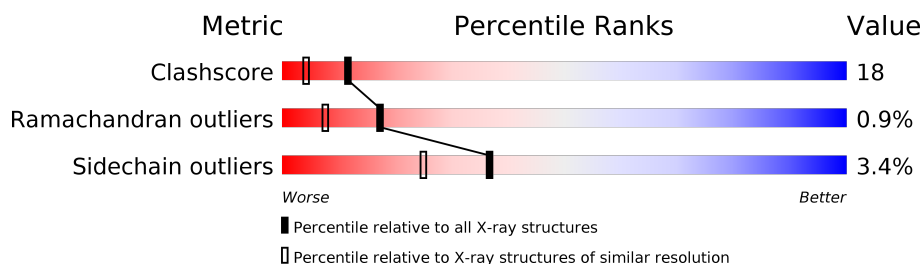
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	
1	C	248	
1	D	248	

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
2	1PN	A	1001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1PN	C	1001	-	-	X	-
2	1PN	D	1001	-	-	X	-

2 Entry composition [i](#)

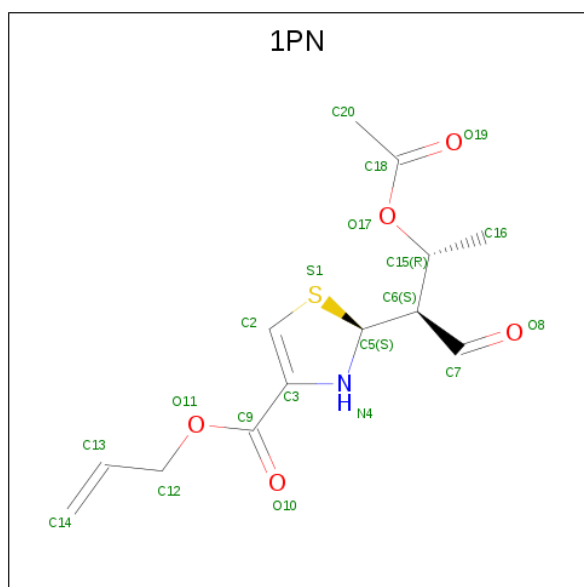
There are 4 unique types of molecules in this entry. The entry contains 7646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIGNAL PEPTIDASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1887	1204	319	356	8			
1	B	211	Total	C	N	O	S	0	0	0
			1679	1077	280	314	8			
1	C	226	Total	C	N	O	S	0	0	0
			1775	1135	295	337	8			
1	D	222	Total	C	N	O	S	0	0	0
			1772	1143	293	330	6			

- Molecule 2 is prop-2-en-1-yl (2S)-2-[(2S,3R)-3-(acetyloxy)-1-oxobutan-2-yl]-2,3-dihydro-1,3-thiazole-4-carboxylate (three-letter code: 1PN) (formula: C₁₃H₁₇NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	13	1	5	1		
2	B	1	Total	C	N	O	S	0	0
			20	13	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			20	13	1	5	1		
2	D	1	Total	C	N	O	S	0	0
			20	13	1	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	111	Total	O	0	0
			111	111		
4	C	122	Total	O	0	0
			122	122		
4	D	86	Total	O	0	0
			86	86		

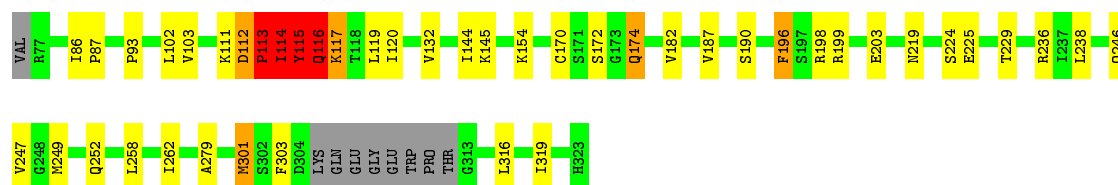
3 Residue-property plots

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.

Note EDS was not executed.

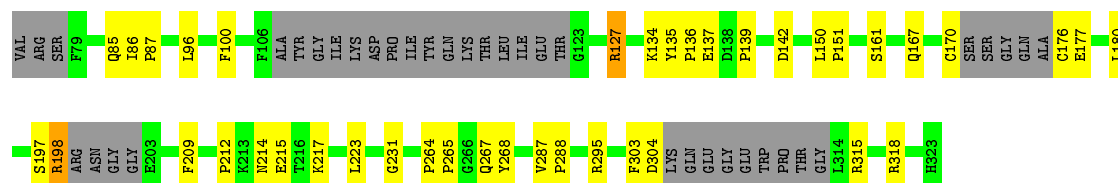
• Molecule 1: SIGNAL PEPTIDASE I

Chain A: 



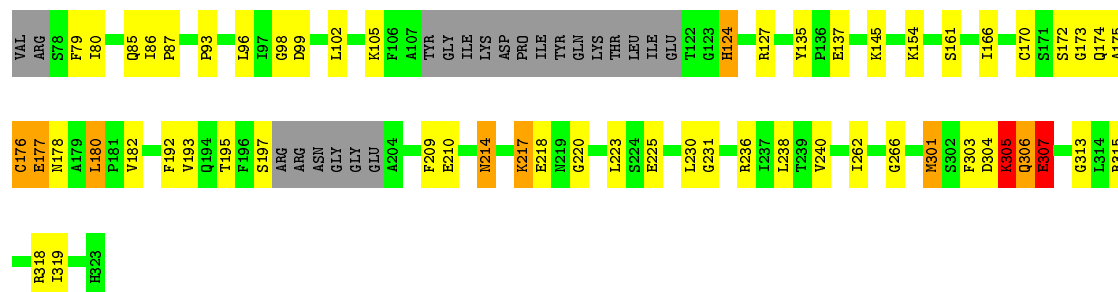
• Molecule 1: SIGNAL PEPTIDASE I

Chain B: 



• Molecule 1: SIGNAL PEPTIDASE I

Chain C: 



• Molecule 1: SIGNAL PEPTIDASE I

Chain D: 



VAL	R77	S78	F79	I80	Y81	E82	I86	P87	P93	F100	K105	F106	I110	K111	D112	P113	I114	Y115	Q116	K117	I118	L119	I120	E121	P125	K126	R127	I130	V131	V132	Y135	P136	E137	D138	P139	K140	L141	I144	K145	D153	I166	Q167	P168	GLY	CYS	SER	SER	GLY
GLN	ALA	CYS	GLU	ASN	A179	L180	P181	V187	D191	S197	ARG	ARG	ASN	GLY	GLY	GLU	ALA	T205	S206	K213	L223	S224	G231	L238	T239	V240	Q246	Q267	P288	R295	P303	D304	LYS	GLN	GLU	GLY	GLY	TRP	PRO	THR	G313	I322	H323					

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.70 Å 113.20 Å 99.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.50 – 1.95	Depositor
% Data completeness (in resolution range)	96.8 (19.50-1.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.220 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7646	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 1PN

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	0.81	5/1935 (0.3%)	1.06	13/2622 (0.5%)
1	B	0.48	0/1721	0.77	0/2330
1	C	0.65	1/1822 (0.1%)	0.90	8/2472 (0.3%)
1	D	0.54	1/1818 (0.1%)	0.76	1/2464 (0.0%)
All	All	0.63	7/7296 (0.1%)	0.88	22/9888 (0.2%)

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	3
1	D	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	ILE	C-N	-17.71	0.93	1.34
1	C	307	GLU	N-CA	16.00	1.78	1.46
1	A	115	TYR	C-N	-13.86	1.02	1.34
1	D	116	GLN	N-CA	10.98	1.68	1.46
1	A	114	ILE	CA-C	-9.01	1.29	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	TYR	N-CA-C	16.08	154.41	111.00
1	A	114	ILE	O-C-N	-15.77	97.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	TYR	N-CA-CB	-12.23	88.58	110.60
1	A	117	LYS	N-CA-CB	11.77	131.79	110.60
1	A	114	ILE	CA-C-N	10.58	140.47	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	114	ILE	Mainchain
1	A	116	GLN	Peptide
1	D	115	TYR	Sidechain,Peptide

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	1887	0	1843	62	0
1	B	1679	0	1635	47	1
1	C	1775	0	1718	82	6
1	D	1772	0	1745	54	8
2	A	20	0	16	8	0
2	B	20	0	16	6	0
2	C	20	0	16	8	0
2	D	20	0	16	8	0
3	B	5	0	0	0	0
4	A	129	0	0	2	1
4	B	111	0	0	2	0
4	C	122	0	0	4	2
4	D	86	0	0	3	0
All	All	7646	0	7005	249	9

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 18.

The worst 5 of 249 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:D:116:GLN:N	1:D:116:GLN:CA	1.68	1.53
1:C:307:GLU:N	1:C:307:GLU:CA	1.78	1.44
1:A:114:ILE:HD12	1:A:115:TYR:CB	1.63	1.27
1:C:177:GLU:HG3	1:C:178:ASN:H	1.11	1.11
1:A:87:PRO:HD2	2:A:1001:1PN:H20	1.37	1.05

The worst 5 of 9 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)
1:C:266:GLY:CA	1:D:115:TYR:OH[4_455]	1.34	0.86
1:D:115:TYR:CD1	4:C:1045:HOH:O[4_555]	1.52	0.68
1:C:266:GLY:N	1:D:115:TYR:CE1[4_455]	1.74	0.46
1:D:115:TYR:CE1	4:C:1045:HOH:O[4_555]	1.76	0.44
1:C:266:GLY:CA	1:D:115:TYR:CZ[4_455]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	235/248 (95%)	221 (94%)	13 (6%)	1 (0%)	34	22
1	B	201/248 (81%)	197 (98%)	3 (2%)	1 (0%)	29	17
1	C	220/248 (89%)	209 (95%)	7 (3%)	4 (2%)	8	2
1	D	214/248 (86%)	207 (97%)	5 (2%)	2 (1%)	17	8
All	All	870/992 (88%)	834 (96%)	28 (3%)	8 (1%)	17	8

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	GLY
1	C	177	GLU

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Mol	Chain	Res	Type
1	C	305	LYS
1	D	113	PRO
1	C	218	GLU

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	205/213 (96%)	198 (97%)	7 (3%)	37	25
1	B	184/213 (86%)	179 (97%)	5 (3%)	44	34
1	C	193/213 (91%)	186 (96%)	7 (4%)	35	23
1	D	194/213 (91%)	187 (96%)	7 (4%)	35	23
All	All	776/852 (91%)	750 (97%)	26 (3%)	37	25

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	LEU
1	C	214	ASN
1	D	246	GLN
1	C	124	HIS
1	C	197	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	ASN
1	C	85	GLN
1	D	167	GLN
1	B	167	GLN
1	C	214	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	1PN	C	1001	1	17,20,20	2.17	2 (11%)	17,26,26	2.15	6 (35%)
3	PO4	B	1002	-	4,4,4	1.39	0	6,6,6	0.46	0
2	1PN	A	1001	1	17,20,20	2.29	3 (17%)	17,26,26	2.09	4 (23%)
2	1PN	D	1001	1	17,20,20	2.11	2 (11%)	17,26,26	2.04	5 (29%)
2	1PN	B	1001	1	17,20,20	2.32	2 (11%)	17,26,26	1.91	5 (29%)

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	1PN	C	1001	1	-	7/18/31/31	0/1/1/1
2	1PN	A	1001	1	-	7/18/31/31	0/1/1/1
2	1PN	D	1001	1	-	8/18/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PN	B	1001	1	-	8/18/31/31	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1PN	C6-C15	-7.94	1.45	1.54
2	B	1001	1PN	C6-C15	-7.79	1.45	1.54
2	C	1001	1PN	C6-C15	-7.22	1.46	1.54
2	D	1001	1PN	C6-C15	-6.94	1.46	1.54
2	B	1001	1PN	C2-S1	4.30	1.80	1.74

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	1PN	O11-C9-C3	-5.12	106.23	112.00
2	C	1001	1PN	O11-C9-C3	-4.88	106.51	112.00
2	D	1001	1PN	O11-C9-C3	-4.88	106.51	112.00
2	B	1001	1PN	O11-C9-C3	-4.51	106.92	112.00
2	C	1001	1PN	O17-C15-C16	3.49	115.15	108.21

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	1PN	C3-C9-O11-C12
2	A	1001	1PN	C3-C9-O11-C12
2	D	1001	1PN	C3-C9-O11-C12
2	B	1001	1PN	C3-C9-O11-C12
2	C	1001	1PN	O10-C9-O11-C12

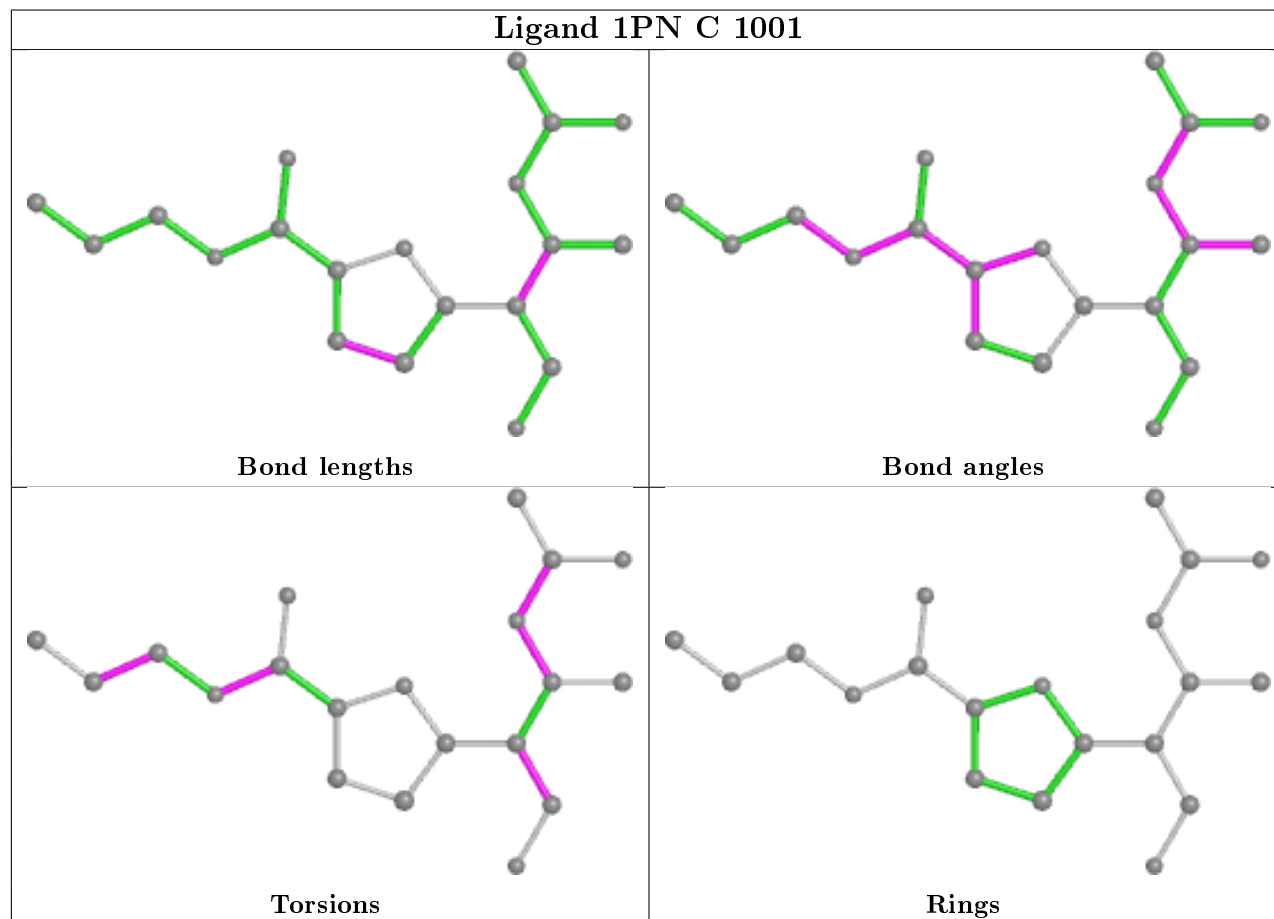
There are no ring outliers.

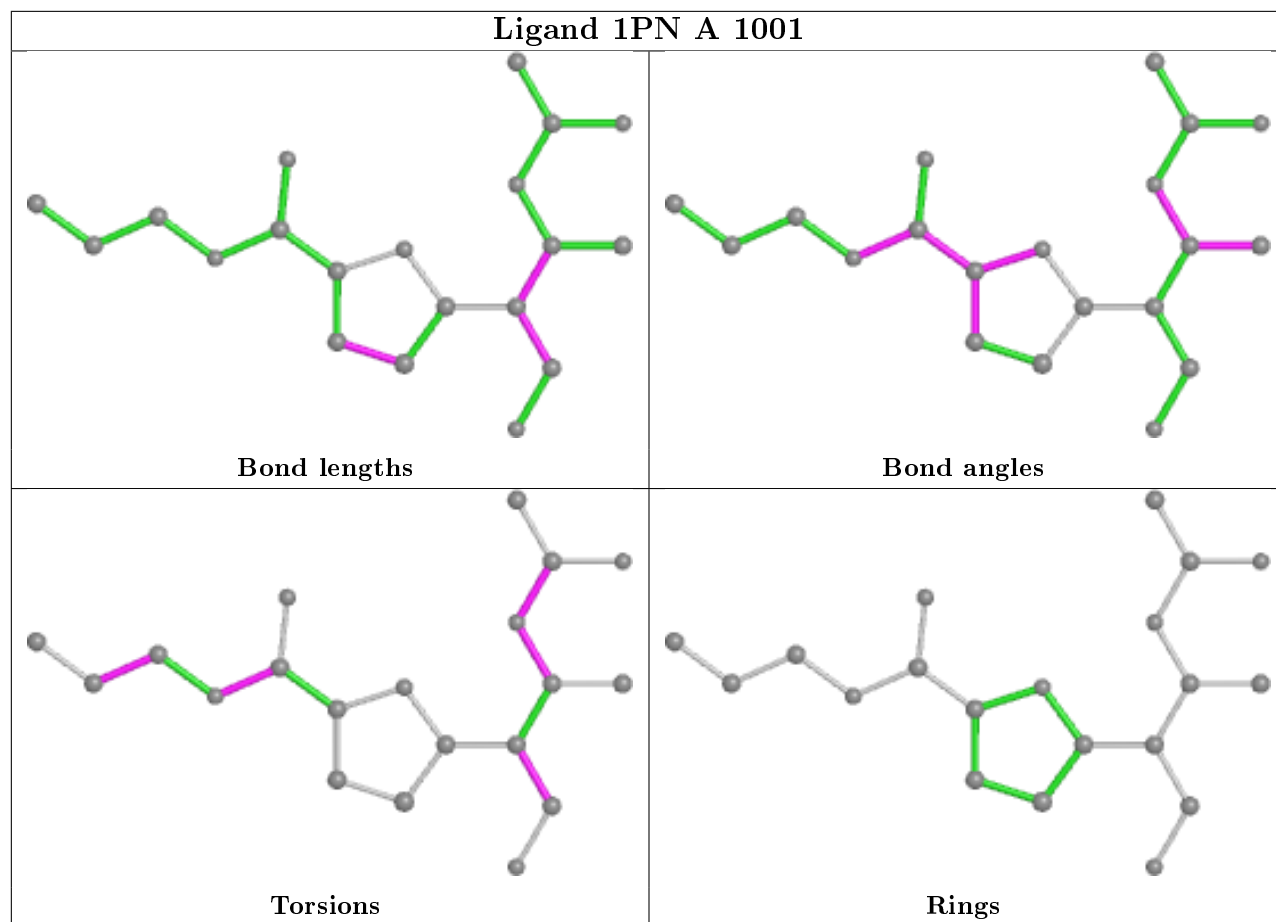
4 monomers are involved in 30 short contacts:

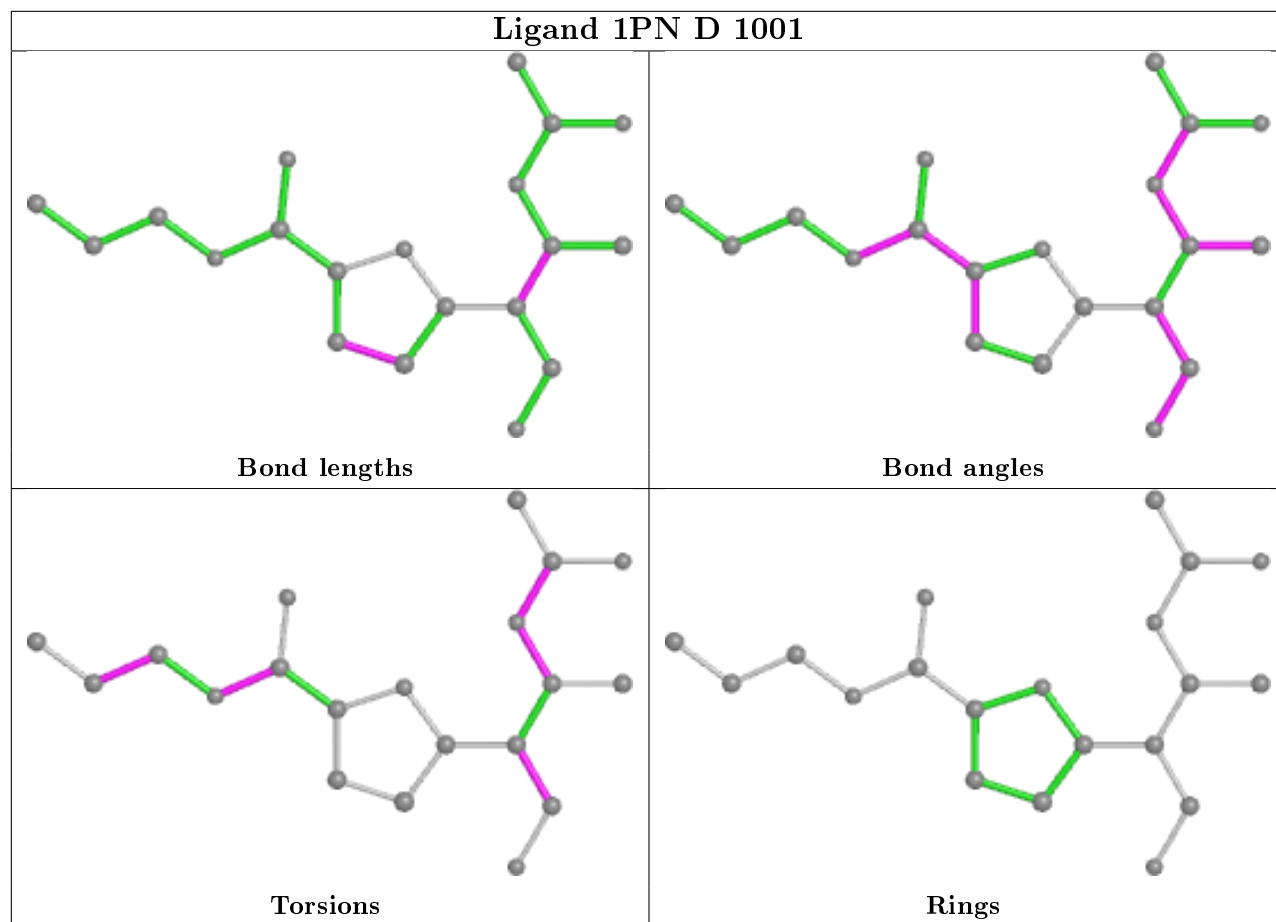
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	1PN	8	0
2	A	1001	1PN	8	0
2	D	1001	1PN	8	0
2	B	1001	1PN	6	0

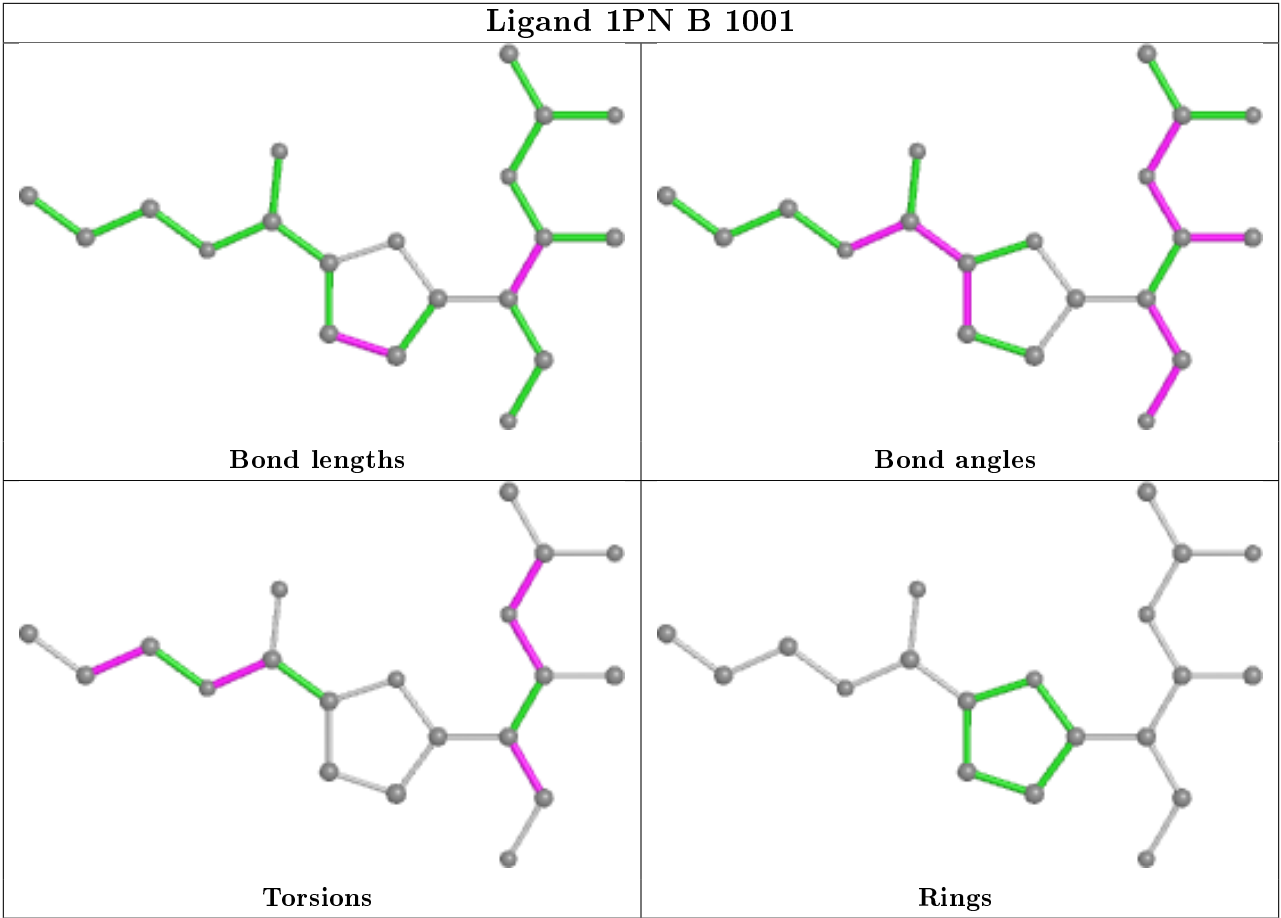
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	115:TYR	C	116:GLN	N	1.02
1	A	114:ILE	C	115:TYR	N	0.93

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.