



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:20 am BST

PDB ID : 6OP5
Title : Crystal Structure of Piper methysticum Styrylpyrone Synthase 1 in complex with p-coumaroyl-CoA
Authors : Pluskal, T.; Weng, J.K.
Deposited on : 2019-04-24
Resolution : 2.70 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

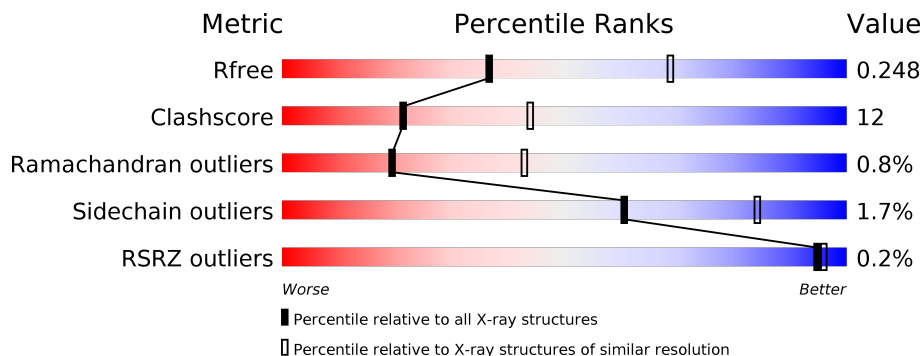
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	397	 74% 21% . .
1	B	397	 68% 28% .
1	D	397	 72% 23% . .
1	E	397	 67% 27% . .
1	F	397	 67% 27% . .
2	C	397	 73% 22% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17920 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.

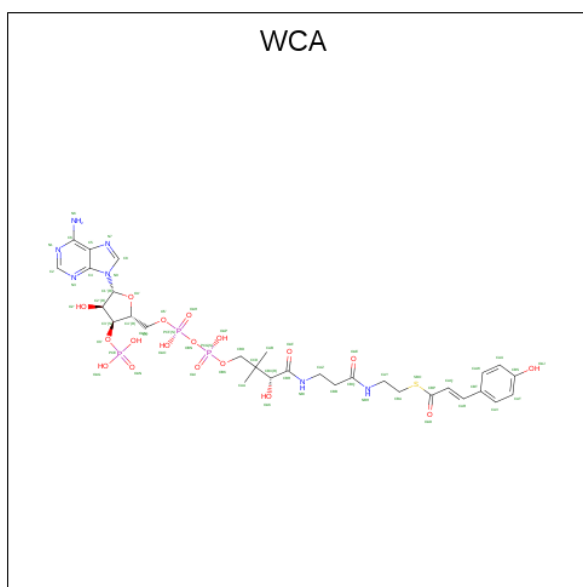
- Molecule 1 is a protein called Styrylpyrone synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2939	1867	502	550	20	0	0	0
1	B	382	2934	1864	501	549	20	0	0	0
1	D	382	2934	1864	501	549	20	0	0	0
1	E	382	2934	1864	501	549	20	0	0	0
1	F	382	2934	1864	501	549	20	0	0	0

- Molecule 2 is a protein called Styrylpyrone synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	382	2945	1873	501	551	20	0	0	0

- Molecule 3 is p-coumaroyl-CoA (three-letter code: WCA) (formula: $C_{30}H_{42}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	59	30	7	18	3	1	0	0
3	B	1	59	30	7	18	3	1	0	0

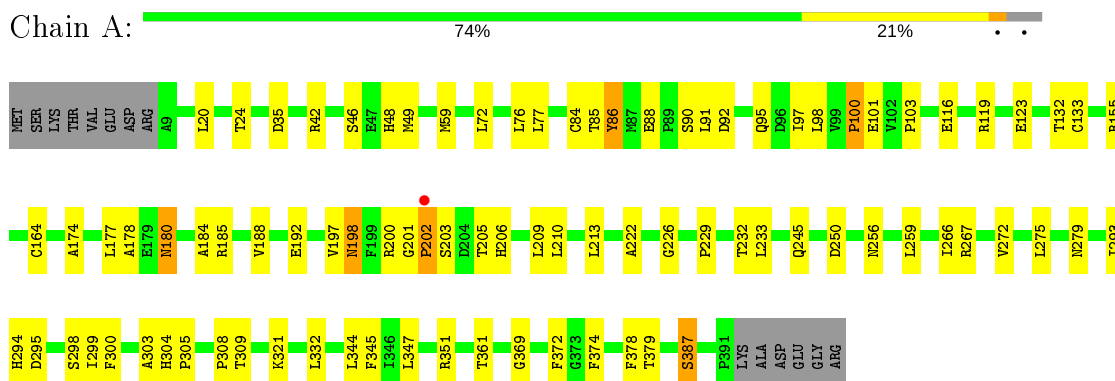
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	36	Total	O	0	0
			36	36		
4	C	33	Total	O	0	0
			33	33		
4	D	32	Total	O	0	0
			32	32		
4	E	21	Total	O	0	0
			21	21		
4	F	21	Total	O	0	0
			21	21		

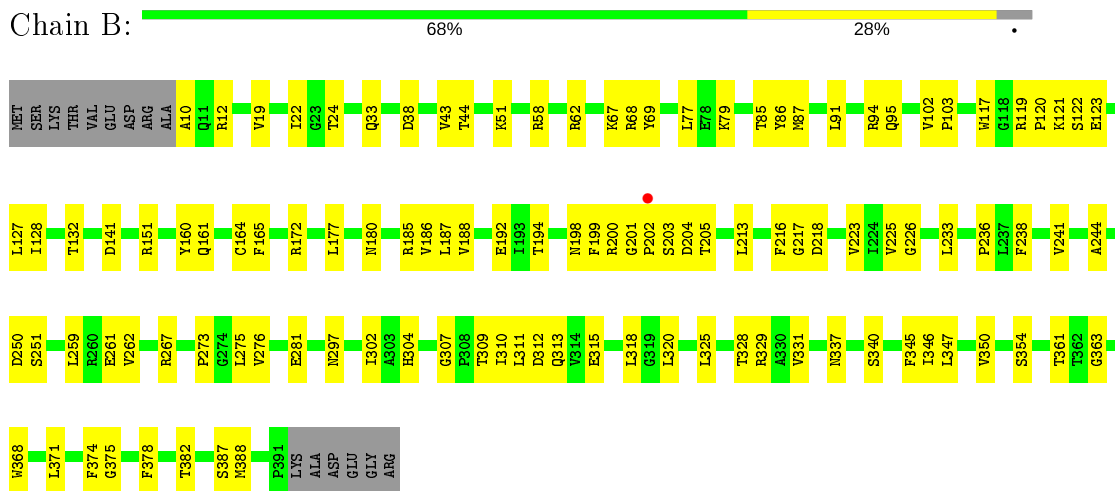
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

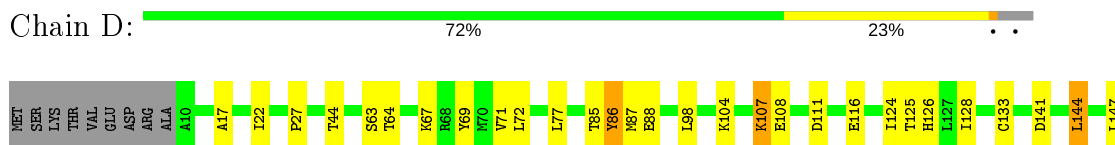
- Molecule 1: Styrylpyrone synthase 1

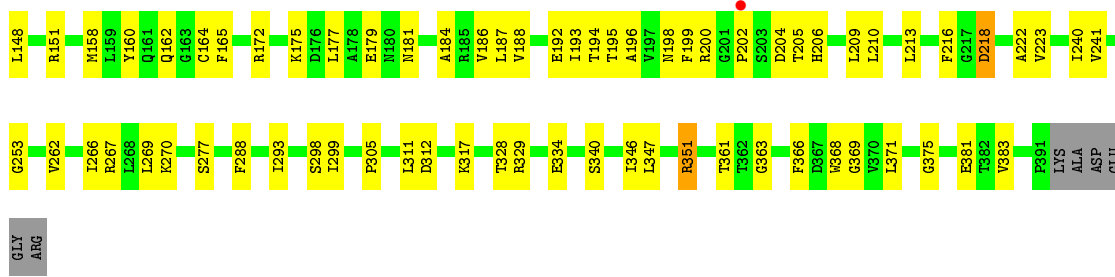


- Molecule 1: Styrylpyrone synthase 1



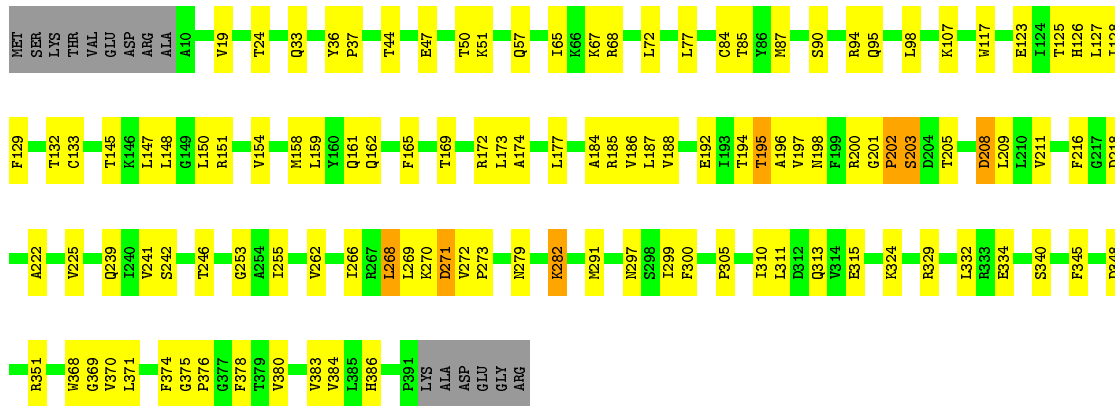
- Molecule 1: Styrylpyrone synthase 1





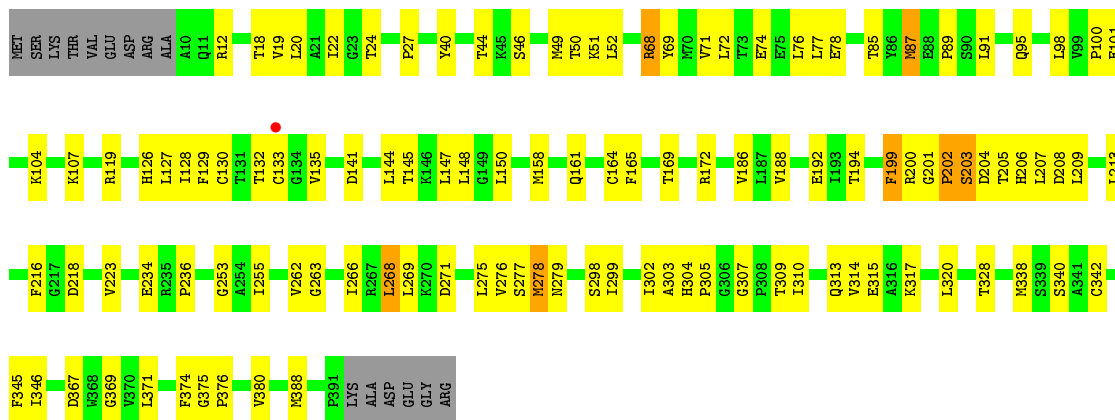
- Molecule 1: Styrylpyrone synthase 1

Chain E: 67% 27%



- Molecule 1: Styrylpyrone synthase 1

Chain F: 67% 27%



- Molecule 2: Styrylpyrone synthase 1

Chain C: 73% 22%



H126	L127	I128	C133	L148	R151	V154	R155	R156	F164	F165	T169	R172	L177	M181	V186	L187	V188	S191	E192	L193	T194	T195	A196	V197	M198	F199	R200	G201	P202	S203	D204	T205	H206	L207	L213	D218	G219	V223	D230	P231	T232	P236
I255	I266	R267	L268	V276	F300	H304	I310	E315	L320	E323	K326	G336	M337	M338	S339	D348	R351	T361	G369	V370	L371	F372	G373	F374	G375	F378	E381	T382	V383	P389	I390	P391	LYS	ALA	ASP	GLU	GLY	ARG				

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	164.40 Å 164.40 Å 87.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.20 – 2.70 82.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (82.20-2.70) 98.7 (82.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.204 , 0.261 0.192 , 0.248	Depositor DCC
R_{free} test set	1967 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 13.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l 0.039 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17920	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: WCA, 60F

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	0.27	0/2996	0.46	0/4060
1	B	0.28	0/2991	0.48	0/4053
1	D	0.27	0/2991	0.46	0/4053
1	E	0.28	0/2991	0.47	0/4053
1	F	0.28	0/2991	0.48	0/4053
2	C	0.27	0/2984	0.45	0/4042
All	All	0.28	0/17944	0.47	0/24314

There are no bond length outliers.

There are no bond angle outliers.

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	2939	0	2978	62	0
1	B	2934	0	2973	90	0
1	D	2934	0	2973	68	0
1	E	2934	0	2973	77	0
1	F	2934	0	2973	84	0
2	C	2945	0	2968	58	0
3	A	59	0	38	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	59	0	38	3	0
4	A	39	0	0	3	0
4	B	36	0	0	5	0
4	C	33	0	0	2	0
4	D	32	0	0	2	0
4	E	21	0	0	3	0
4	F	21	0	0	1	0
All	All	17920	0	17914	428	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 12.

The worst 5 of 428 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:F:255:ILE:HD13	1:F:268:LEU:HG	1.25	1.10
1:B:86:TYR:H	1:B:200:ARG:NE	1.53	1.04
1:B:86:TYR:HB3	1:B:200:ARG:CZ	1.89	1.02
1:B:86:TYR:H	1:B:200:ARG:HE	1.02	0.99
1:A:86:TYR:H	1:A:200:ARG:HE	1.03	0.98

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 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	381/397 (96%)	357 (94%)	19 (5%)	5 (1%)	12 30
1	B	380/397 (96%)	360 (95%)	19 (5%)	1 (0%)	41 66
1	D	380/397 (96%)	355 (93%)	23 (6%)	2 (0%)	29 54
1	E	380/397 (96%)	351 (92%)	25 (7%)	4 (1%)	14 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	380/397 (96%)	350 (92%)	26 (7%)	4 (1%)	14	34
2	C	379/397 (96%)	351 (93%)	26 (7%)	2 (0%)	29	54
All	All	2280/2382 (96%)	2124 (93%)	138 (6%)	18 (1%)	19	43

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	PRO
2	C	195	THR
1	D	195	THR
1	E	202	PRO
1	A	198	ASN

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 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	318/330 (96%)	314 (99%)	4 (1%)	69	87
1	B	318/330 (96%)	312 (98%)	6 (2%)	57	82
1	D	318/330 (96%)	314 (99%)	4 (1%)	69	87
1	E	318/330 (96%)	312 (98%)	6 (2%)	57	82
1	F	318/330 (96%)	309 (97%)	9 (3%)	43	73
2	C	317/329 (96%)	313 (99%)	4 (1%)	69	87
All	All	1907/1979 (96%)	1874 (98%)	33 (2%)	60	84

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	107	LYS
1	E	57	GLN
1	F	278	MET
1	D	144	LEU
1	D	218	ASP

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

Mol	Chain	Res	Type
1	B	95	GLN
2	C	57	GLN
2	C	245	GLN
1	E	162	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	60F	C	164	2	14,17,18	0.90	1 (7%)	13,21,23	4.13	2 (15%)

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	60F	C	164	2	-	4/10/12/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	164	60F	C1'-C3	2.01	1.53	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	164	60F	CB-SG-C1	13.48	119.07	100.42
2	C	164	60F	C1'-C3-C2	-5.87	113.47	126.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	164	60F	SG-C1-C2-C3
2	C	164	60F	C2'-C1'-C3-C2
2	C	164	60F	C6'-C1'-C3-C2
2	C	164	60F	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	164	60F	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	WCA	B	801	-	52,62,62	3.29	14 (26%)	65,91,91	2.12	11 (16%)
3	WCA	A	801	-	52,62,62	3.28	12 (23%)	65,91,91	2.27	11 (16%)

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	WCA	B	801	-	-	27/52/72/72	0/4/4/4
3	WCA	A	801	-	-	19/52/72/72	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	WCA	O4'-C1'	14.06	1.60	1.41
3	B	801	WCA	O4'-C1'	13.70	1.60	1.41
3	A	801	WCA	C2'-C1'	-12.10	1.35	1.53
3	B	801	WCA	C2'-C1'	-12.01	1.35	1.53
3	B	801	WCA	O4'-C4'	-6.82	1.29	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	WCA	C5-C6-N6	9.42	134.67	120.35
3	B	801	WCA	C5-C6-N6	8.71	133.59	120.35
3	A	801	WCA	N6-C6-N1	-7.25	103.53	118.57
3	A	801	WCA	CBA-SBO-CBP	6.97	108.55	99.80
3	B	801	WCA	CBA-SBO-CBP	6.89	108.45	99.80

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	WCA	CAR-CAQ-CBP-OAD
3	B	801	WCA	CAR-CAQ-CBP-SBO
3	B	801	WCA	CAQ-CBP-SBO-CBA
3	B	801	WCA	OAD-CBP-SBO-CBA
3	B	801	WCA	CAY-CBA-SBO-CBP

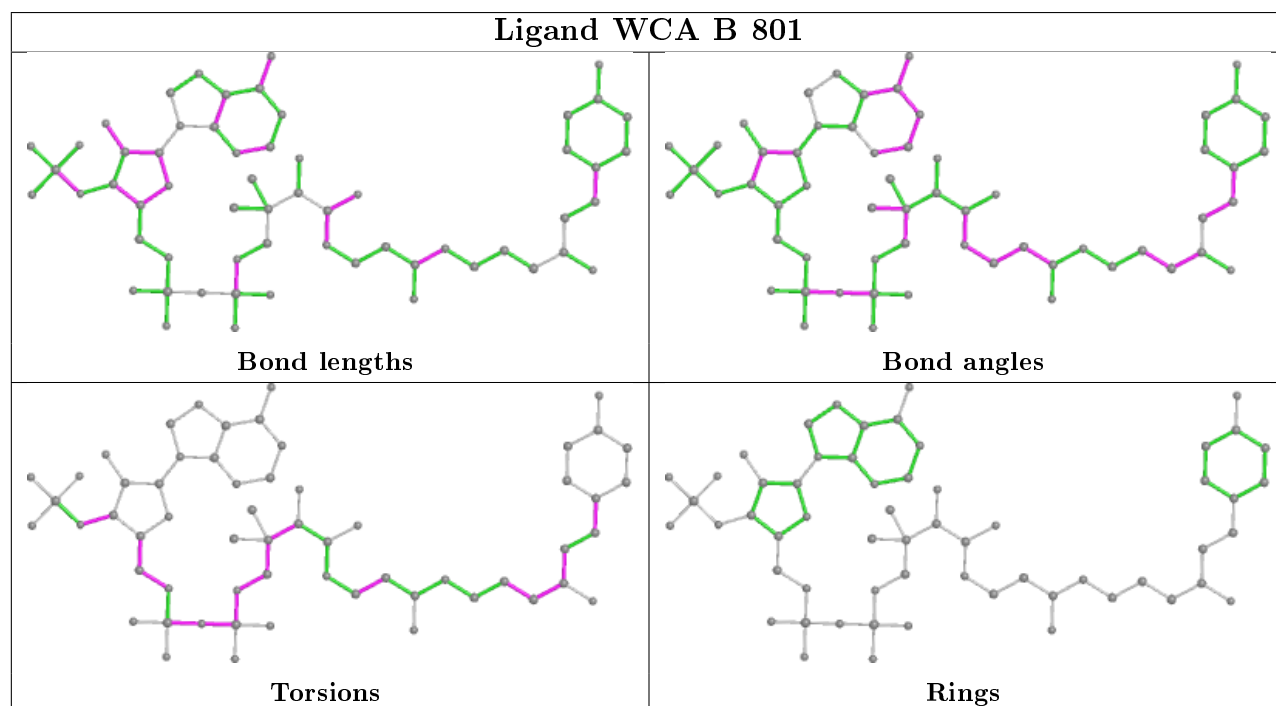
There are no ring outliers.

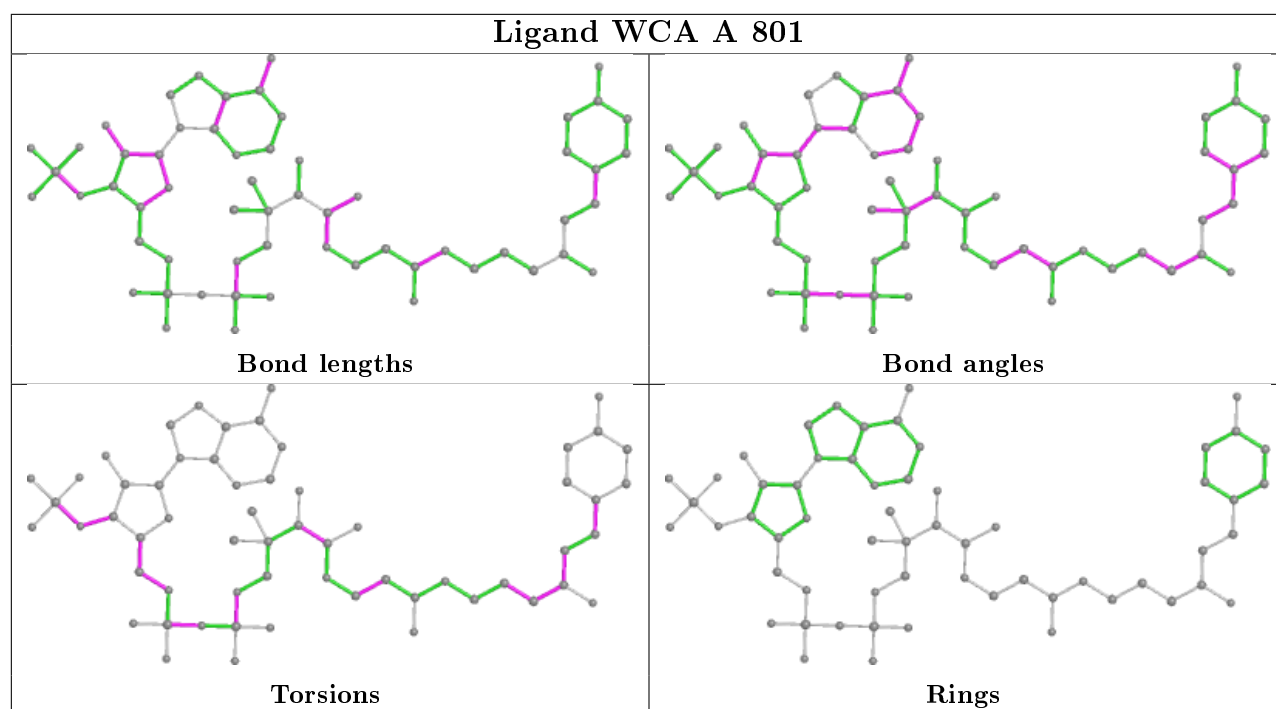
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	WCA	3	0
3	A	801	WCA	5	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/397 (96%)	-0.59	1 (0%) 94 95	23, 35, 54, 72	0
1	B	382/397 (96%)	-0.57	1 (0%) 94 95	23, 35, 47, 61	0
1	D	382/397 (96%)	-0.57	1 (0%) 94 95	23, 34, 47, 67	0
1	E	382/397 (96%)	-0.57	0 100 100	26, 38, 49, 66	0
1	F	382/397 (96%)	-0.60	1 (0%) 94 95	26, 36, 48, 61	0
2	C	381/397 (95%)	-0.53	1 (0%) 94 95	24, 37, 56, 68	0
All	All	2292/2382 (96%)	-0.57	5 (0%) 95 96	23, 36, 50, 72	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	PRO	3.5
1	B	202	PRO	3.5
2	C	10	ALA	3.1
1	D	202	PRO	2.3
1	F	133	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	60F	C	164	17/18	0.93	0.16	32,39,55,60	0

6.3 Carbohydrates [i](#)

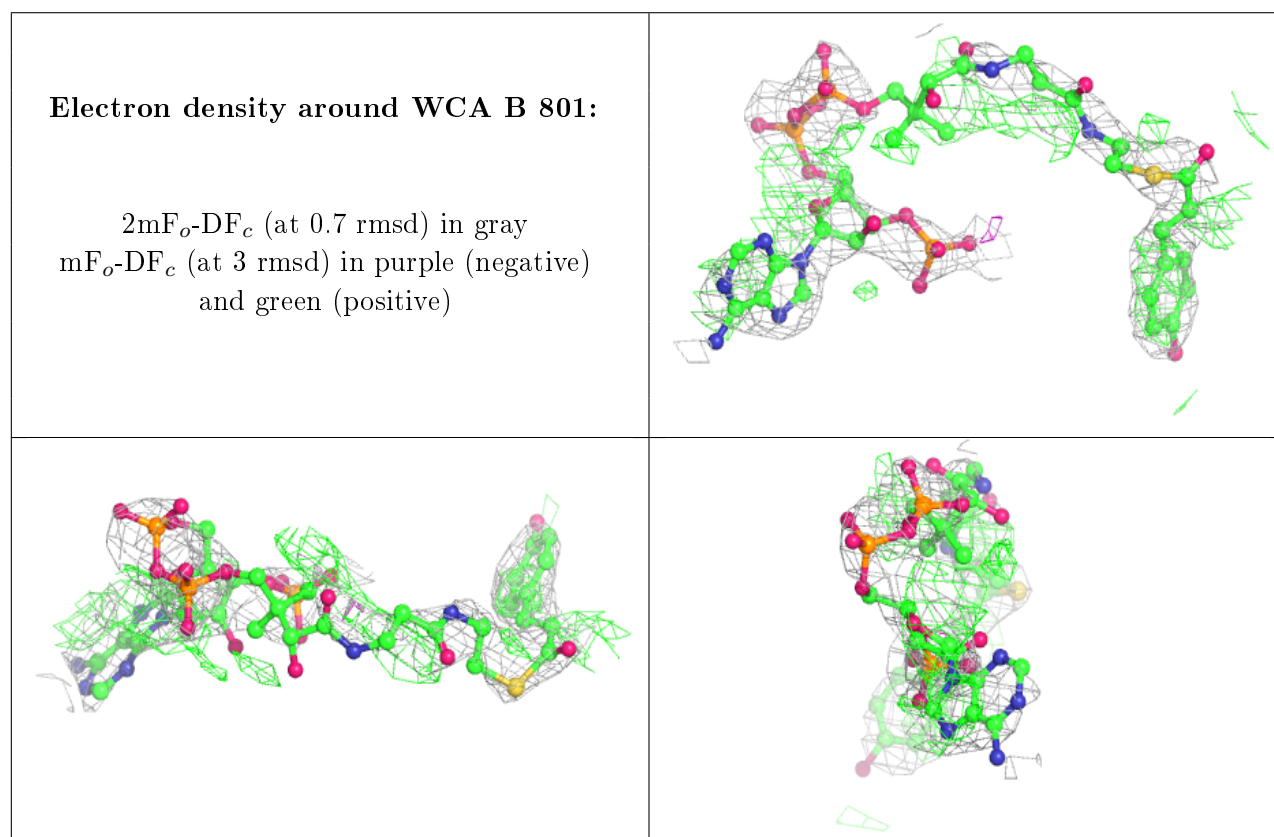
There are no carbohydrates in this entry.

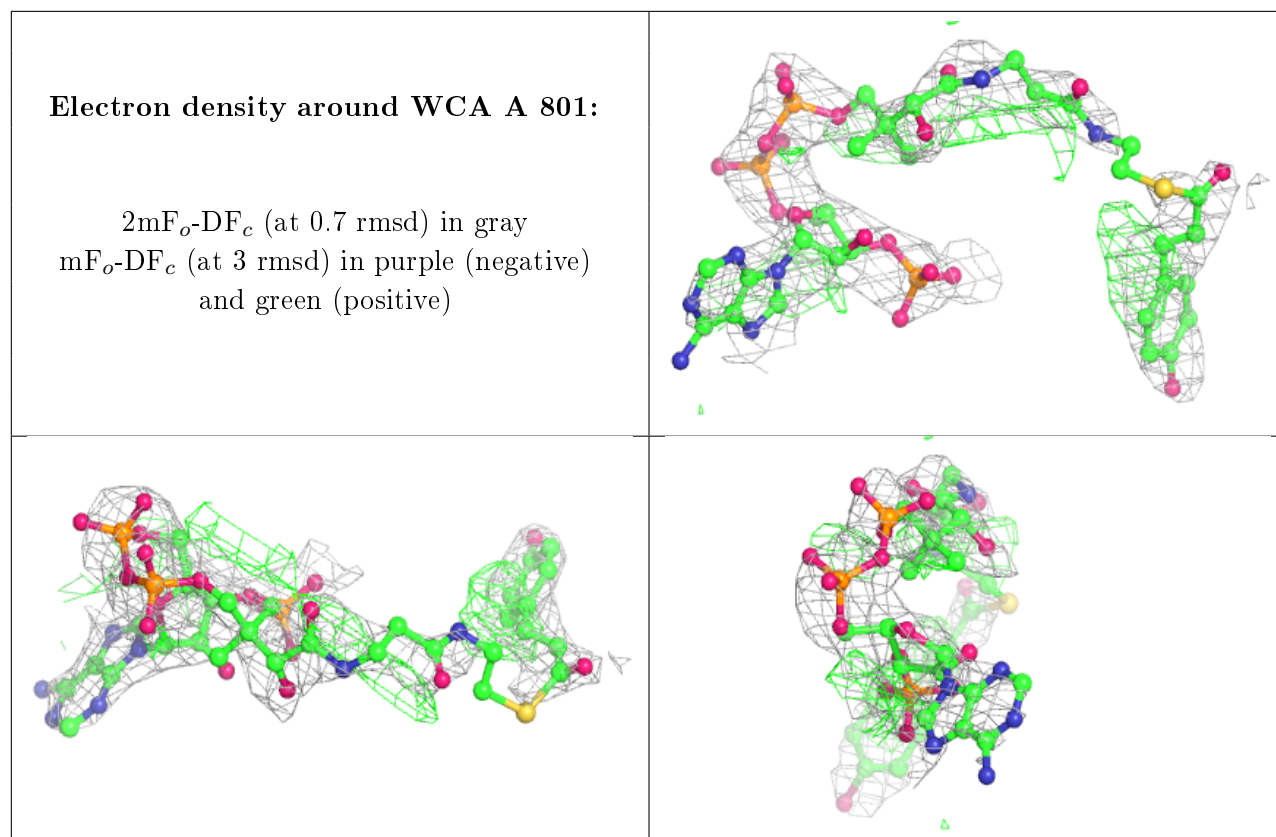
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	WCA	B	801	59/59	0.81	0.33	30,43,54,57	59
3	WCA	A	801	59/59	0.84	0.28	26,37,46,53	59

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.