Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 04:11 pm BST

PDB ID	:	9GS1 / pdb_00009gs1
Title	:	Crystal structure of Arabidopsis thaliana Acyl-ACP Thioesterase (At-FatA) complexed with Oxaziclomefone
Authors	:	Montgomery, M.G.
Deposited on	:	2024-09-13
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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:

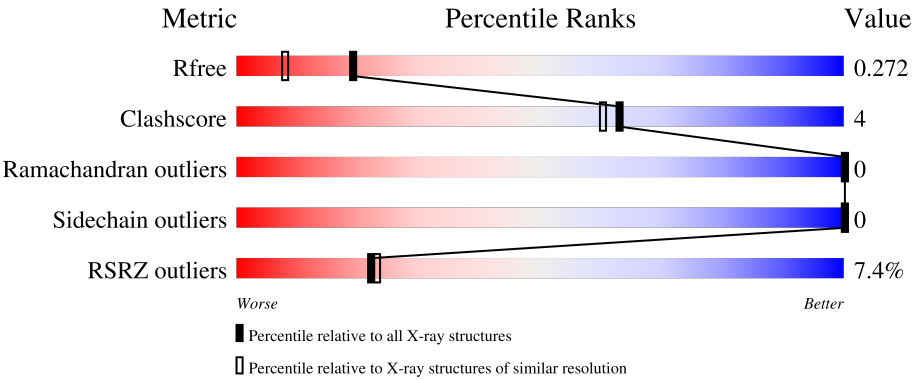
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 of 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 <=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	AaA	295	8% 81% 7% 13%
1	BaB	295	5% 80% 7% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4415 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.

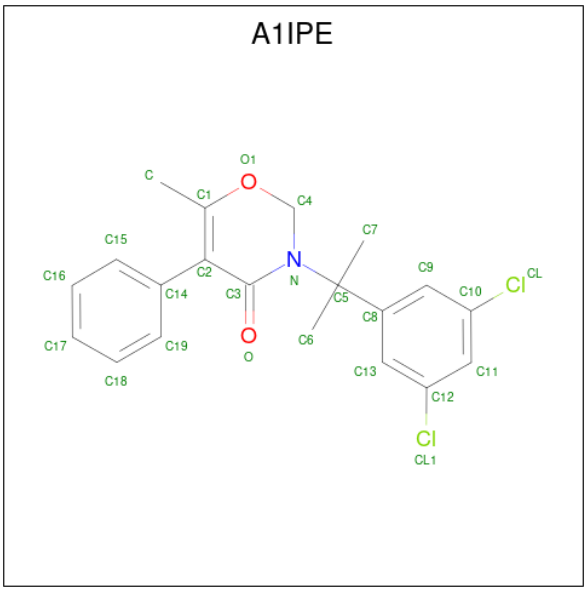
- Molecule 1 is a protein called Oleoyl-acyl carrier protein thioesterase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AaA	258	Total	C	N	O	S	0	2	0
			2091	1310	366	405	10			
1	BaB	257	Total	C	N	O	S	0	4	0
			2100	1316	369	405	10			

There are 14 discrepancies between the modelled and reference sequences:

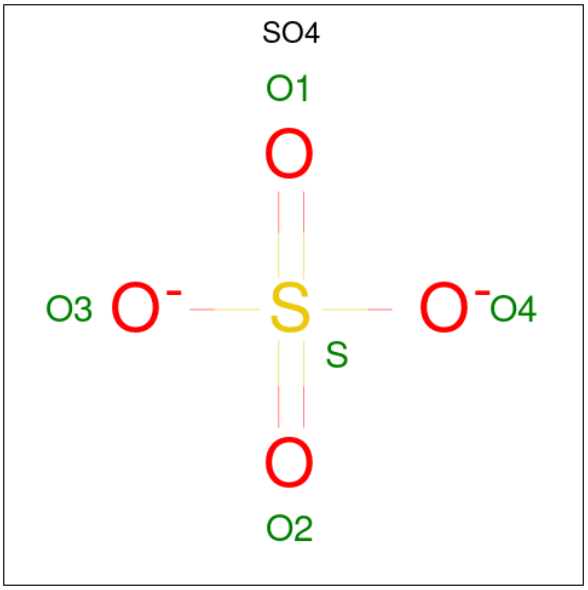
Chain	Residue	Modelled	Actual	Comment	Reference
AaA	74	MET	-	initiating methionine	UNP Q42561
AaA	363	HIS	-	expression tag	UNP Q42561
AaA	364	HIS	-	expression tag	UNP Q42561
AaA	365	HIS	-	expression tag	UNP Q42561
AaA	366	HIS	-	expression tag	UNP Q42561
AaA	367	HIS	-	expression tag	UNP Q42561
AaA	368	HIS	-	expression tag	UNP Q42561
BaB	74	MET	-	initiating methionine	UNP Q42561
BaB	363	HIS	-	expression tag	UNP Q42561
BaB	364	HIS	-	expression tag	UNP Q42561
BaB	365	HIS	-	expression tag	UNP Q42561
BaB	366	HIS	-	expression tag	UNP Q42561
BaB	367	HIS	-	expression tag	UNP Q42561
BaB	368	HIS	-	expression tag	UNP Q42561

- Molecule 2 is Oxaziclomefone (CCD ID: A1IPE) (formula: $C_{20}H_{19}Cl_2NO_2$) (labeled as "Ligand of Interest" by depositor).



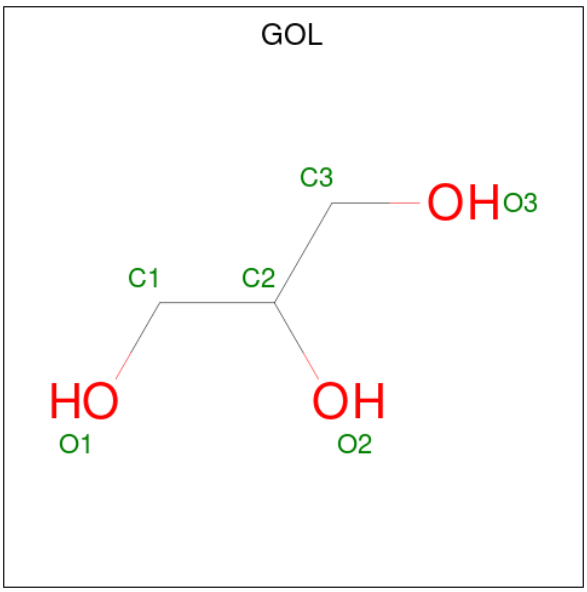
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AaA	1	Total	C	Cl	N	O	0	0
			25	20	2	1	2		
2	BaB	1	Total	C	Cl	N	O	0	0
			25	20	2	1	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AaA	1	Total	O	S	0	0
			5	4	1		
3	BaB	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

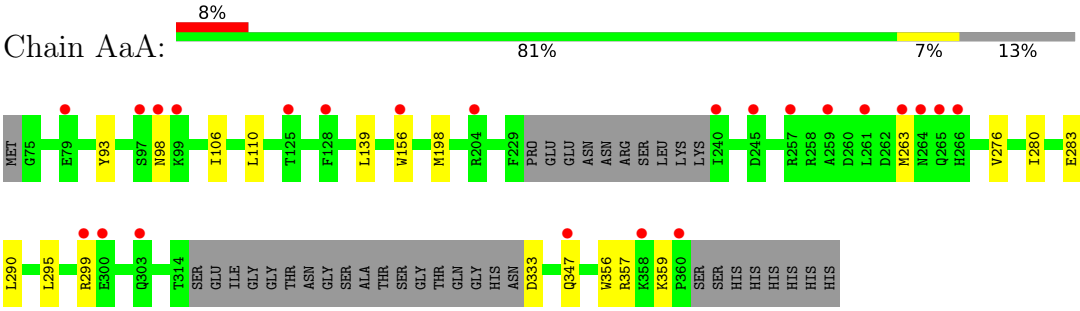
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AaA	82	Total O 82 82	0	0
5	BaB	76	Total O 76 76	0	0

3 Residue-property plots (i)

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 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.

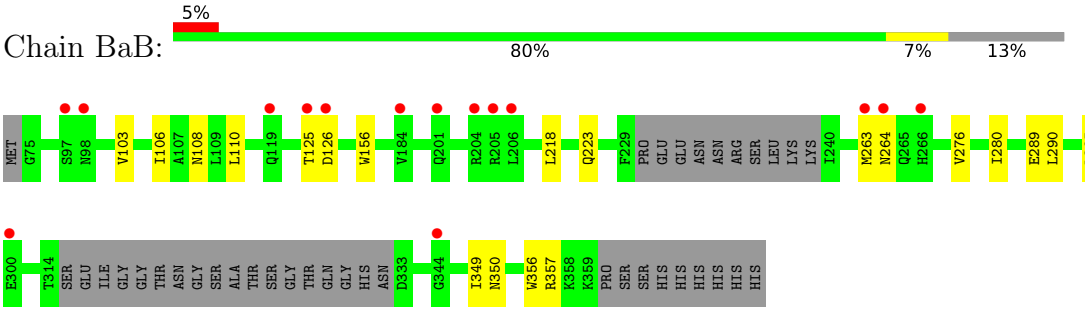
• Molecule 1: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic

Chain AaA:



• Molecule 1: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic

Chain BaB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.15Å 97.84Å 126.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.42 – 1.90 20.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.42-1.90) 99.3 (20.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.236 , 0.272 0.242 , 0.272	Depositor DCC
R_{free} test set	2350 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4415	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IPE, SO4, GOL

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	AaA	1.00	0/2136	1.27	0/2895
1	BaB	1.03	0/2147	1.25	0/2908
All	All	1.01	0/4283	1.26	0/5803

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

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	AaA	2091	0	2055	24	0
1	BaB	2100	0	2071	20	0
2	AaA	25	0	0	0	0
2	BaB	25	0	0	0	0
3	AaA	5	0	0	0	0
3	BaB	5	0	0	0	0
4	BaB	6	0	8	0	0
5	AaA	82	0	0	0	0
5	BaB	76	0	0	0	0
All	All	4415	0	4134	33	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 4.

All (33) 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:AaA:299:ARG:CZ	1:AaA:347:GLN:OE1	1.79	1.30
1:AaA:299:ARG:NH2	1:AaA:347:GLN:OE1	1.82	1.09
1:AaA:263:MET:HE1	1:BaB:156:TRP:CE3	2.08	0.88
1:AaA:156:TRP:CE3	1:BaB:263:MET:HE1	2.19	0.78
1:BaB:218:LEU:HG	1:BaB:223:GLN:HE22	1.61	0.65
1:AaA:276:VAL:HG21	1:AaA:295:LEU:HD21	1.81	0.62
1:BaB:276:VAL:HG21	1:BaB:295:LEU:HD21	1.80	0.61
1:AaA:299:ARG:NE	1:AaA:347:GLN:OE1	2.32	0.61
1:AaA:156:TRP:CZ3	1:BaB:263:MET:SD	2.93	0.61
1:AaA:156:TRP:CZ3	1:BaB:263:MET:HE1	2.37	0.59
1:AaA:98:ASN:HD22	1:AaA:359:LYS:HE2	1.71	0.55
1:AaA:263:MET:HE1	1:BaB:156:TRP:HE3	1.68	0.55
1:AaA:156:TRP:CE3	1:BaB:263:MET:CE	2.95	0.49
1:AaA:290:LEU:C	1:AaA:290:LEU:HD23	2.38	0.49
1:BaB:280:ILE:HD13	1:BaB:356:TRP:CZ2	2.48	0.48
1:AaA:263:MET:HE1	1:BaB:156:TRP:CZ3	2.47	0.48
1:AaA:156:TRP:CZ3	1:BaB:263:MET:CE	2.98	0.47
1:AaA:156:TRP:CZ3	1:BaB:125:THR:HB	2.49	0.47
1:BaB:103:VAL:HG21	1:BaB:290[B]:LEU:HD23	1.98	0.46
1:AaA:280:ILE:HD13	1:AaA:356:TRP:CZ2	2.51	0.45
1:BaB:349:ILE:HG22	1:BaB:350:ASN:OD1	2.16	0.45
1:AaA:139:LEU:HD13	1:AaA:198:MET:HE3	1.99	0.44
1:AaA:283:GLU:H	1:AaA:283:GLU:CD	2.26	0.44
1:AaA:156:TRP:CE3	1:BaB:263:MET:SD	3.11	0.43
1:BaB:289:GLU:OE1	1:BaB:357:ARG:NH1	2.52	0.42
1:BaB:106:ILE:O	1:BaB:110:LEU:HG	2.19	0.42
1:AaA:289:GLU:OE1	1:AaA:357:ARG:NH1	2.53	0.41
1:AaA:106:ILE:O	1:AaA:110:LEU:HG	2.19	0.41
1:AaA:333:ASP:HA	1:AaA:356:TRP:O	2.20	0.41
1:BaB:126:ASP:O	1:BaB:264:ASN:ND2	2.54	0.41
1:AaA:93:TYR:CE2	1:BaB:108:ASN:HB3	2.56	0.41
1:AaA:98:ASN:HD22	1:AaA:359:LYS:CE	2.33	0.40

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	AaA	254/295 (86%)	251 (99%)	3 (1%)	0	100	100
1	BaB	255/295 (86%)	253 (99%)	2 (1%)	0	100	100
All	All	509/590 (86%)	504 (99%)	5 (1%)	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 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	AaA	234/263 (89%)	234 (100%)	0	100	100
1	BaB	235/263 (89%)	235 (100%)	0	100	100
All	All	469/526 (89%)	469 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
3	SO4	AaA	402	-	4,4,4	0.31	0	6,6,6	0.10	0
2	A1IPE	AaA	401	-	25,27,27	0.92	1 (4%)	33,40,40	0.76	0
4	GOL	BaB	403	-	5,5,5	0.15	0	5,5,5	0.59	0
3	SO4	BaB	402	-	4,4,4	0.63	0	6,6,6	0.13	0
2	A1IPE	BaB	401	-	25,27,27	0.97	2 (8%)	33,40,40	0.89	2 (6%)

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	A1IPE	BaB	401	-	-	0/15/33/33	0/3/3/3
4	GOL	BaB	403	-	-	2/4/4/4	-
2	A1IPE	AaA	401	-	-	0/15/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	401	A1IPE	C2-C1	-2.64	1.32	1.39
2	AaA	401	A1IPE	C2-C1	-2.29	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	401	A1IPE	O1-C4	-2.10	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BaB	401	A1IPE	C4-N-C3	2.06	124.60	120.62
2	BaB	401	A1IPE	C7-C5-C8	-2.00	104.55	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

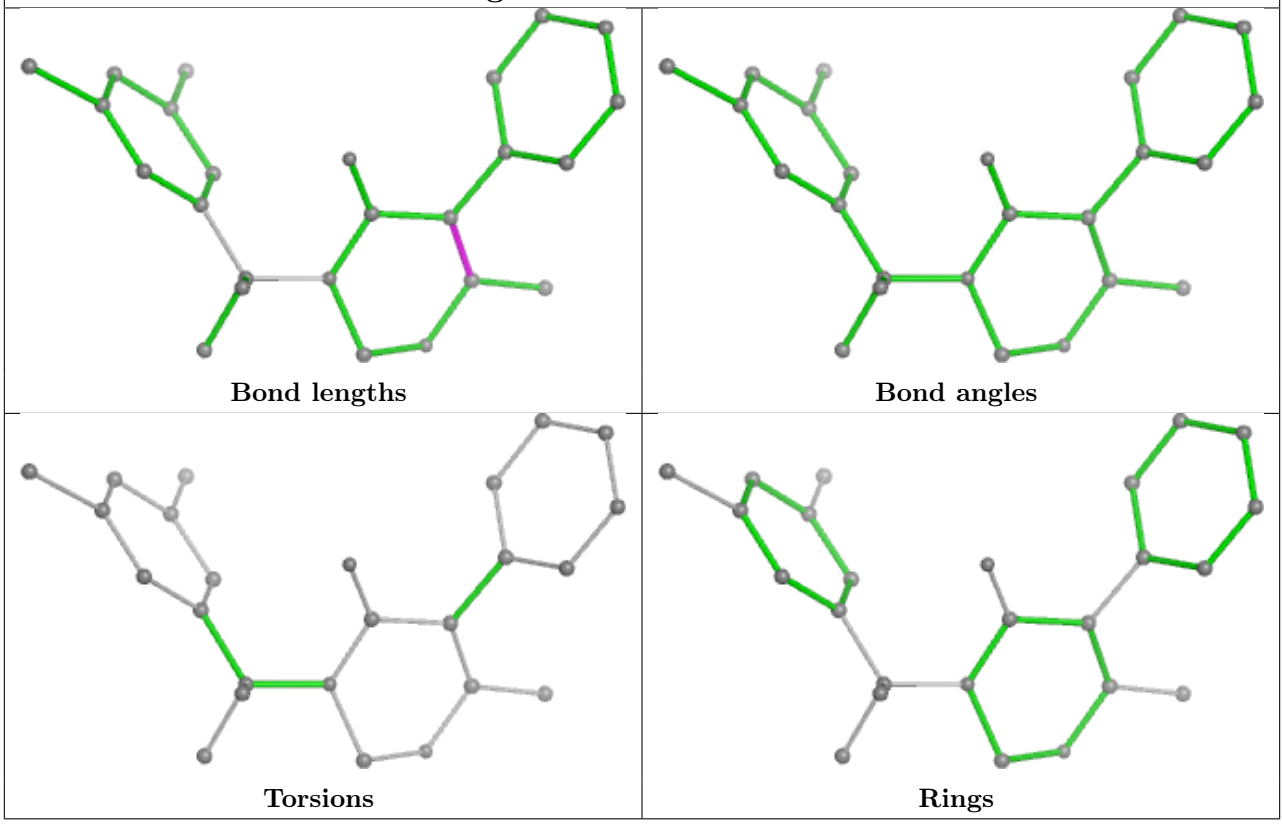
Mol	Chain	Res	Type	Atoms
4	BaB	403	GOL	C1-C2-C3-O3
4	BaB	403	GOL	O2-C2-C3-O3

There are no ring outliers.

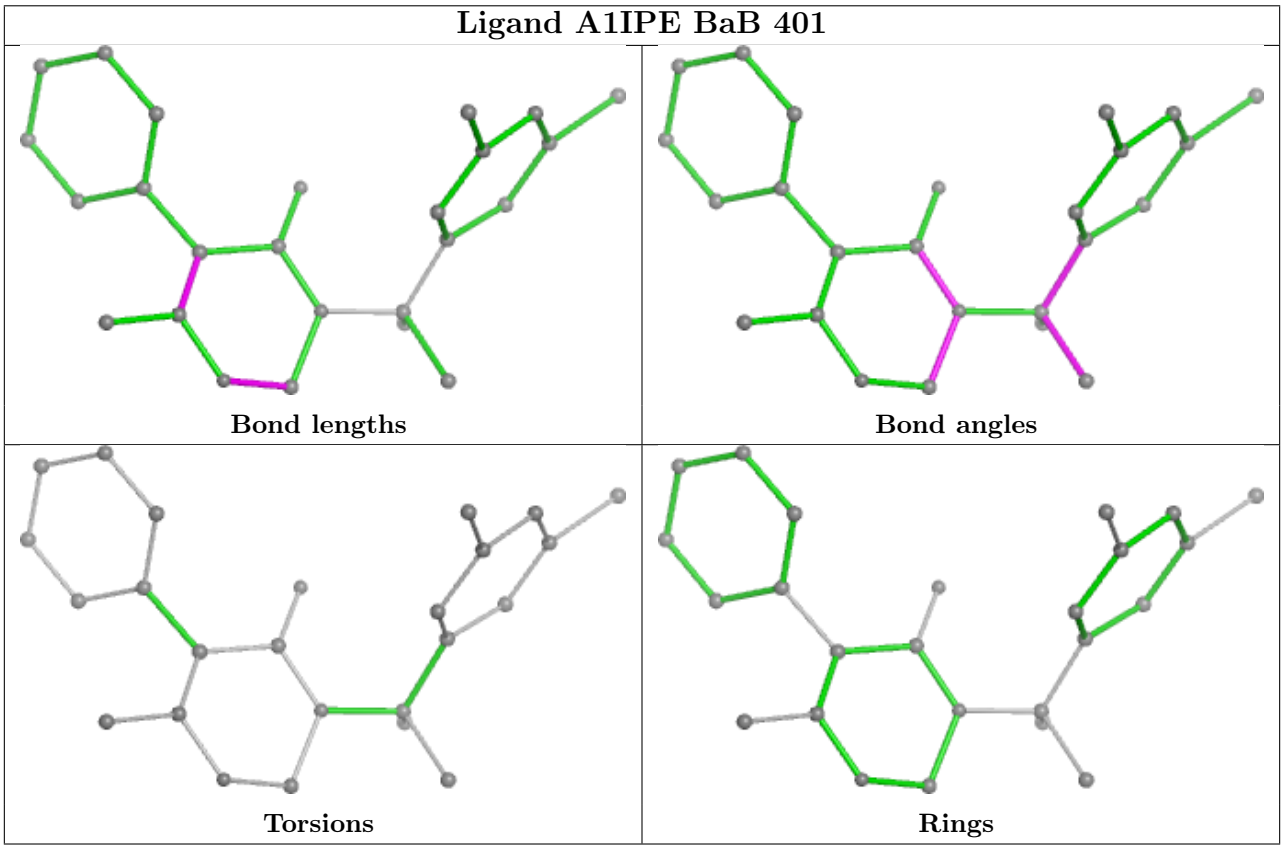
No monomer is involved in short contacts.

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 then 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.

Ligand A1IPE AaA 401



Ligand A1IPE BaB 401



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	AaA	258/295 (87%)	0.50	23 (8%)	17	17	13, 27, 52, 69	2 (0%)
1	BaB	257/295 (87%)	0.50	15 (5%)	30	31	9, 26, 45, 65	4 (1%)
All	All	515/590 (87%)	0.50	38 (7%)	22	23	9, 27, 48, 69	6 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	126	ASP	4.8
1	AaA	360	PRO	4.7
1	BaB	266	HIS	4.5
1	AaA	263	MET	3.8
1	BaB	344	GLY	3.6
1	BaB	98	ASN	3.4
1	AaA	128	PHE	3.3
1	AaA	266	HIS	3.2
1	BaB	264	ASN	3.2
1	BaB	263	MET	3.1
1	AaA	265	GLN	3.1
1	BaB	184	VAL	3.1
1	BaB	119	GLN	2.9
1	AaA	347	GLN	2.9
1	AaA	204	ARG	2.8
1	AaA	299	ARG	2.8
1	BaB	206	LEU	2.7
1	AaA	261	LEU	2.6
1	AaA	125	THR	2.6
1	BaB	205	ARG	2.6
1	AaA	99	LYS	2.5
1	AaA	245	ASP	2.5
1	BaB	125	THR	2.5
1	AaA	156	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	BaB	204	ARG	2.4
1	BaB	97	SER	2.4
1	AaA	264	ASN	2.4
1	AaA	240	ILE	2.3
1	AaA	300	GLU	2.3
1	AaA	358	LYS	2.2
1	AaA	79	GLU	2.2
1	BaB	201	GLN	2.2
1	AaA	257	ARG	2.2
1	AaA	303	GLN	2.1
1	AaA	259	ALA	2.1
1	AaA	97	SER	2.1
1	AaA	98	ASN	2.1
1	BaB	300	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

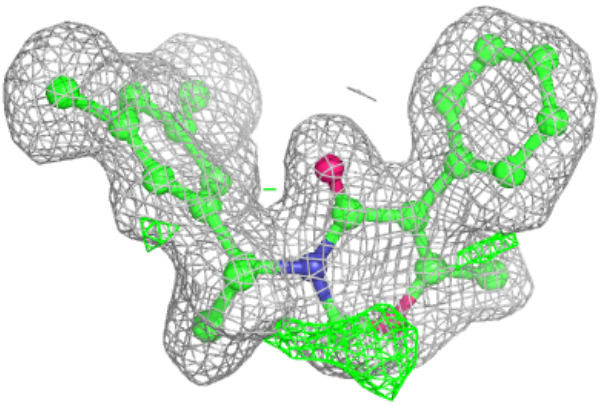
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

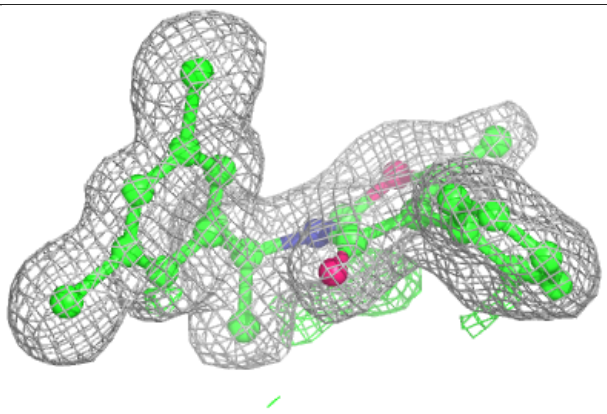
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	AaA	402	5/5	0.81	0.11	56,57,60,66	0
4	GOL	BaB	403	6/6	0.83	0.14	32,34,38,39	0
2	A1IPE	AaA	401	25/25	0.97	0.06	15,17,19,20	0
3	SO4	BaB	402	5/5	0.97	0.09	30,35,41,42	0
2	A1IPE	BaB	401	25/25	0.97	0.07	16,19,21,22	0

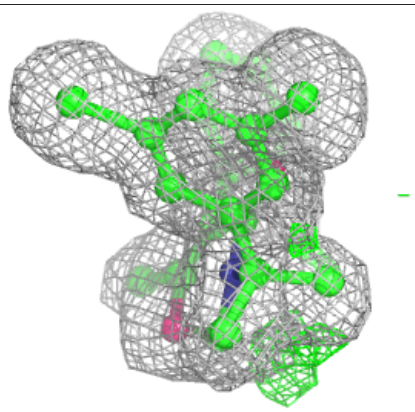
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1IPE AaA 401:

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

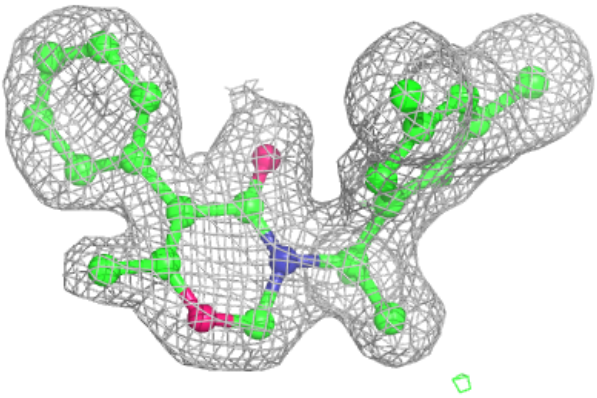


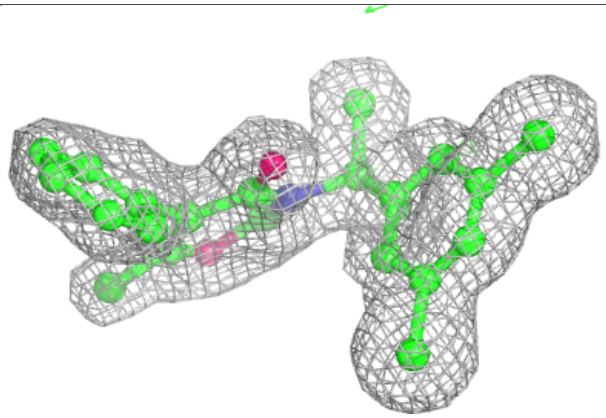


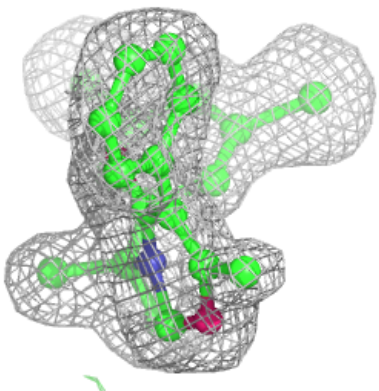


Electron density around A1IPE BaB 401:

$2mF_o$-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)

There are no such residues in this entry.