



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:22 PM UTC

PDB ID : 6S37 / pdb_00006s37
Title : Ligand binding domain of the P. putida receptor PcaY_PP in complex with salicylic acid
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Deposited on : 2019-06-24
Resolution : 2.30 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 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

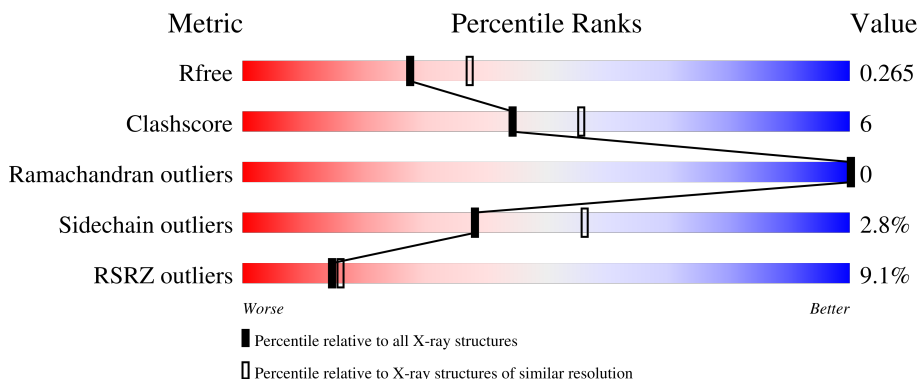
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	550	
1	B	550	

2 Entry composition [i](#)

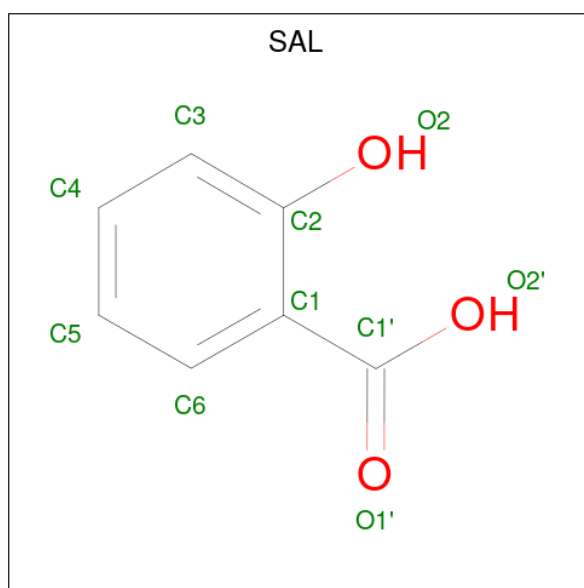
There are 4 unique types of molecules in this entry. The entry contains 2411 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aromatic acid chemoreceptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	19	0
			1237	746	234	252	5			
1	B	126	Total	C	N	O	S	0	17	0
			1106	671	208	222	5			

- Molecule 2 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	31	Total	O	0	0
			31	31		

ARG	GLN	LEU	VAL	MET
GLU	ALA	GLU	ALA	GLN
VAL	GLY	VAL	ARG	GLN
ASP	THR	ILE	ASN	SER
ARG	GLU	ARG	ALA	GLN
ASN	ALA	SER	ILE	ARG
LEU	ALA	VAL	THR	ASP
LEU	VAL	SER	THR	THR
ASN	ALA	GLU	SER	GLY
ILE	SER	GLN	THR	GLN
ARG	MET	THR	THR	GLN
GLU	GLN	ASN	THR	ILE
LEU	ALA	LEU	SER	ASN
SER	SER	LEU	GLU	ASN
ASN	THR	ALA	SER	CYS
HIS	THR	ALA	ASN	ALA
SER	ARG	ASN	GLN	ARG
ALA	ALA	ALA	LEU	GLN
ALA	GLN	ILE	ALA	LEU
GLY	SER	ILE	ALA	ASP
ALA	THR	GLU	GLN	ASP
GLN	LEU	THR	ARG	THR
GLN	VAL	ARG	THR	ALA
THR	THR	ALA	GLN	ALA
SER	THR	ALA	VAL	LEU
GLU	LEU	GLY	SER	ASN
ALA	ALA	GLU	SER	ALA
SER	SER	ALA	GLU	ALA
LYS	GLY	GLY	ASN	VAL
ALA	ALA	ARG	ILE	THR
LEU	VAL	GLY	ASP	GLU
SER	LEU	PHE	GLY	GLU
GLY	LEU	ALA	THR	SER
LEU	GLY	VAL	GLU	ALA
VAL	ILE	VAL	ALA	ASN
GLY	TYR	ALA	MET	ASN
GLU	SER	ASP	THR	LEU
MET	ALA	GLU	ARG	ARG
THR	ILE	VAL	GLU	GLN
ALA	GLY	ARG	ILE	GLN
LEU	GLU	THR	GLN	GLY
VAL	ILE	LEU	THR	GLN
GLY	ASN	ALA	SER	GLU
ARG	GLU	TYR	SER	LEU
PHE	ARG	ARG	ALA	GLU
LYS	ASN	THR	HIS	GLN
VAL	LEU	GLN	LEU	ALA
	VAL	GLN	GLN	ALA
	ILE	SER	THR	THR
	ALA	THR	LEU	ALA
	SER	GLN	VAL	VAL
	ALA	ALA	GLY	THR
	SER	ILE	ARG	THR
	GLN	MET	ASP	THR
	GLU	ILE	ILE	ALA
	ALA	GLY	GLY	VAL
	VAL	SER	LYS	GLU
	ALA	VAL	VAL	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.84Å 69.40Å 93.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.44 – 2.30 40.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.44-2.30) 99.0 (40.44-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.195 , 0.255 0.204 , 0.265	Depositor DCC
R_{free} test set	681 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2411	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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: SAL, ACT

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	0.11	0/1245	0.30	0/1670
1	B	0.11	0/1114	0.25	0/1493
All	All	0.11	0/2359	0.28	0/3163

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	1237	0	1203	15	0
1	B	1106	0	1089	15	0
2	A	10	0	5	0	0
3	A	4	0	3	1	0
4	A	23	0	0	1	0
4	B	31	0	0	2	0
All	All	2411	0	2300	28	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 6.

The worst 5 of 28 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:B:147[A]:ARG:NH1	4:B:601:HOH:O	2.23	0.72
1:A:110:ASP:O	1:A:114[A]:GLU:HG2	2.06	0.55
1:A:83[A]:GLN:NE2	1:A:146:THR:O	2.33	0.52
1:B:110:ASP:O	1:B:114[B]:GLU:HG3	2.10	0.51
1:A:60[B]:ASP:OD2	1:B:173:GLN:NE2	2.41	0.50

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	156/550 (28%)	156 (100%)	0	0	100	100
1	B	141/550 (26%)	141 (100%)	0	0	100	100
All	All	297/1100 (27%)	297 (100%)	0	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	A	131/438 (30%)	119 (91%)	12 (9%)	8	11
1	B	117/438 (27%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	248/876 (28%)	236 (95%)	12 (5%)	38	35

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117[B]	ARG
1	A	118[A]	GLU
1	A	187[B]	MET
1	A	118[B]	GLU
1	A	59[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	B	102	ASN
1	B	158	ASN
1	B	142	GLN
1	A	174	GLN

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 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	SAL	A	601	-	10,10,10	1.10	0	13,13,13	0.87	0
3	ACT	A	602	-	3,3,3	1.35	0	3,3,3	1.53	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	SAL	A	601	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

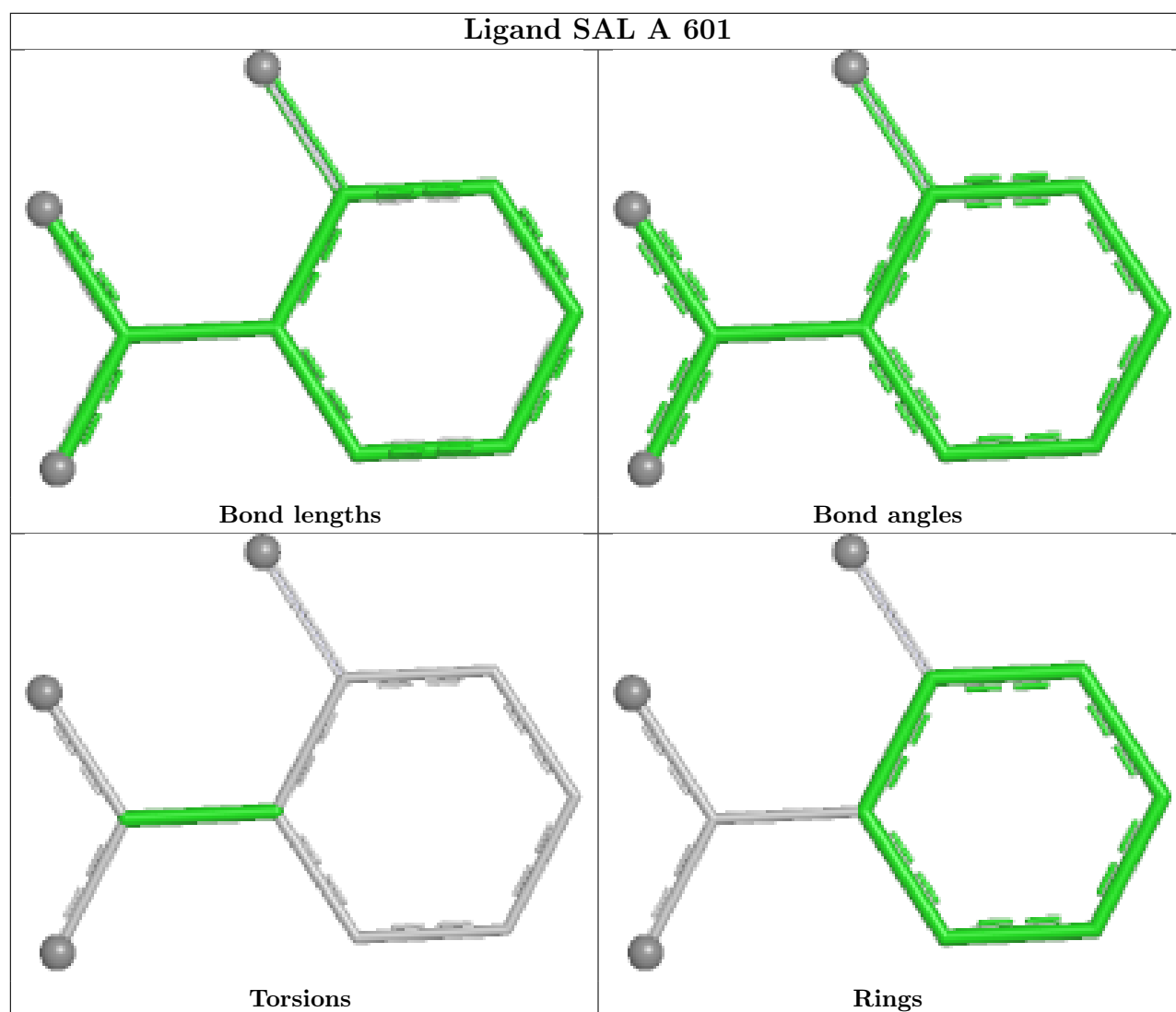
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ACT	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.

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	139/550 (25%)	0.66	17 (12%) 8 9	16, 44, 82, 107	19 (13%)
1	B	126/550 (22%)	0.21	7 (5%) 30 32	12, 35, 73, 95	17 (13%)
All	All	265/1100 (24%)	0.44	24 (9%) 15 16	12, 40, 79, 107	36 (13%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	ALA	6.1
1	A	156[A]	LYS	5.6
1	B	180	SER	4.2
1	A	126	THR	4.2
1	A	188	LEU	4.0

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](#)

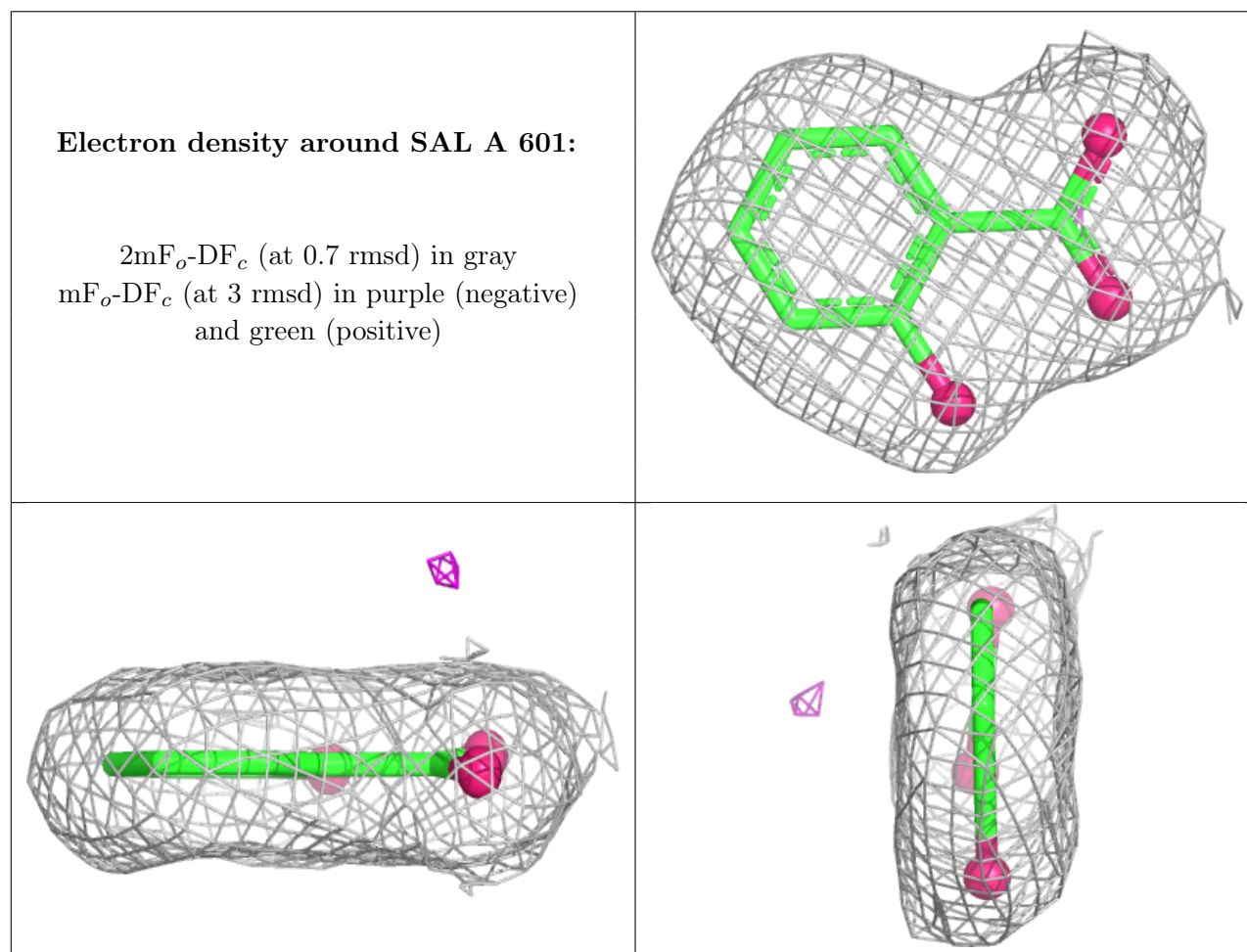
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	ACT	A	602	4/4	0.82	0.18	64,67,68,68	0
2	SAL	A	601	10/10	0.95	0.07	21,32,37,45	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.