



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:33 PM UTC

PDB ID : 6S1A / pdb_00006s1a
Title : Ligand binding domain of the P. putida receptor PcaY_PP
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Deposited on : 2019-06-18
Resolution : 2.11 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

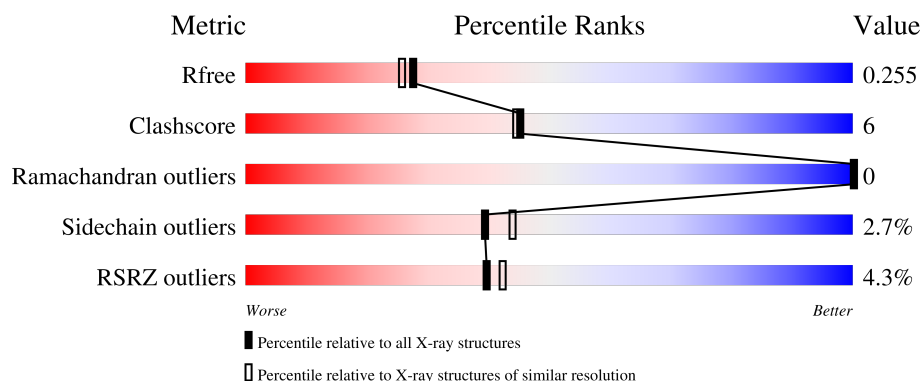
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	% 22% •• 75%
1	B	550	% 21% 5% 75%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2605 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	140	Total	C	N	O	S	0	15	0
			1223	740	231	247	5			
1	B	138	Total	C	N	O	S	0	27	0
			1297	778	246	268	5			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		

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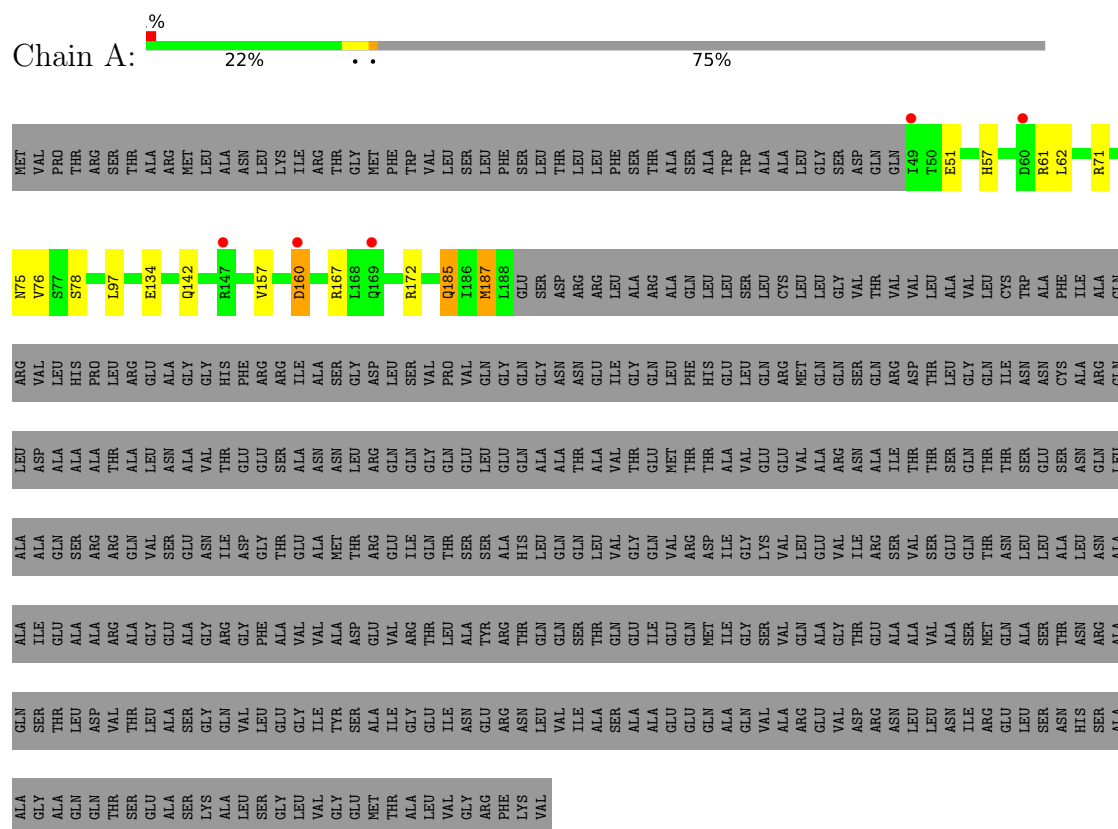
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	49	Total	O	0	0
			49	49		

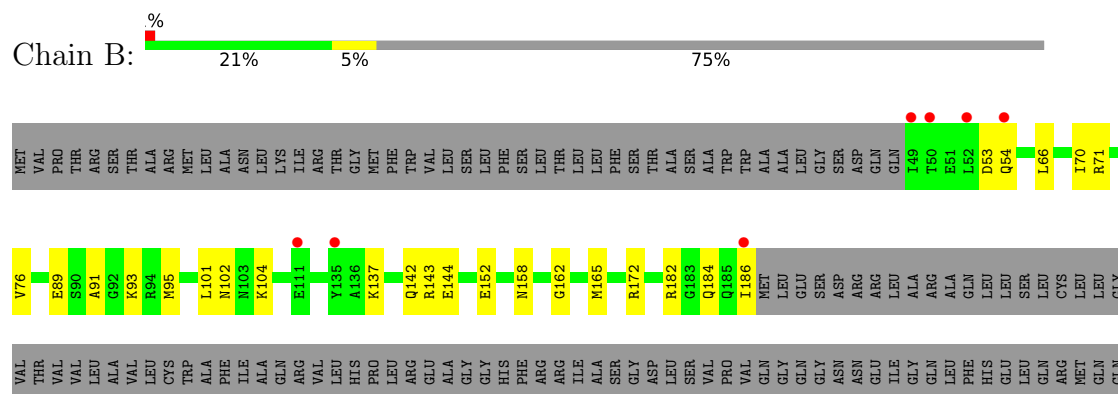
3 Residue-property plots [i](#)

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: Aromatic acid chemoreceptor



• Molecule 1: Aromatic acid chemoreceptor



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.52Å 69.23Å 90.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.51 – 2.11 38.51 – 2.11	Depositor EDS
% Data completeness (in resolution range)	88.0 (38.51-2.11) 88.1 (38.51-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.212 , 0.260 (Not available) , 0.255	Depositor DCC
R_{free} test set	706 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	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	2605	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% 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

5.1 Standard geometry

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

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	0.32	0/1231	0.36	0/1650
1	B	0.18	0/1305	0.33	0/1746
All	All	0.26	0/2536	0.35	0/3396

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	A	1223	0	1199	13	0
1	B	1297	0	1252	19	0
2	B	5	0	0	0	0
3	A	31	0	0	1	0
3	B	49	0	0	4	0
All	All	2605	0	2451	30	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.

All (30) 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:70:ILE:HD13	1:B:165[A]:MET:HG2	1.57	0.86
1:B:137[A]:LYS:HE2	3:B:710:HOH:O	1.82	0.79
1:B:104[A]:LYS:NZ	3:B:704:HOH:O	2.25	0.69
1:B:162:GLY:HA2	1:B:165[B]:MET:HE2	1.78	0.65
1:B:182[B]:ARG:NH1	3:B:707:HOH:O	2.30	0.65
1:A:76:VAL:HG11	1:A:142:GLN:HB3	1.82	0.61
1:B:54[B]:GLN:NE2	3:B:711:HOH:O	2.34	0.61
1:A:134:GLU:OE2	1:A:167:ARG:NH2	2.36	0.58
1:B:95[B]:MET:HE1	1:B:143:ARG:HA	1.86	0.57
1:B:66:LEU:HD22	1:B:172:ARG:HB2	1.90	0.54
1:A:157:VAL:HA	1:A:160[A]:ASP:HB2	1.90	0.54
1:B:76:VAL:HG11	1:B:142:GLN:HB3	1.90	0.54
1:B:91:ALA:O	1:B:95[B]:MET:HG2	2.08	0.53
1:B:152[B]:GLU:CD	1:B:152[B]:GLU:H	2.17	0.52
1:A:62:LEU:HG	1:A:172:ARG:HG3	1.93	0.49
1:A:78:SER:HB3	1:B:158[A]:ASN:HD21	1.76	0.49
1:A:51[B]:GLU:OE1	1:A:51[B]:GLU:N	2.42	0.46
1:A:187[A]:MET:HB3	1:A:187[A]:MET:HE3	1.78	0.45
1:A:57:HIS:HD2	1:A:61:ARG:HG3	1.82	0.44
1:B:184:GLN:C	1:B:186:ILE:H	2.26	0.43
1:A:185:GLN:HE21	1:A:185:GLN:HB2	1.56	0.42
1:B:71[B]:ARG:HB3	1:B:101:LEU:HD13	2.00	0.42
1:B:162:GLY:HA2	1:B:165[B]:MET:HG3	2.03	0.41
1:B:95[A]:MET:HE2	1:B:95[A]:MET:HB2	1.80	0.41
1:A:75:ASN:OD1	1:A:97[A]:LEU:HD23	2.21	0.41
1:B:93[B]:LYS:HE3	1:B:93[B]:LYS:HB2	1.87	0.41
1:B:102:ASN:HD22	1:B:143:ARG:HH22	1.69	0.41
1:A:57:HIS:CD2	1:A:61:ARG:HG3	2.56	0.40
1:A:71:ARG:HD2	1:B:165[A]:MET:HG3	2.03	0.40
1:A:172:ARG:NH1	3:A:604:HOH:O	2.41	0.40

There are no symmetry-related clashes.

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	154/550 (28%)	153 (99%)	1 (1%)	0	100	100
1	B	163/550 (30%)	162 (99%)	1 (1%)	0	100	100
All	All	317/1100 (29%)	315 (99%)	2 (1%)	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	129/438 (30%)	124 (96%)	5 (4%)	28	29
1	B	138/438 (32%)	132 (96%)	6 (4%)	26	26
All	All	267/876 (30%)	256 (96%)	11 (4%)	39	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160[A]	ASP
1	A	160[B]	ASP
1	A	185	GLN
1	A	187[A]	MET
1	A	187[B]	MET
1	B	53[A]	ASP
1	B	53[B]	ASP
1	B	89[A]	GLU
1	B	89[B]	GLU
1	B	144[A]	GLU
1	B	144[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	83	GLN

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	173	GLN
1	A	174	GLN
1	B	102	ASN
1	B	142	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](#)

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](#)

1 ligand 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	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.06	0

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.

No monomer is involved in short contacts.

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	140/550 (25%)	0.40	5 (3%)	46	49	16, 34, 56, 81	15 (10%)
1	B	138/550 (25%)	0.51	7 (5%)	33	36	15, 34, 71, 88	27 (19%)
All	All	278/1100 (25%)	0.46	12 (4%)	40	42	15, 34, 59, 88	42 (15%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	ILE	3.8
1	B	186	ILE	3.2
1	B	135	TYR	2.9
1	B	52	LEU	2.7
1	B	49	ILE	2.5
1	B	111[A]	GLU	2.4
1	A	160[A]	ASP	2.3
1	A	147[A]	ARG	2.2
1	B	54[A]	GLN	2.1
1	A	60[A]	ASP	2.1
1	B	50	THR	2.1
1	A	169	GLN	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 oligosaccharides in this entry.

6.4 Ligands

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
2	SO4	B	601	5/5	0.83	0.11	65,65,66,68	0

6.5 Other polymers

There are no such residues in this entry.