



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:29 am GMT

PDB ID : 1I7S
Title : ANTHRANILATE SYNTHASE FROM SERRATIA MARCESCENS IN
COMPLEX WITH ITS END PRODUCT INHIBITOR L-TRYPTOPHAN
Authors : Spraggon, G.; Kim, C.; Nguyen-Huu, X.; Yee, M.-C.; Yanofsky, C.; Mills, S.E.
Deposited on : 2001-03-10
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

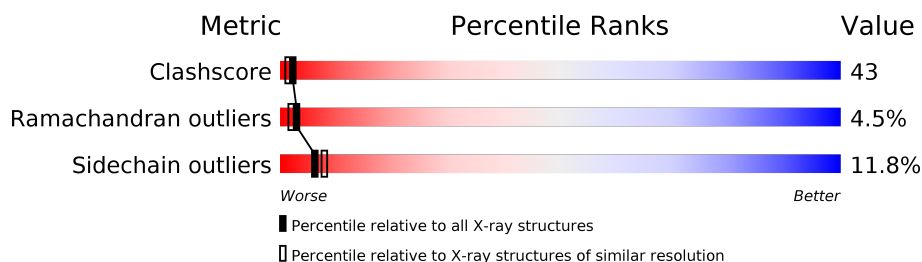
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	519	
1	C	519	
2	B	193	
2	D	193	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10880 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 ANTHRANILATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3966	2474	721	753	18			
1	C	511	Total	C	N	O	S	0	0	0
			3966	2474	721	753	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ARG	PRO	SEE REMARK 999	UNP P00897
A	83	LEU	VAL	see remark 999	UNP P00897
A	130	ILE	LEU	see remark 999	UNP P00897
A	164	LEU	VAL	see remark 999	UNP P00897
A	459	VAL	HIS	see remark 999	UNP P00897
A	461	ASN	HIS	see remark 999	UNP P00897
A	492	PRO	ARG	see remark 999	UNP P00897
A	493	GLU	ARG	see remark 999	UNP P00897
C	60	ARG	PRO	see remark 999	UNP P00897
C	83	LEU	VAL	see remark 999	UNP P00897
C	130	ILE	LEU	see remark 999	UNP P00897
C	164	LEU	VAL	see remark 999	UNP P00897
C	459	VAL	HIS	see remark 999	UNP P00897
C	461	ASN	HIS	see remark 999	UNP P00897
C	492	PRO	ARG	see remark 999	UNP P00897
C	493	GLU	ARG	see remark 999	UNP P00897

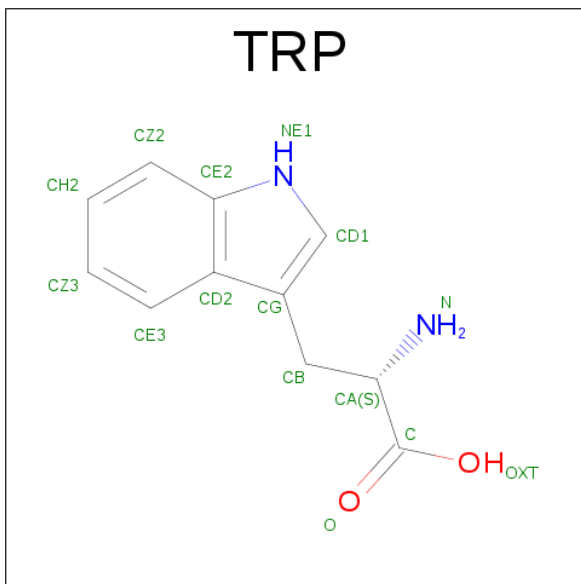
- Molecule 2 is a protein called TRPG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1459	917	265	267	10			
2	D	192	Total	C	N	O	S	0	0	0
			1459	917	265	267	10			

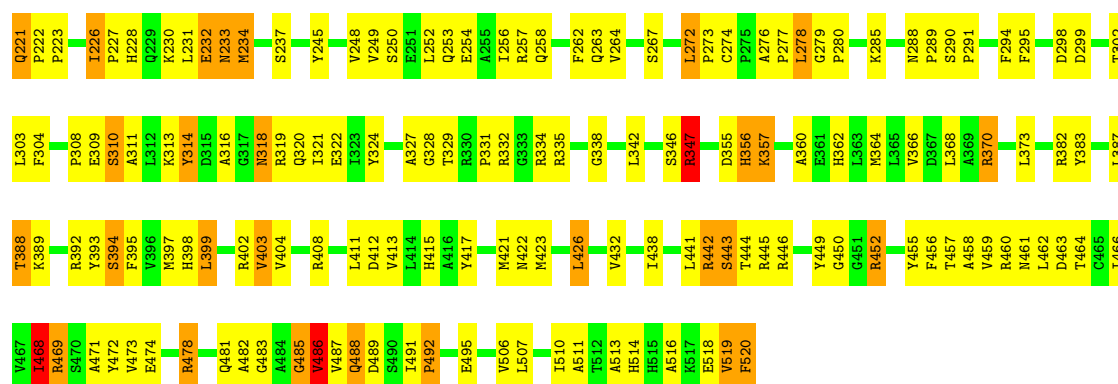
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	PHE	SER	see remark 999	UNP P00900
D	152	PHE	SER	see remark 999	UNP P00900

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).

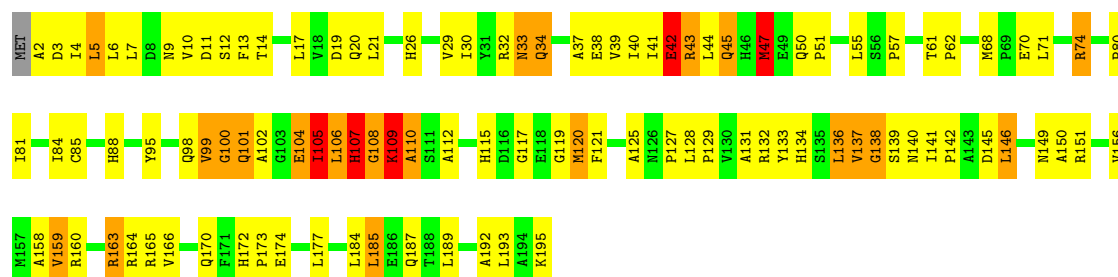


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		



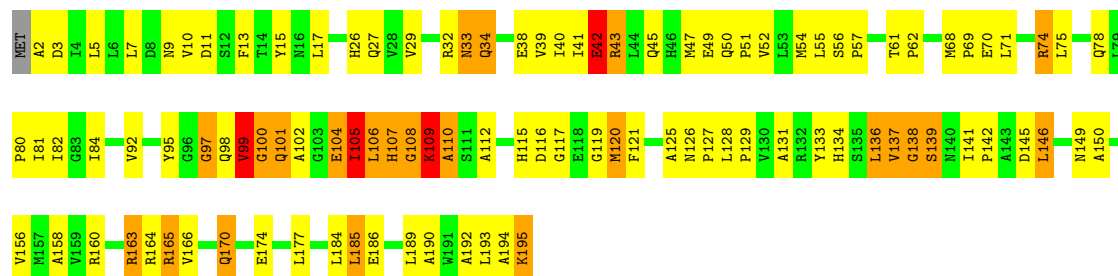
• Molecule 2: TRPG

Chain B: 45% 41% 11% ••



• Molecule 2: TRPG

Chain D: 46% 40% 12% ••



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 21	Depositor
Cell constants a, b, c, α , β , γ	72.27Å 123.56Å 179.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (44.90-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0, REFMAC	Depositor
R, R_{free}	0.247 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10880	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.84	0/4035	1.00	9/5474 (0.2%)
1	C	0.86	1/4035 (0.0%)	1.02	13/5474 (0.2%)
2	B	1.05	4/1487 (0.3%)	1.11	8/2015 (0.4%)
2	D	0.92	3/1487 (0.2%)	1.05	5/2015 (0.2%)
All	All	0.89	8/11044 (0.1%)	1.03	35/14978 (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	1
1	C	0	1
2	D	0	1
All	All	0	3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	GLU	CD-OE1	10.95	1.37	1.25
2	B	42	GLU	CD-OE2	8.64	1.35	1.25
2	B	42	GLU	CD-OE1	8.27	1.34	1.25
2	B	42	GLU	CB-CG	6.91	1.65	1.52
2	D	42	GLU	CB-CG	6.02	1.63	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	146	LEU	N-CA-C	-10.50	82.66	111.00
2	B	146	LEU	N-CA-C	-9.77	84.62	111.00
1	A	408	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	B	47	MET	CG-SD-CE	-8.08	87.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	370	ARG	NE-CZ-NH1	8.06	124.33	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	PHE	Sidechain
1	C	314	TYR	Sidechain
2	D	15	TYR	Sidechain

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	3966	0	3940	337	0
1	C	3966	0	3940	324	0
2	B	1459	0	1459	137	0
2	D	1459	0	1459	145	0
3	A	15	0	9	1	0
3	C	15	0	9	2	0
All	All	10880	0	10816	923	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 43.

The worst 5 of 923 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:A:263:GLN:NE2	1:A:364:MET:HG2	1.42	1.32
1:C:263:GLN:NE2	1:C:364:MET:HG2	1.44	1.28
2:D:41:ILE:HG22	2:D:45:GLN:HE21	1.15	1.09
1:C:263:GLN:HE22	1:C:364:MET:HG2	0.92	1.06
2:B:163:ARG:NH1	2:B:163:ARG:H	1.54	1.05

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	507/519 (98%)	449 (89%)	36 (7%)	22 (4%)	3	2
1	C	507/519 (98%)	449 (89%)	39 (8%)	19 (4%)	4	3
2	B	190/193 (98%)	162 (85%)	18 (10%)	10 (5%)	2	1
2	D	190/193 (98%)	158 (83%)	20 (10%)	12 (6%)	1	0
All	All	1394/1424 (98%)	1218 (87%)	113 (8%)	63 (4%)	3	2

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	21	PRO
1	A	139	ASP
1	A	201	GLN
1	A	221	GLN

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	422/434 (97%)	374 (89%)	48 (11%)	7	9
1	C	422/434 (97%)	372 (88%)	50 (12%)	6	8
2	B	152/153 (99%)	132 (87%)	20 (13%)	5	5
2	D	152/153 (99%)	134 (88%)	18 (12%)	6	8
All	All	1148/1174 (98%)	1012 (88%)	136 (12%)	6	8

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	145	ASP
1	C	83	LEU
2	D	101	GLN
2	B	163	ARG
1	C	21	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	101	GLN
1	C	168	GLN
2	D	89	GLN
2	B	115	HIS
1	C	27	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 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	TRP	A	601	-	11,16,16	1.15	2 (18%)	11,22,22	0.83	0
3	TRP	C	701	-	11,16,16	1.24	2 (18%)	11,22,22	0.74	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
3	TRP	A	601	-	-	0/3/8/8	0/2/2/2
3	TRP	C	701	-	-	0/3/8/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	TRP	CB-CG	-2.04	1.45	1.51
3	C	701	TRP	CD1-NE1	2.07	1.40	1.36
3	C	701	TRP	CZ3-CE3	2.43	1.42	1.36
3	A	601	TRP	CZ3-CE3	2.61	1.42	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TRP	1	0
3	C	701	TRP	2	0

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.