



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:33 am GMT

PDB ID : 2A4M  
Title : Structure of Trprs II bound to ATP  
Authors : Buddha, M.R.; Crane, B.R.  
Deposited on : 2005-06-29  
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](mailto: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.

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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

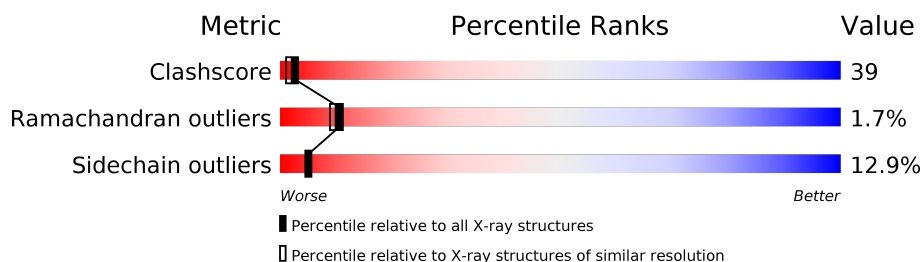
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	331	
1	B	331	
1	C	331	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRP	C	500	-	-	X	-

## 2 Entry composition [i](#)

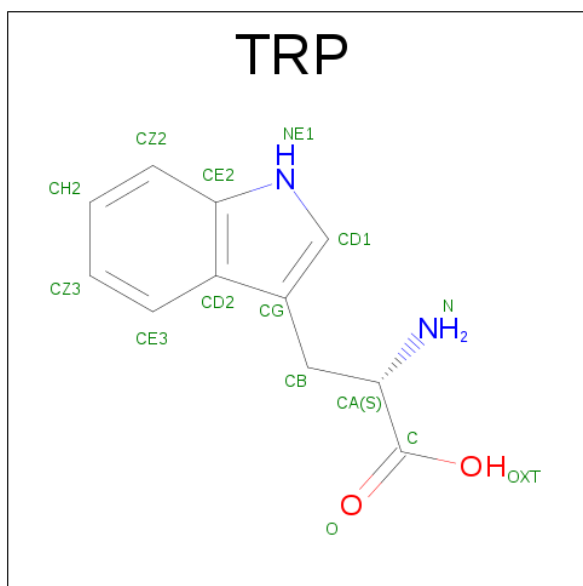
There are 3 unique types of molecules in this entry. The entry contains 8788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophanyl-tRNA synthetase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	2	0	0
			2544	1599	468	471	6			
1	B	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2527	1591	462	468	6			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total 382	O 382	0	0
3	B	395	Total 395	O 395	0	0
3	C	414	Total 414	O 414	0	0



Note EDS was not executed.

- Chain A:

52% 41% 7%

A21 A22 A23 A24 A25 A26 A27 A30 A36 A37 A38 A39 A40 A43 A44 A45 A46 A47 A48 A49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 A61 A62 A63 A64 A65 A66 A67 A68 A69 A70 A74 A75 A76 A77 A78 A81 A84 A85 A86 A87 A89 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A114 A117 A118 A119 A123 A127 A130 A134 A135 A136 A137 A138 A139 A140 A141 A142 A143 A149 A150 A154 A165 A166 A167 A168 A169 A170 A171 A172 A173 A174 A175 A178 A184 A185 A189 A196 Q200 Q201 Q202 Q206 Q207 Q208 Q211 Q212 Q213 Q214 Q215 Q218 Q222 Q223 Q224 Q225 Q226 Q230 Q231 Q232 Q233 Q234 Q235 Q236 Q237 Q238 Q239 Q240 Q241 Q242 Q243 Q244 Q245 Q246 Q247 Q248 Q249 Q250 Q251 Q252 Q253 Q254 Q255 Q257 Q258 Q259 Q260 Q261 Q262 Q263 Q264 Q267 Q270 Q273 Q276 Q277 Q278 Q279 Q280 Q281 Q282 Q283 Q284 Q285 Q286 Q289 Q290 Q291 Q292 Q293 Q294 Q295 Q296 Q297 Q298 Q299 Q300 Q301 Q302 Q305 Q308 Q309 Q310 Q311 Q312 Q316 Q317 Q318 Q321 Q322 Q325 Q328 Q333 Q337 Q344 Q345 Q346 Q347 Q348 Q349 Q350 Q351

- Chain B:

Category	Percentage	Tokens
Blue	10%	A304, P305, I306, R307, M240, V241, T242, H246, L247, R248, A249, S250, P251, G253, R254, V255, E256, P259, V260, F261, T262, F263, F267, D268, P269, D270, R273, V274, A276, L277, Y281, R282, A283, L286, G287, D288, V289, K290, V291, K292, K293, H294, L295, L296, D297, V298, L299, N300, G301, V302, L303
Green	41%	R235, V237, M240, V241, T242, H246, L247, R248, A249, S250, P251, G253, R254, V255, E256, P259, V260, F261, T262, F263, F267, D268, P269, D270, R273, V274, A276, L277, Y281, R282, A283, L286, G287, D288, V289, K290, V291, K292, K293, H294, L295, L296, D297, V298, L299, N300, G301, V302, L303
Yellow	51%	L188, L192, D93, P94, G95, K96, T97, T98, C99, Q102, S103, A104, V105, L108, A109, E110, L111, T112, V113, L116, N117, L118, V119, L120, T121, S122, H123, L124, R125, K126, N127, P128, T129, V130, E133, I134, K137, G138, Y139, R142, V143, F148, V149, A150, P151, Y151, V152, S153, A156, D157, A160
Red	8%	L165, V168, Q172, L173, P174, M175, L176, Q178, T179, V183, R184, R185, A191, P192, V193, E196, A199, Q200, L201, S202, R203, V204, P205, R206, L207, P208, G209, L210, D211, G212, Q213, A214, K215, M216, S217, K218, S219, L220, N221, N222, A223, L224, A225, L226, S229, A230, D231, E232, V233, L234

- Chain C:  52% 37% 10%

P271	L173	K96	A21
A272	M175	T97	R22
R273	P174	T98	P23
A276	L176	C99	R24
L277	E177	V100	V25
K278	Q178	V101	L26
D279	T179	Q102	T27
T278	R180	S103	
Q280		A104	R30
L286	R185	V105	P31
G287	L189	F106	T32
D288	L189	E107	
V289	V193	L108	L35
K290	E196	A109	H36
V291	P197	E110	L37
K292	L196	L111	
K293	G200	T112	L40
H294	L201	V113	A41
L295	S202	L116	G42
V298	R203	N117	S43
L299	V204	T120	L44
N300	P205	H123	Q45
	L210	M127	N46
	M216	T128	R47
R307	A223	V130	Q51
T308	I224	K131	E55
R309	S229	E133	L56
R310	A230	Q136	F57
A311	D231	K137	V58
E314	E232	P144	L59
R315	V233	A145	L60
L321	R235	G146	V63
T325	M238	V149	Q64
E326	D243	Y150	A65
G327	P244	P151	D68
T328	L247	V152	H69
A329	R248	S153	F70
R330		Q154	D71
G331	R254	A155	
R332	V255	A156	E74
	E256	D157	Q75
Q337	G257	I158	V76
T338	N258	L165	R77
L339	P259	V166	E78
G340	V260	P167	N79
Q341		V168	V80
V342	F267	G169	L81
R343	D268	D170	A82
	P269	D171	V83
R347	D270	O172	A84
H351	P270		L85
			L92
			D93
			P94
			Q95

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.58Å 58.57Å 85.15Å 90.00° 96.64° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	0.3 (30.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.36	0/2591	0.64	0/3519
1	B	0.32	0/2558	0.61	0/3478
1	C	0.43	0/2574	0.71	2/3499 (0.1%)
All	All	0.37	0/7723	0.65	2/10496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLN	N-CA-C	-5.79	95.36	111.00
1	C	44	LEU	CB-CA-C	5.71	121.05	110.20

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	2544	0	2568	183	0
1	B	2511	0	2507	236	0
1	C	2527	0	2539	190	0
2	C	15	0	9	6	0
3	A	382	0	0	12	0
3	B	395	0	0	6	0
3	C	414	0	0	11	0
All	All	8788	0	7623	599	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 39.

The worst 5 of 599 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:193:VAL:HG21	1:B:341:GLN:HB3	1.20	1.14
1:C:120:THR:HG23	1:C:123:HIS:H	1.13	1.08
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.21	1.06
1:C:337:GLN:HA	1:C:337:GLN:HE21	1.16	1.05
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.11	1.05

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	329/331 (99%)	305 (93%)	19 (6%)	5 (2%)	12	11
1	B	329/331 (99%)	299 (91%)	21 (6%)	9 (3%)	6	4
1	C	329/331 (99%)	309 (94%)	17 (5%)	3 (1%)	20	23
All	All	987/993 (99%)	913 (92%)	57 (6%)	17 (2%)	11	9

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	ALA
1	C	202	SER
1	A	22	ARG
1	B	208	PRO
1	B	214	ALA

### 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	264/264 (100%)	228 (86%)	36 (14%)	4	4
1	B	256/264 (97%)	225 (88%)	31 (12%)	6	6
1	C	260/264 (98%)	226 (87%)	34 (13%)	5	5
All	All	780/792 (98%)	679 (87%)	101 (13%)	5	5

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	ARG
1	B	215	LYS
1	C	286	LEU
1	B	142	ARG
1	B	165	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
1	B	172	GLN
1	C	294	HIS
1	B	46	ASN
1	B	69	HIS

### 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 [i](#)

There are no carbohydrates 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	TRP	C	500	-	11,16,16	0.56	0	11,22,22	0.95	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	TRP	C	500	-	-	0/3/8/8	0/2/2/2

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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	TRP	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.