



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2018 – 07:30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

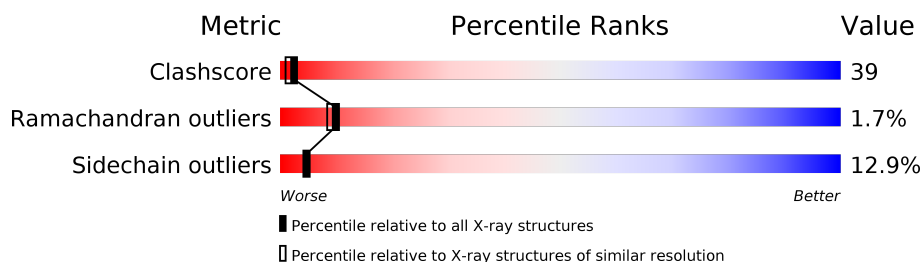
1 Overall quality at a glance

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	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (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 ≥ 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](#)

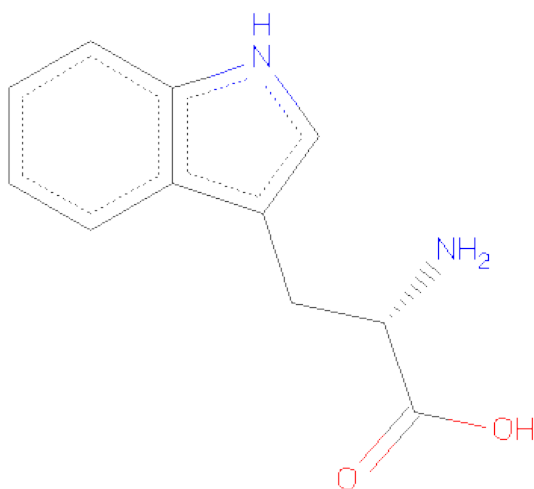
There are 3 unique types of molecules in this entry. The entry contains 8788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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:

R273	A276	L277	K278	D279	K280	Y281	A283	K284	G285	L286	V289	K290	V291	K292	K293	K294	L295	V296	D297	V298	L299	N300	G301	V302	P305	T308	R309	R310	R310	A311	E312	K316	P317	D318	L321	R322	T325	T328	E333	Q337	R344	A345	K346	R347	F348	F349	G350	R351			
Q200	L201	R206	L207	P208	D211	G212	K213	Q214	K215	K218	N222	K223	L224	A225	L226	A230	D231	E232	V233	A234	K235	K236	V237	M238	G239	M240	L241	T242	D243	P244	G245	H246	L247	R248	A249	S250	P252	G253	R254	V255	E256	G257	N258	P259	V260	F261	T262	F263	L264	D270	
P94	Q95	K96	T97	T98	G99	V100	V101	S103	A104	Y114	N117	L118	V119	H123	N127	V130	I134	A135	Q136	K137	G138	Y139	G140	E141	R142	V143	V149	Y150	Q154	L155	V156	P157	V168	G169	D170	D171	Q172	L173	P174	M175	Q178	R184	R185	L189	F196						
A21	R22	R23	R24	V25	L26	T27	R30	H36	L37	G38	H39	L40	S43	L44	Q45	M46	R47	V48	R49	L50	Q51	D52	E53	A54	E55	L56	F57	V58	L59	L60	A61	D62	V63	Q64	L66	T67	D68	H69	F70	E74	Q75	V76	R77	V80	L81	A84	L85	D86	Y87	L92	D93

- Chain B:

Category	Count
A304	1
P305	1
I306	1
R307	1
R310	1
E314	1
P317	1
V320	1
L321	1
F322	1
V323	1
V324	1
T325	1
R330	1
E333	1
Q337	1
T338	1
Q341	1
V342	1
R343	1
L348	1
H351	1
R235	1
K236	1
V237	1
K240	1
V241	1
T242	1
H246	1
L247	1
R248	1
A249	1
S250	1
T251	1
F252	1
G253	1
R254	1
V255	1
E256	1
P259	1
V260	1
F261	1
T262	1
F263	1
F267	1
D268	1
P269	1
D270	1
R273	1
V274	1
Q275	1
A276	1
L277	1
K278	1
V281	1
R282	1
A283	1
L286	1
G287	1
D288	1
V289	1
K290	1
V291	1
K292	1
K293	1
R294	1
L295	1
T296	1
D297	1
V298	1
L299	1
K300	1
G301	1
V302	1
L303	1
L165	1
V168	1
G169	1
Q172	1
L173	1
P174	1
M175	1
L176	1
E177	1
Q178	1
T179	1
V183	1
R184	1
R185	1
A191	1
P192	1
V193	1
E196	1
A199	1
Q200	1
L201	1
S202	1
R203	1
V204	1
P205	1
R206	1
L207	1
P208	1
G209	1
L210	1
G211	1
G212	1
Q213	1
A214	1
K215	1
M216	1
S217	1
K218	1
S219	1
L220	1
G221	1
N222	1
A223	1
I224	1
A225	1
L226	1
S229	1
A230	1
D231	1
E232	1
V233	1
A234	1
L188	1
L92	1
D93	1
P94	1
G95	1
K96	1
T97	1
T98	1
C99	1
Q102	1
S103	1
A104	1
V105	1
L108	1
A109	1
E110	1
L111	1
T112	1
V113	1
L116	1
N117	1
L118	1
V119	1
T120	1
V121	1
S122	1
H123	1
L124	1
R125	1
Q126	1
N127	1
P128	1
T129	1
V130	1
E133	1
I134	1
K137	1
G138	1
V139	1
R142	1
V143	1
F148	1
V149	1
A150	1
P151	1
V152	1
S153	1
A156	1
D157	1
A160	1
A21	1
R22	1
P23	1
R24	1
V25	1
L26	1
T27	1
R30	1
G33	1
A34	1
L35	1
H36	1
L37	1
G38	1
H39	1
L40	1
A41	1
L44	1
R47	1
V48	1
R49	1
L50	1
Q51	1
D52	1
E53	1
A54	1
E55	1
L56	1
F57	1
V58	1
L59	1
L60	1
A61	

- Chain C:  52% 37% 10%

P271	A272	R273	A276	L277	K278	D279	Q280	L286	G287	D288	V289	R290	V291	K292	R293	H294	L295	V298	L299	N300	L303	A304	R307	T308	R309	R310	A311	E314	R315	L321	T325	E326	G327	T328	A329	R330	G331	R332	Q337	T338	L339	G340	Q341	R343	R347	H351					
L173	P174	M175	L176	E177	Q178	T179	R180	R185	L189	V193	E196	P197	Q200	L201	S202	R203	V204	P205	L210	M216	A223	I224	S229	A230	D231	E232	V233	A234	R235	M238	D243	P244	L247	R248	R254	V255	E256	G257	N258	P259	V260	F267	D268	P269	D270						
K96	T97	T98	C99	V100	L26	Q102	S103	A104	V105	P106	E107	L108	A109	E110	L111	T112	V113	L116	N117	T120	H123	N127	P128	T129	V130	K131	A132	E133	Q136	K137	P144	A145	G146	V149	Y150	P151	V152	S153	Q154	A155	A156	D157	I158	L165	V166	P167	V168	G169	D170	D171	Q172
A21	R22	P23	R24	V25	L26	T27	R30	P31	T32	L35	H36	L37	L40	A41	G42	S43	L44	Q45	N46	R47	Q51	E55	L56	F57	V58	L59	L60	V63	Q64	A65	D68	H69	F70	D71	E74	Q75	V76	R77	E78	N79	V80	L81	A82	V83	A84	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, α , β , γ	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 ²)	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%)	11	11
1	B	329/331 (99%)	299 (91%)	21 (6%)	9 (3%)	5	4
1	C	329/331 (99%)	309 (94%)	17 (5%)	3 (1%)	19	22
All	All	987/993 (99%)	913 (92%)	57 (6%)	17 (2%)	10	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%)	5	6
1	C	260/264 (98%)	226 (87%)	34 (13%)	4	4
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	0.57	0	11,22,22	0.97	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.