wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:22 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

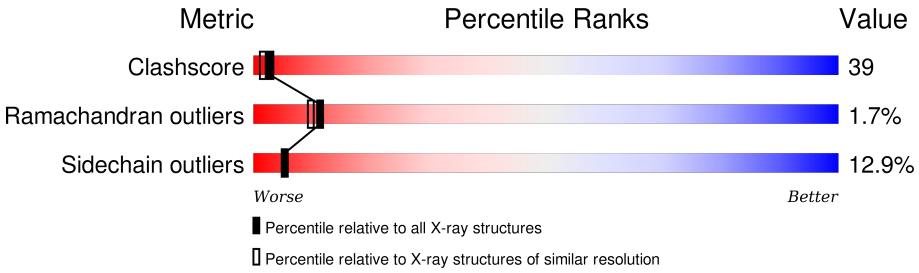
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 <=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	52% 41% 7%
1	B	331	41% 51% 8%
1	C	331	52% 37% 10%

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

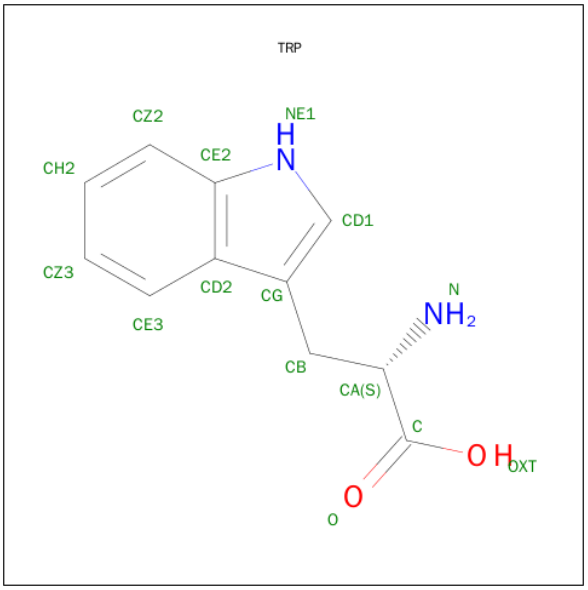
There are 3 unique types of molecules in this entry. The entry contains 8788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O 382 382	0	0
3	B	395	Total O 395 395	0	0
3	C	414	Total O 414 414	0	0

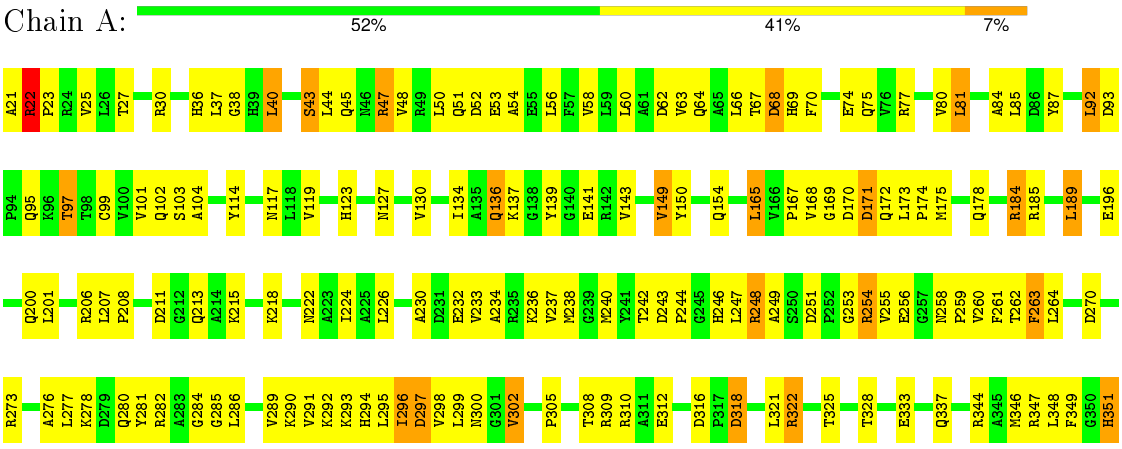
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

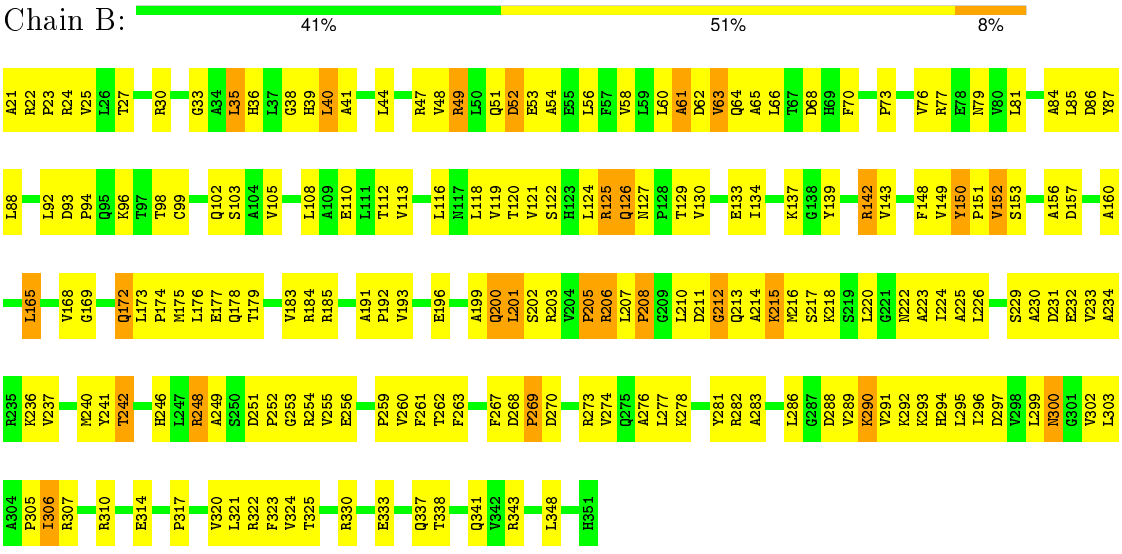
• Molecule 1: Tryptophanyl-tRNA synthetase II

Chain A:



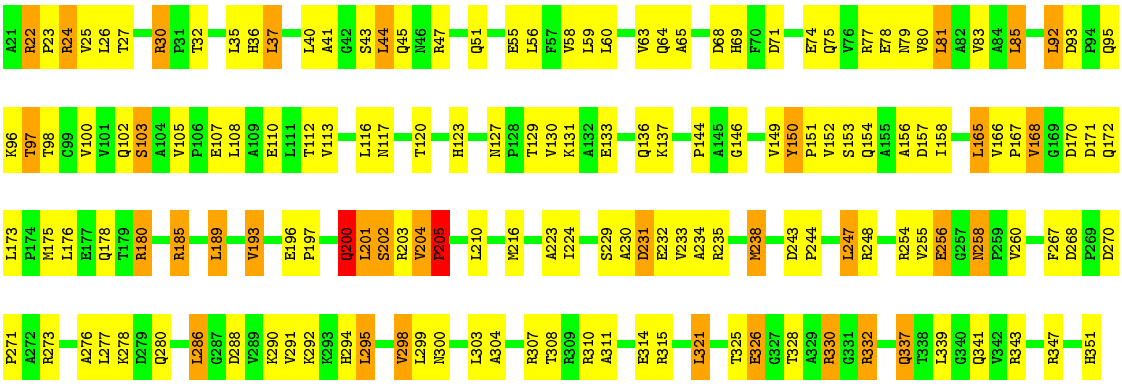
• Molecule 1: Tryptophanyl-tRNA synthetase II

Chain B:



• Molecule 1: Tryptophanyl-tRNA synthetase II

Chain C:


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
K96 T97 T98 C99 V100 V101 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
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
P271 A272 R273 A276 I277 K278 D279 Q280 L286 G287 D288 V289 K290 V291 K292 K293 H294 L295 V298 L299 N300 L303 A304 R307 T308 R309 R310 A311 E314 R315 I321 T325 E326 G327 T328 A329 R330 G331 R332 Q337 T338 L339 G340 Q341 V342 R343 R347 H351

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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	0.36	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(^{o})	Ideal(^{o})
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

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:HE21	1:C:337:GLN:HA	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%)	13	12
1	B	329/331 (99%)	299 (91%)	21 (6%)	9 (3%)	6	4
1	C	329/331 (99%)	309 (94%)	17 (5%)	3 (1%)	21	24
All	All	987/993 (99%)	913 (92%)	57 (6%)	17 (2%)	11	10

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%)	5	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	-	12,16,16	0.59	0	7,22,22	1.11	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.