



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 06:57 AM EDT

PDB ID : 3LXU  
Title : Crystal Structure of Tripeptidyl Peptidase 2 (TPP II)  
Authors : Chuang, C.K.  
Deposited on : 2010-02-25  
Resolution : 3.14 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

<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

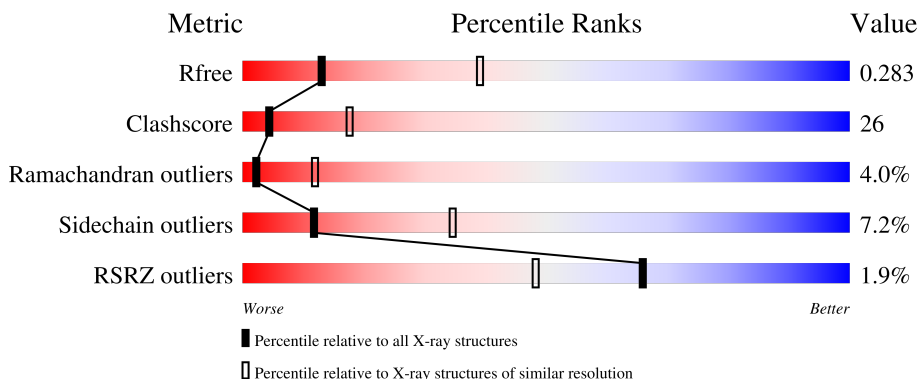
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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))
$R_{free}$	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

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  $\geq 3$ , 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	X	1354	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9464 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.

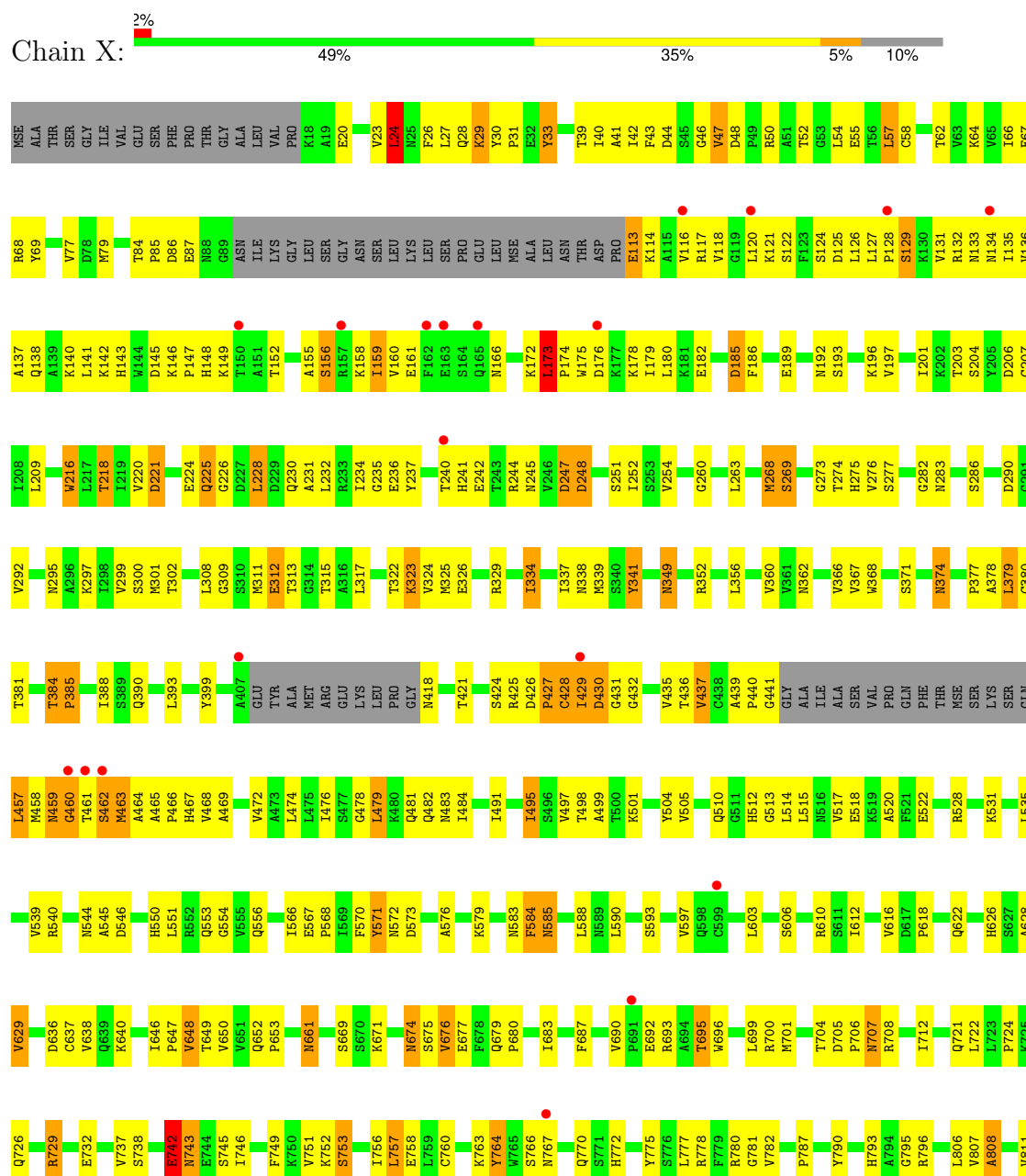
- Molecule 1 is a protein called Tripeptidyl-peptidase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	1217	Total	C	N	O	S	Se	0	0	0
			9464	5958	1648	1816	17	25			

### 3 Residue-property plots

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: Tripeptidyl-peptidase 2



E1322	L1323	I1326	L1330	G1331	H1332	E1333	H1334	I1335	V1338	I1339	M1340	R1341	M1342	M1343	I1344	T1345	A1346	F1347	P1348	R1352	L1353	F1354																															
L1244	S1245	K1246	K1247	G1248	I1249	A1250	V1251	L1254	L1257	C1260	I1261	K1262	D1263	S1264	L1265	A1266	E1267	I1268	N1269	E1270	L1271	Y1272	T1273	E1274	K1277	A1281	N1282	K1285	A1286	I1287	Q1288	F1289	W1292	H1297	G1298	H1299	Y1300	M1303	Y1304	K1305	Y1306	V1307	V1308	K1309	L1310	I1311	H1319	F1320	V1321				
L1160	P1161	L1162	T1163	T1170	S1171	P1172	P1173	E1174	A1175	S1178	Q1186	V1189	R1190	S1191	A1192	I1196	V1197	K1198	L1199	A1200	D1201	K1202	V1203	I1204	Q1205	E1206	T1207	D1208	A1211	L1212	Y1216	G1217	L1218	A1227	K1228	I1229	K1230	T1231	N1232	M1233	D1234	K1235	Q1236	K1237	N1238	T1239	L1240	I1241	E1242	A1243			
ALA	ALA	GLY	ASP	GLY	ILE	SER	SER	VAL	GLN	ASN	ASP	PRO	PRO	VAL	PRO	ASP	SER	SER	GLY	PRO	ALA	SER	LYS	G1099	K1100	A1101	N1102	D1105	R1111	D1112	F1113	Q1114	C1115	S1116	Q1117	I1118	V1119	K1120	C1121	E1122	L1123	E1124	M1125	I1129	L1145	L1146	L1147	I1151	E1152	S1153	N1154	Q1155	L1156
Q812	P813	Q814	L815	Q816	L817	K818	N819	A820	E821	V822	V823	L824	K825	P826	T827	E828	S832	I841	P842	D843	G844	R845	Y848	Q849	N850	L851	L852	A853	F854	D863	I866	Y867	I870	F871	N872	D873	L874	L875	Y876	E877	A878	E881	S882	Q883	M884	W885	M886	L887	F888	D889	A890	N891	
K892	A893	T897	Q898	K908	Y914	T915	T916	R917	L918	R921	H922	R925	L928	E929	K930	I931	A934	K941	L942	L948	Q956	Q961	R962	K963	L969	R970	L971	I978	Q983	T987	A993	Q994	C995	L998	V1003	F1004	P1005	Q1006	D1007	E1008	A1009	V1099											
G1010	R1011	R1012	V1013	A1014	F1018	T1019	Y1020	I1021	L1022	E1026	LYS	LYS	SER	HIS	THR	ASN	GLY	SER	SER	ASN	GLY	SER	SER	ALA	ALA	GLY	SER	THR	ALA	ALA	VAL	THR	THR	ALA	ASP	PRO	ALA	PRO	ALA	ALA	THR	THR	PRO	GLN	ALA	ALA	THR	THR	VAL	THR	THR	ASN	PRO

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.37Å 126.37Å 213.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.14 50.00 – 3.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.14) 99.2 (50.00-3.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.241 , 0.293 0.240 , 0.283	Depositor DCC
$R_{free}$ test set	1548 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	X	0.22	0/9621	0.41	0/12999

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	X	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	384	THR	Peptide
1	X	462	SER	Peptide

### 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	X	9464	0	9342	492	0
All	All	9464	0	9342	492	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 26.

The worst 5 of 492 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:X:429:ILE:CD1	1:X:722:LEU:HD13	1.87	1.03
1:X:457:LEU:HD13	1:X:458:MSE:H	1.30	0.97
1:X:729:ARG:HH11	1:X:729:ARG:HG2	1.31	0.94
1:X:793:HIS:HD2	1:X:795:GLY:H	1.10	0.90
1:X:116:VAL:HG22	1:X:117:ARG:H	1.35	0.88

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	X	1207/1354 (89%)	1001 (83%)	158 (13%)	48 (4%)	<b>2</b> <b>12</b>

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	129	SER
1	X	225	GLN
1	X	385	PRO
1	X	429	ILE
1	X	571	TYR

### 5.3.2 Protein sidechains [i](#)

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	X	1027/1116 (92%)	953 (93%)	74 (7%)	12 34

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	851	LEU
1	X	1265	LEU
1	X	897	THR
1	X	1118	ILE
1	X	349	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	812	GLN
1	X	1117	GLN
1	X	849	GLN
1	X	956	GLN
1	X	1142	GLN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	X	1192/1354 (88%)	-0.04	23 (1%)	66 48	53, 86, 137, 179	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	150	THR	3.8
1	X	462	SER	3.2
1	X	767	ASN	3.2
1	X	407	ALA	3.1
1	X	134	ASN	2.9

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.