



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:44 AM UTC

PDB ID : 3LXU / pdb_00003lxu
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

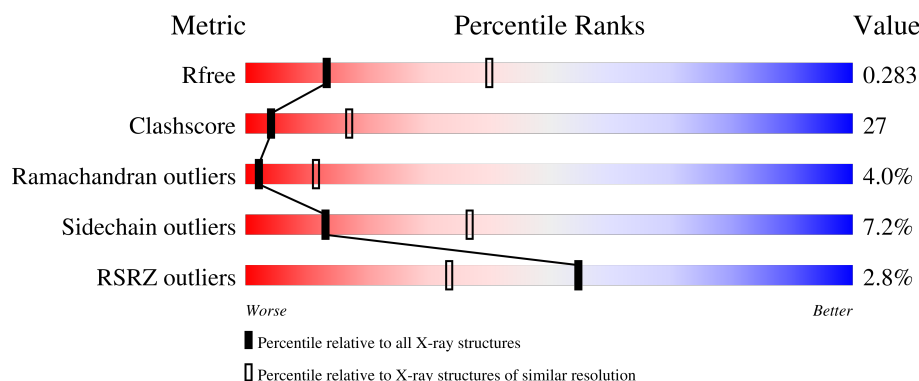
1 Overall quality at a glance

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}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (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 ≥ 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 [i](#)

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.

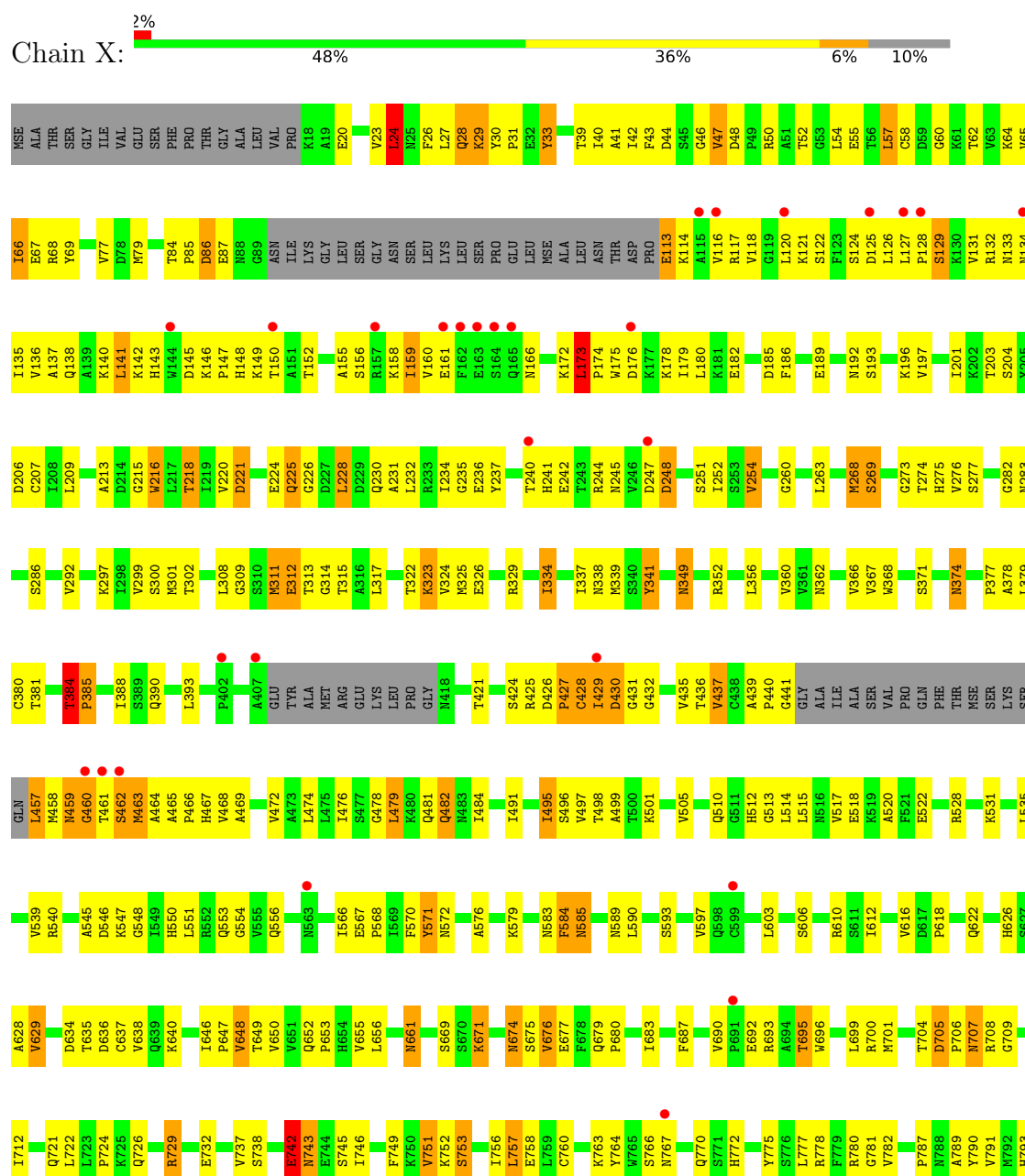
- Molecule 1 is a protein called Tripeptidyl-peptidase 2.

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



Y1304	M1232	I1129	ALA	C995	Q883	A794
K1305	M1233	L1145	THR	L998	M884	G795
Y1306	D1234	L1146	PRO	V1003	W885	R796
V1307	K1235	L1147	GLN	F1004	M886	L806
V1308	Q1236	L1147	ALA	F1005	F887	V807
K1309	K1237	I1151	ALA	P1006	D888	A808
L1310	M1238	E1152	THR	Q1006	D889	
I1311	T1239	S1153	SER	D1007	A890	V811
	L1240	S1153	VAL	E1008	N891	
H1319	T1241	N1154	THR	E1009	K892	Q812
F1320	E1242	Q1155	ASN	V1009	A893	P813
V1321	A1243	L1156	PRO	G1010	L894	Q814
E1322	I1244		ALA	R1011	L815	L815
L1323	S1245	L1160	ALA	R1012	Q816	Q816
	K1246	P1161	GLY	A1013	L817	L817
I1326	L1247	L1162	ASP	A1014	K818	K818
	G1248	T1163	GLY		N819	N819
L1330	I1249		ILE	F1018	A820	A820
G1331	A1250	T1170	SER	T1019	P821	P821
H1332	V1251	S1171	VAL	Y1020	V822	V822
E1333		P1172	GLN	I1021	V823	V823
H1334	L1254	P1173	ASN	I1022	R917	L824
I1335		E1174	ASP	N1023	K825	K825
	L1257	A1175	PRO	E1026	P826	P826
V1338			PRO	LYS	T827	T827
I1339	G1260	S1178	VAL	LYS	E828	E828
N1340	I1261		ASP	LYS	S832	S832
R1341	K1262	Q1186	SER	K924		
M1342	D1263		SER	R925		
M1343	S1264	V1189	GLY		T841	T841
I1344	L1265	R1190	SER	ASN	P842	P842
T1345	A1266	S1191	PRO	GLY	D843	D843
A1346	E1267	A1192	ALA	SER	G844	G844
F1347	T1268		SER	ASN	R845	R845
P1348	I1269	I1196	PRO	ASN		
	E1270	V1197	LYS	GLY	Y848	Y848
	I1271	K1198	SER	SER	Q849	Q849
R1352	Y1272	L1199	LYS	SER	N850	N850
L1353	T1273	A1200	G1099	ALA	L851	L851
F1354	E1274	D1201	K1100	ALA	L852	L852
		K1202	A1101	GLY	A853	A853
		V1203	N1102	SER	F854	F854
	K1277			THR		
		Q1205	D1105	ALA	D863	D863
	N1282	E1206	R1111	THR	I866	I866
K1285		T1207	D1112	ALA	Y867	Y867
A1286		D1208	F1113	ALA		
I1287			Q1114	ALA	I870	I870
Q1288		A1211	C1115	VAL	P871	P871
F1289		L1212	S1116	THR	N872	N872
		Y1216	Q1117	THR	D873	D873
		G1217	V1119	ALA	L874	L874
		L1218	K1120	ASN	L875	L875
			C1121	ALA	Y876	Y876
		A1227	F1122	LYS	E877	E877
		K1228	L1123	PRO	A878	A878
		I1229	E1124	LYS		
		K1230	M1125	ALA	E881	E881
		T1231	PRO	PRO	Q894	Q894

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.28	0/9621	0.74	12/12999 (0.1%)

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.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	X	1172	PRO	N-CA-C	5.88	117.88	110.70
1	X	1170	THR	CB-CA-C	-5.63	110.06	116.54
1	X	705	ASP	CA-C-N	5.49	126.70	119.84
1	X	705	ASP	C-N-CA	5.49	126.70	119.84
1	X	384	THR	CA-C-N	-5.41	114.81	120.38

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	514	0
All	All	9464	0	9342	514	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 27.

The worst 5 of 514 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%)	2 11

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

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Mol	Chain	Res	Type
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%)	13 37

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

Mol	Chain	Res	Type
1	X	930	LYS
1	X	1265	LEU
1	X	1019	THR
1	X	1203	VAL
1	X	349	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	770	GLN
1	X	857	ASN
1	X	1269	ASN
1	X	772	HIS
1	X	793	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 95th 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 ²)	Q<0.9
1	X	1192/1354 (88%)	0.10	33 (2%) 55 33	53, 86, 137, 179	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	150	THR	4.0
1	X	462	SER	3.4
1	X	767	ASN	3.3
1	X	407	ALA	3.2
1	X	134	ASN	3.0

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 oligosaccharides 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.