



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:59 am BST

PDB ID : 1AZW
Title : PROLINE IMINOPEPTIDASE FROM XANTHOMONAS CAMPESTRIS
PV. CITRI
Authors : Medrano, F.J.; Alonso, J.; Garcia, J.L.; Romero, A.; Bode, W.; Gomis-Ruth,
F.X.
Deposited on : 1997-11-22
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

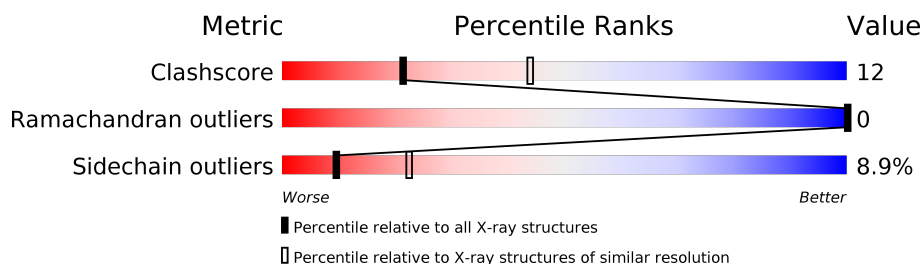
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5227 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 PROLINE IMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	29	0	0
			2514	1599	452	456	7			
1	B	313	Total	C	N	O	S	26	0	0
			2514	1599	452	456	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLN	ALA	CONFLICT	UNP P52279
A	122	THR	ASP	CONFLICT	UNP P52279
A	123	HIS	PRO	CONFLICT	UNP P52279
A	124	PRO	SER	CONFLICT	UNP P52279
A	125	GLN	ALA	CONFLICT	UNP P52279
A	126	GLN	ALA	CONFLICT	UNP P52279
A	127	VAL	GLY	CONFLICT	UNP P52279
A	128	THR	HIS	CONFLICT	UNP P52279
A	129	GLU	GLN	CONFLICT	UNP P52279
B	121	GLN	ALA	CONFLICT	UNP P52279
B	122	THR	ASP	CONFLICT	UNP P52279
B	123	HIS	PRO	CONFLICT	UNP P52279
B	124	PRO	SER	CONFLICT	UNP P52279
B	125	GLN	ALA	CONFLICT	UNP P52279
B	126	GLN	ALA	CONFLICT	UNP P52279
B	127	VAL	GLY	CONFLICT	UNP P52279
B	128	THR	HIS	CONFLICT	UNP P52279
B	129	GLU	GLN	CONFLICT	UNP P52279

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		

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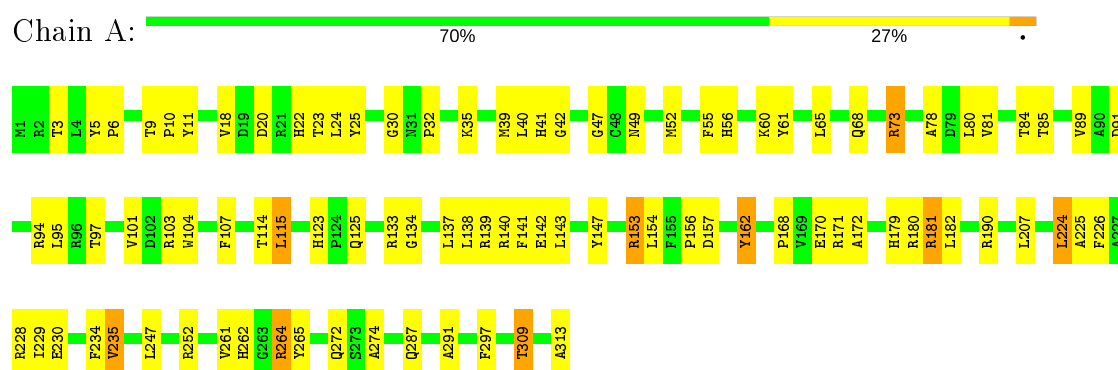
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	108	Total 108	O 108	0	0

3 Residue-property plots

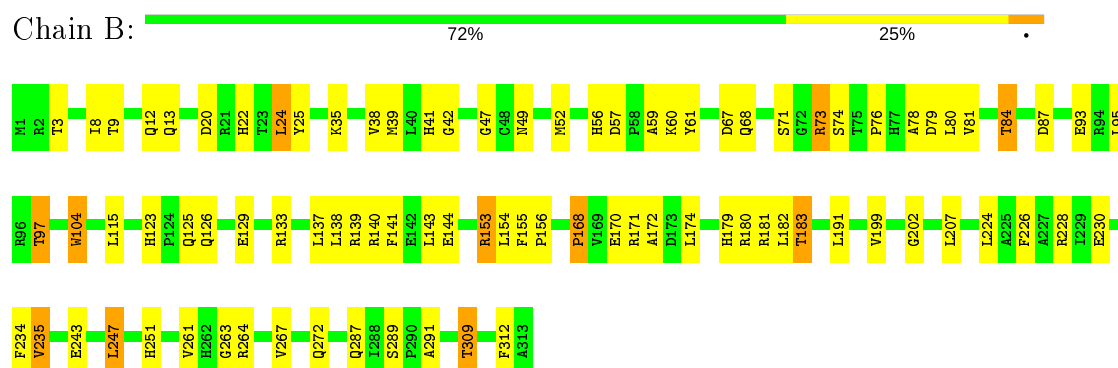
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: PROLINE IMINOPEPTIDASE



• Molecule 1: PROLINE IMINOPEPTIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.20 Å 167.80 Å 85.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.5 (7.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.192 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5227	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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	0.53	0/2591	0.74	0/3525
1	B	0.49	0/2591	0.69	0/3525
All	All	0.51	0/5182	0.71	0/7050

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain

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	2514	0	2386	63	0
1	B	2514	0	2386	58	0
2	A	91	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	108	0	0	3	0
All	All	5227	0	4772	116	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 12.

All (116) 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:A:49:ASN:OD1	1:A:52:MET:HG3	1.79	0.82
1:B:138:LEU:HD23	1:B:143:LEU:HD21	1.68	0.75
1:B:153:ARG:HG3	1:B:153:ARG:HH11	1.54	0.72
1:A:168:PRO:HA	1:A:171:ARG:HD3	1.73	0.71
1:B:41:HIS:HE1	1:B:68:GLN:H	1.38	0.70
1:A:262:HIS:ND1	1:A:274:ALA:HB2	2.09	0.68
1:A:172:ALA:CB	1:B:140:ARG:HD2	2.24	0.67
1:A:41:HIS:HE1	1:A:68:GLN:H	1.42	0.66
1:A:226:PHE:O	1:A:230:GLU:HB2	1.96	0.65
1:A:56:HIS:HA	1:A:309:THR:HG21	1.79	0.64
1:B:139:ARG:NH1	1:B:141:PHE:CZ	2.66	0.64
1:B:41:HIS:HD2	1:B:42:GLY:O	1.80	0.64
1:A:123:HIS:HE1	2:A:324:HOH:O	1.83	0.62
1:B:139:ARG:NH1	1:B:141:PHE:CE2	2.68	0.61
1:A:252:ARG:HD3	2:A:352:HOH:O	2.02	0.60
1:B:138:LEU:CD2	1:B:143:LEU:HD21	2.32	0.60
1:B:56:HIS:HA	1:B:309:THR:HG21	1.84	0.60
1:B:68:GLN:O	1:B:71:SER:HB3	2.01	0.60
1:B:140:ARG:O	1:B:140:ARG:HG3	2.02	0.59
1:B:76:PRO:HG2	1:B:79:ASP:HB2	1.85	0.59
1:A:85:THR:O	1:A:89:VAL:HG23	2.03	0.59
1:B:25:TYR:CG	1:B:73:ARG:HG3	2.37	0.59
1:B:35:LYS:HD3	1:B:61:TYR:HE1	1.69	0.58
1:A:154:LEU:C	1:A:156:PRO:HD3	2.24	0.58
1:B:140:ARG:HD3	1:B:144:GLU:OE2	2.03	0.58
1:B:35:LYS:HD3	1:B:61:TYR:CE1	2.38	0.58
1:B:84:THR:HG21	2:B:332:HOH:O	2.03	0.58
1:B:226:PHE:O	1:B:230:GLU:HB2	2.03	0.57
1:A:35:LYS:HD3	1:A:61:TYR:CE1	2.39	0.57
1:A:230:GLU:HG2	1:A:234:PHE:CE2	2.40	0.56
1:B:171:ARG:HG3	1:B:174:LEU:HD21	1.87	0.56
1:A:264:ARG:HG2	1:A:265:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD12	1:A:228:ARG:HD2	1.88	0.56
1:A:39:MET:CE	1:A:107:PHE:HB3	2.35	0.56
1:A:114:THR:HG21	1:A:138:LEU:HD12	1.88	0.56
1:B:170:GLU:HA	2:B:322:HOH:O	2.06	0.55
1:B:154:LEU:C	1:B:156:PRO:HD3	2.28	0.55
1:A:9:THR:HG22	1:A:10:PRO:HD2	1.89	0.54
1:B:8:ILE:HG12	1:B:9:THR:N	2.23	0.54
1:B:57:ASP:OD2	1:B:59:ALA:HB3	2.08	0.54
1:A:39:MET:HE1	1:A:107:PHE:HB3	1.90	0.53
1:A:41:HIS:CE1	1:A:68:GLN:H	2.26	0.53
1:B:179:HIS:O	1:B:183:THR:HB	2.07	0.53
1:A:103:ARG:HD2	1:A:125:GLN:O	2.09	0.52
1:A:30:GLY:O	1:A:32:PRO:HD3	2.10	0.52
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.73	0.52
1:B:207:LEU:HD22	1:B:291:ALA:O	2.09	0.52
1:A:55:PHE:O	1:A:309:THR:HG21	2.08	0.52
1:B:123:HIS:HB3	1:B:126:GLN:HG2	1.92	0.51
1:A:9:THR:CG2	1:A:10:PRO:HD2	2.41	0.51
1:B:139:ARG:HA	1:B:243:GLU:HG3	1.92	0.51
1:A:170:GLU:CD	1:A:181:ARG:HH22	2.15	0.50
1:A:140:ARG:HD2	1:B:172:ALA:CB	2.42	0.50
1:A:139:ARG:NH1	1:A:141:PHE:CZ	2.81	0.49
1:A:139:ARG:HG3	1:A:142:GLU:OE2	2.13	0.49
1:A:133:ARG:HD2	1:A:134:GLY:N	2.28	0.48
1:B:168:PRO:O	1:B:171:ARG:HB2	2.14	0.48
1:A:235:VAL:HG13	1:B:180:ARG:CZ	2.44	0.48
1:B:129:GLU:HG2	1:B:312:PHE:CD1	2.49	0.48
1:B:22:HIS:HE1	1:B:81:VAL:O	1.96	0.48
1:B:191:LEU:HD12	1:B:224:LEU:CD2	2.44	0.47
1:A:41:HIS:HD2	1:A:42:GLY:O	1.98	0.47
1:B:78:ALA:O	1:B:228:ARG:NH1	2.47	0.47
1:A:25:TYR:CG	1:A:73:ARG:HG3	2.50	0.47
1:B:93:GLU:O	1:B:97:THR:HB	2.14	0.47
1:B:251:HIS:HE1	2:B:384:HOH:O	1.98	0.47
1:A:39:MET:HG3	1:A:65:LEU:HG	1.97	0.47
1:A:180:ARG:CZ	1:B:235:VAL:HG13	2.45	0.47
1:A:41:HIS:CE1	1:A:47:GLY:HA2	2.50	0.47
1:A:138:LEU:HD23	1:A:143:LEU:HD21	1.96	0.46
1:A:190:ARG:HD3	1:A:224:LEU:HD11	1.97	0.46
1:B:76:PRO:HG2	1:B:79:ASP:CB	2.46	0.46
1:A:39:MET:HE1	1:A:107:PHE:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:O	1:A:228:ARG:NH1	2.49	0.46
1:A:22:HIS:HE1	1:A:81:VAL:O	1.99	0.45
1:A:123:HIS:CD2	2:A:387:HOH:O	2.69	0.45
1:A:91:ASP:OD1	1:A:94:ARG:NH1	2.50	0.45
1:B:140:ARG:HG3	1:B:144:GLU:HG3	1.99	0.45
1:A:39:MET:HE1	1:A:107:PHE:CG	2.52	0.45
1:A:68:GLN:NE2	1:A:115:LEU:HD12	2.32	0.45
1:B:234:PHE:N	1:B:234:PHE:CD1	2.82	0.45
1:A:5:TYR:HB3	1:A:6:PRO:HD2	1.98	0.44
1:B:24:LEU:HA	1:B:74:SER:OG	2.18	0.44
1:A:157:ASP:N	1:A:157:ASP:OD1	2.51	0.44
1:A:230:GLU:HG2	1:A:234:PHE:CZ	2.51	0.44
1:A:207:LEU:HD22	1:A:291:ALA:O	2.18	0.44
1:B:49:ASN:OD1	1:B:52:MET:HG3	2.17	0.44
1:A:147:TYR:HB3	1:A:162:TYR:OH	2.17	0.43
1:A:123:HIS:CE1	2:A:324:HOH:O	2.66	0.43
1:B:41:HIS:CD2	1:B:47:GLY:H	2.35	0.43
1:A:39:MET:HE1	1:A:56:HIS:HE1	1.83	0.43
1:A:224:LEU:CD1	1:A:228:ARG:HD2	2.48	0.43
1:B:133:ARG:HA	1:B:261:VAL:O	2.18	0.43
1:B:139:ARG:HH21	1:B:247:LEU:HD21	1.84	0.43
1:B:84:THR:HB	1:B:87:ASP:OD2	2.19	0.42
1:A:225:ALA:O	1:A:229:ILE:HG13	2.19	0.42
1:A:25:TYR:CD1	1:A:25:TYR:C	2.92	0.42
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.72	0.42
1:B:155:PHE:CE2	1:B:267:VAL:HG21	2.53	0.42
1:A:55:PHE:CZ	1:A:297:PHE:CE1	3.07	0.42
1:A:133:ARG:HA	1:A:261:VAL:O	2.19	0.42
1:A:40:LEU:HD13	1:A:115:LEU:HB3	2.02	0.42
1:A:11:TYR:CE2	1:A:32:PRO:HG3	2.55	0.41
1:B:199:VAL:O	1:B:202:GLY:N	2.52	0.41
1:A:179:HIS:HE1	2:A:329:HOH:O	2.03	0.41
1:B:8:ILE:HG12	1:B:9:THR:H	1.85	0.41
1:A:18:VAL:HG11	1:A:24:LEU:HD22	2.03	0.41
1:A:172:ALA:HB1	1:B:140:ARG:HD2	2.02	0.41
1:B:263:GLY:HA2	1:B:289:SER:HB2	2.03	0.41
1:A:60:LYS:HE2	1:A:313:ALA:HB1	2.03	0.40
1:B:57:ASP:OD2	1:B:60:LYS:HD3	2.21	0.40
1:B:12:GLN:NE2	1:B:13:GLN:O	2.54	0.40
1:B:38:VAL:HB	1:B:104:TRP:CZ3	2.56	0.40
1:B:67:ASP:HB3	1:B:71:SER:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:O	1:B:156:PRO:HD3	2.22	0.40
1:B:155:PHE:HE2	1:B:267:VAL:HG21	1.87	0.40

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	311/313 (99%)	294 (94%)	17 (6%)	0	100	100
1	B	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
All	All	622/626 (99%)	587 (94%)	35 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	A	258/258 (100%)	236 (92%)	22 (8%)	10	24
1	B	258/258 (100%)	234 (91%)	24 (9%)	9	21
All	All	516/516 (100%)	470 (91%)	46 (9%)	9	22

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	20	ASP
1	A	23	THR
1	A	73	ARG
1	A	80	LEU
1	A	84	THR
1	A	95	LEU
1	A	97	THR
1	A	101	VAL
1	A	104	TRP
1	A	115	LEU
1	A	137	LEU
1	A	153	ARG
1	A	181	ARG
1	A	182	LEU
1	A	224	LEU
1	A	235	VAL
1	A	247	LEU
1	A	264	ARG
1	A	272	GLN
1	A	287	GLN
1	A	309	THR
1	B	3	THR
1	B	20	ASP
1	B	24	LEU
1	B	39	MET
1	B	73	ARG
1	B	80	LEU
1	B	84	THR
1	B	95	LEU
1	B	97	THR
1	B	104	TRP
1	B	115	LEU
1	B	125	GLN
1	B	137	LEU
1	B	153	ARG
1	B	168	PRO
1	B	181	ARG
1	B	182	LEU
1	B	183	THR
1	B	235	VAL
1	B	247	LEU
1	B	264	ARG

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Mol	Chain	Res	Type
1	B	272	GLN
1	B	287	GLN
1	B	309	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	121	GLN
1	A	123	HIS
1	A	126	GLN
1	A	272	GLN
1	A	285	GLN
1	A	287	GLN
1	B	22	HIS
1	B	41	HIS
1	B	121	GLN
1	B	164	ASN
1	B	179	HIS
1	B	217	HIS
1	B	251	HIS
1	B	285	GLN
1	B	287	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

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.