



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:12 PM GMT

PDB ID : 4BTA
Title : CRYSTAL STRUCTURE OF THE PEPTIDE(PRO-PRO-GLY)₃ BOUND
COMPLEX OF N- TERMINAL DOMAIN AND PEPTIDE SUBSTRATE
BINDING DOMAIN OF PROLYL-4 HYDROXYLASE (RESIDUES 1-244)
TYPE I FROM HUMAN
Authors : Anantharajan, J.; Koski, M.K.; Pekkala, M.; Wierenga, R.K.
Deposited on : 2013-06-14
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

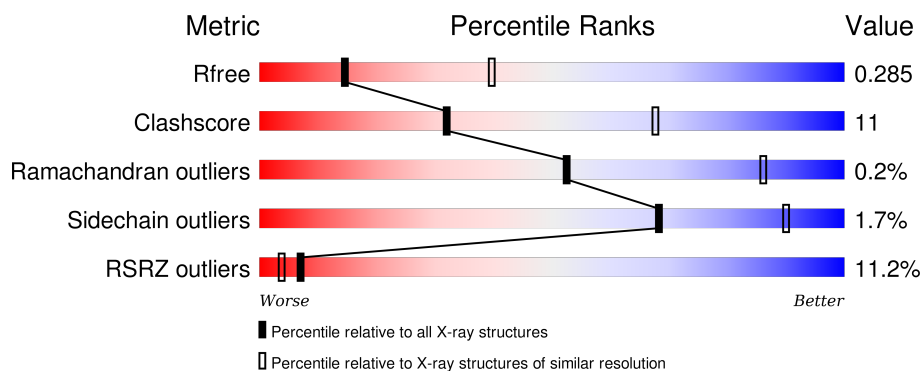
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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.

Mol	Chain	Length	Quality of chain
1	A	251	
1	B	251	
2	C	9	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3692 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 PROLYL 4-HYDROXYLASE SUBUNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1919	1222	311	380	6			
1	B	211	Total	C	N	O	S	0	0	0
			1718	1093	276	344	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P13674
A	-5	HIS	-	EXPRESSION TAG	UNP P13674
A	-4	HIS	-	EXPRESSION TAG	UNP P13674
A	-3	HIS	-	EXPRESSION TAG	UNP P13674
A	-2	HIS	-	EXPRESSION TAG	UNP P13674
A	-1	HIS	-	EXPRESSION TAG	UNP P13674
A	0	HIS	-	EXPRESSION TAG	UNP P13674
B	-6	MET	-	EXPRESSION TAG	UNP P13674
B	-5	HIS	-	EXPRESSION TAG	UNP P13674
B	-4	HIS	-	EXPRESSION TAG	UNP P13674
B	-3	HIS	-	EXPRESSION TAG	UNP P13674
B	-2	HIS	-	EXPRESSION TAG	UNP P13674
B	-1	HIS	-	EXPRESSION TAG	UNP P13674
B	0	HIS	-	EXPRESSION TAG	UNP P13674

- Molecule 2 is a protein called PROLINE RICH PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			55	36	9	10			

- Molecule 1: PROLYL 4-HYDROXYLASE SUBUNIT ALPHA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	234.66 Å 47.85 Å 60.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.80 – 2.95 33.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.80-2.95) 99.6 (33.80-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.227 , 0.279 0.231 , 0.285	Depositor DCC
R_{free} test set	747 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 14996 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3692	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.67	0/1954	0.93	3/2637 (0.1%)
1	B	0.51	0/1746	0.79	0/2357
2	C	0.47	0/60	1.03	0/83
All	All	0.60	0/3760	0.87	3/5077 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	LEU	CA-CB-CG	7.77	133.18	115.30
1	A	120	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	A	124	TYR	CA-CB-CG	5.91	124.62	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	PRO	Peptide

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	1919	0	1895	44	0
1	B	1718	0	1692	40	0
2	C	55	0	53	6	0
All	All	3692	0	3640	78	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 11.

All (78) 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:101:ARG:NH2	1:B:82:GLU:OE1	1.98	0.96
1:A:60:PHE:O	1:A:66:ASN:ND2	2.08	0.86
1:A:82:GLU:OE1	1:B:101:ARG:NH2	2.13	0.80
1:B:192:ASP:OD1	1:B:193:TYR:N	2.19	0.76
1:B:157:ALA:HB1	1:B:162:ASP:HB3	1.68	0.75
1:A:211:THR:HG21	1:A:231:PHE:HE2	1.51	0.72
1:A:29:ILE:HD11	1:B:39:ILE:HG22	1.72	0.71
1:A:152:GLU:HG3	1:B:72:LYS:HZ2	1.57	0.70
1:B:187:LYS:HE2	1:B:217:LEU:HD22	1.79	0.65
1:A:204:LEU:HD11	1:A:234:ILE:HD11	1.82	0.62
1:A:69:LYS:NZ	1:B:149:ASP:OD2	2.19	0.60
1:B:99:ILE:O	1:B:102:GLN:HG3	2.01	0.60
1:B:152:GLU:O	1:B:156:VAL:HG13	2.02	0.59
1:B:213:LYS:O	1:B:217:LEU:HD12	2.04	0.57
1:A:152:GLU:HG3	1:B:72:LYS:NZ	2.20	0.57
1:B:105:PRO:HB2	1:B:109:ASP:HB2	1.87	0.56
1:B:153:LEU:O	1:B:156:VAL:HG22	2.07	0.55
1:A:129:ASP:O	1:A:133:LYS:HG2	2.07	0.55
1:B:40:LYS:O	1:B:44:GLU:HG3	2.07	0.54
1:B:131:ILE:HD12	1:B:132:SER:N	2.22	0.53
1:A:66:ASN:OD1	1:A:67:ALA:N	2.41	0.53
1:B:30:LYS:NZ	1:B:34:ASP:OD1	2.42	0.52
1:B:233:TYR:HD2	1:B:234:ILE:HD12	1.74	0.52
1:A:129:ASP:OD1	1:A:133:LYS:HE2	2.11	0.51
1:A:207:ALA:O	1:A:211:THR:HG23	2.11	0.50
1:B:44:GLU:HB3	1:B:48:ARG:HH12	1.75	0.50
1:A:158:TYR:OH	2:C:8:PRO:HD2	2.11	0.50
1:A:222:GLN:CD	1:A:222:GLN:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:PRO:N	2:C:9:GLY:HA3	2.27	0.50
1:B:156:VAL:O	1:B:159:THR:OG1	2.28	0.49
1:A:183:SER:OG	1:A:185:ILE:HG22	2.12	0.49
1:A:106:ASN:OD1	1:A:108:GLU:HB3	2.13	0.49
1:A:68:PHE:CE1	1:B:114:ALA:HB2	2.47	0.48
1:B:29:ILE:O	1:B:33:GLU:HG3	2.13	0.48
1:A:198:VAL:HG11	1:A:206:LYS:HB3	1.96	0.48
1:A:204:LEU:HD21	1:A:234:ILE:HG13	1.96	0.47
1:A:194:LEU:HG	1:A:210:LEU:HD13	1.96	0.47
1:B:151:PHE:CD1	1:B:190:VAL:HG22	2.50	0.46
1:B:221:HIS:CE1	1:B:223:ARG:HG2	2.51	0.46
1:A:186:ASP:N	1:A:186:ASP:OD1	2.38	0.46
1:B:150:CYS:SG	1:B:169:TRP:HE3	2.39	0.45
1:A:151:PHE:CE2	1:A:155:LYS:HD3	2.52	0.45
1:B:131:ILE:HD13	1:B:169:TRP:CH2	2.52	0.45
1:A:140:LYS:HA	1:A:141:HIS:HA	1.66	0.45
1:A:58:GLU:N	1:A:58:GLU:OE1	2.40	0.45
1:A:223:ARG:NH1	2:C:8:PRO:HA	2.32	0.45
1:A:11:MET:HA	1:A:14:LEU:HD12	1.98	0.45
1:A:106:ASN:C	1:B:75:ASN:HD21	2.21	0.44
2:C:7:PRO:C	2:C:9:GLY:HA3	2.38	0.44
1:B:73:ARG:HA	1:B:77:GLU:HB2	2.00	0.44
1:A:60:PHE:O	1:A:66:ASN:CG	2.57	0.43
1:B:187:LYS:HG2	1:B:188:VAL:N	2.33	0.43
1:B:233:TYR:CD2	1:B:234:ILE:HD12	2.53	0.43
1:B:101:ARG:HA	1:B:104:PHE:CD1	2.53	0.43
1:A:167:GLU:OE2	1:A:206:LYS:NZ	2.44	0.43
1:A:136:LEU:HB3	1:A:137:PRO:CD	2.48	0.43
1:A:238:GLU:C	1:A:239:LYS:HG3	2.38	0.43
1:B:185:ILE:HD11	1:B:189:SER:HB3	2.01	0.43
1:A:198:VAL:HG13	1:A:203:ASP:HB3	2.00	0.43
1:A:130:THR:HG23	1:A:135:ASN:HB2	2.00	0.43
2:C:4:PRO:HA	2:C:5:PRO:HD3	1.89	0.43
1:A:64:PRO:HG2	1:B:120:LEU:HD22	2.00	0.42
1:B:187:LYS:HE2	1:B:217:LEU:HD13	2.00	0.42
1:A:155:LYS:O	1:A:159:THR:HG23	2.19	0.42
1:B:32:GLU:HG2	1:B:89:MET:HB2	2.02	0.42
1:A:238:GLU:O	1:A:239:LYS:HG3	2.19	0.42
1:A:228:LEU:O	1:A:232:GLU:HG3	2.20	0.42
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.61	0.42
2:C:1:PRO:HA	2:C:2:PRO:HD3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:O	1:A:44:GLU:HG3	2.20	0.42
1:A:14:LEU:HD22	1:B:74:LEU:HD13	2.02	0.41
1:B:48:ARG:HH11	1:B:48:ARG:HG3	1.84	0.41
1:B:48:ARG:NH1	1:B:48:ARG:HG3	2.36	0.41
1:A:211:THR:HG21	1:A:231:PHE:CE2	2.41	0.41
1:A:57:PRO:O	1:A:61:VAL:HG13	2.21	0.41
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.88	0.40
1:B:12:THR:O	1:B:15:ILE:HG13	2.22	0.40
1:A:74:LEU:N	1:A:74:LEU:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	235/251 (94%)	229 (97%)	5 (2%)	1 (0%)	39	78
1	B	205/251 (82%)	203 (99%)	2 (1%)	0	100	100
2	C	7/9 (78%)	7 (100%)	0	0	100	100
All	All	447/511 (88%)	439 (98%)	7 (2%)	1 (0%)	52	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLY

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	210/224 (94%)	207 (99%)	3 (1%)	74	92
1	B	189/224 (84%)	185 (98%)	4 (2%)	61	88
2	C	6/6 (100%)	6 (100%)	0	100	100
All	All	405/454 (89%)	398 (98%)	7 (2%)	68	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	120	LEU
1	A	139	VAL
1	B	102	GLN
1	B	152	GLU
1	B	187	LYS
1	B	223	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	75	ASN

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 ⓘ

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	A	237/251 (94%)	0.27	8 (3%) 49 30	62, 103, 166, 221	0
1	B	211/251 (84%)	0.99	40 (18%) 2 1	71, 160, 218, 265	0
2	C	9/9 (100%)	2.14	3 (33%) 0 0	130, 145, 163, 178	0
All	All	457/511 (89%)	0.64	51 (11%) 7 4	62, 114, 207, 265	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	LEU	7.8
2	C	1	PRO	6.7
1	B	205	ASP	6.5
1	B	216	GLU	5.1
1	B	209	LEU	4.5
1	B	159	THR	4.3
1	B	175	ARG	4.1
1	A	61	VAL	3.9
1	B	217	LEU	3.9
1	A	60	PHE	3.8
1	B	147	ALA	3.8
1	B	233	TYR	3.7
1	B	126	LEU	3.7
1	B	204	LEU	3.7
1	B	8	ILE	3.7
1	B	124	TYR	3.5
1	B	208	LEU	3.4
1	B	160	GLU	3.4
1	B	193	TYR	3.4
1	B	164	TYR	3.3
2	C	2	PRO	3.3
1	B	178	ASP	3.0
1	B	182	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	158	TYR	2.9
1	B	117	LEU	2.9
1	B	121	GLN	2.8
1	B	219	PRO	2.7
1	A	238	GLU	2.6
1	B	177	LEU	2.6
1	B	212	LYS	2.6
1	A	141	HIS	2.6
1	B	179	GLU	2.6
2	C	4	PRO	2.5
1	B	123	THR	2.5
1	B	168	LEU	2.4
1	B	15	ILE	2.4
1	A	56	ASP	2.4
1	B	191	LEU	2.4
1	A	63	HIS	2.3
1	B	10	GLN	2.3
1	B	7	SER	2.3
1	B	163	TYR	2.2
1	A	59	GLY	2.2
1	B	211	THR	2.2
1	B	153	LEU	2.2
1	B	129	ASP	2.1
1	B	188	VAL	2.1
1	A	199	TYR	2.1
1	B	127	ASP	2.1
1	B	228	LEU	2.1
1	B	187	LYS	2.0

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 carbohydrates 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.