wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NPZ
Title	:	Prolactin Receptor (PRLR) Complexed with the Natural Hormone (PRL)
Authors	:	Van Agthoven, J.; England, P.; Goffin, V.; Broutin, I.
Deposited on	:	2010-06-29
Resolution	:	3.35 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 (1)) were used in the production of this report:

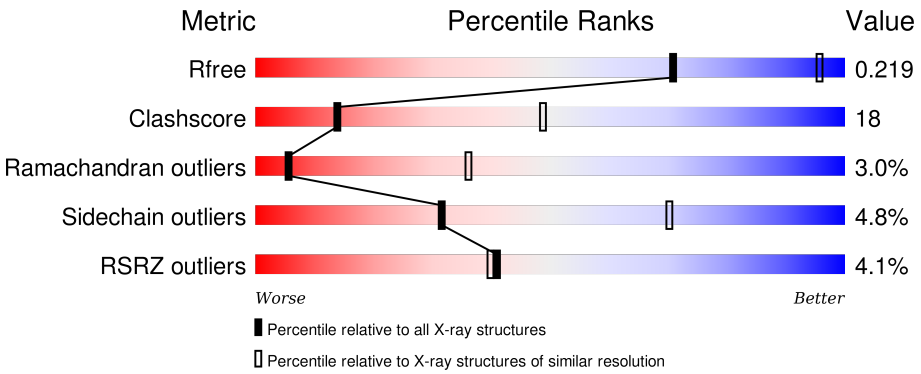
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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.

Mol	Chain	Length	Quality of chain
1	A	199	4%; 53%; 35%; 6%; 7%
2	B	220	%; 62%; 29%; •; 8%
2	C	220	6%; 55%; 32%; •; 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4817 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 Prolactin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1507	949	266	283	9	0	0	0

- Molecule 2 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	202	1666	1072	267	319	8	0	0	0
2	C	199	1644	1058	264	314	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ARG	-	EXPRESSION TAG	UNP P05710
B	212	SER	-	EXPRESSION TAG	UNP P05710
B	213	ARG	-	EXPRESSION TAG	UNP P05710
B	214	SER	-	EXPRESSION TAG	UNP P05710
B	215	HIS	-	EXPRESSION TAG	UNP P05710
B	216	HIS	-	EXPRESSION TAG	UNP P05710
B	217	HIS	-	EXPRESSION TAG	UNP P05710
B	218	HIS	-	EXPRESSION TAG	UNP P05710
B	219	HIS	-	EXPRESSION TAG	UNP P05710
B	220	HIS	-	EXPRESSION TAG	UNP P05710
C	211	ARG	-	EXPRESSION TAG	UNP P05710
C	212	SER	-	EXPRESSION TAG	UNP P05710
C	213	ARG	-	EXPRESSION TAG	UNP P05710
C	214	SER	-	EXPRESSION TAG	UNP P05710
C	215	HIS	-	EXPRESSION TAG	UNP P05710
C	216	HIS	-	EXPRESSION TAG	UNP P05710
C	217	HIS	-	EXPRESSION TAG	UNP P05710
C	218	HIS	-	EXPRESSION TAG	UNP P05710

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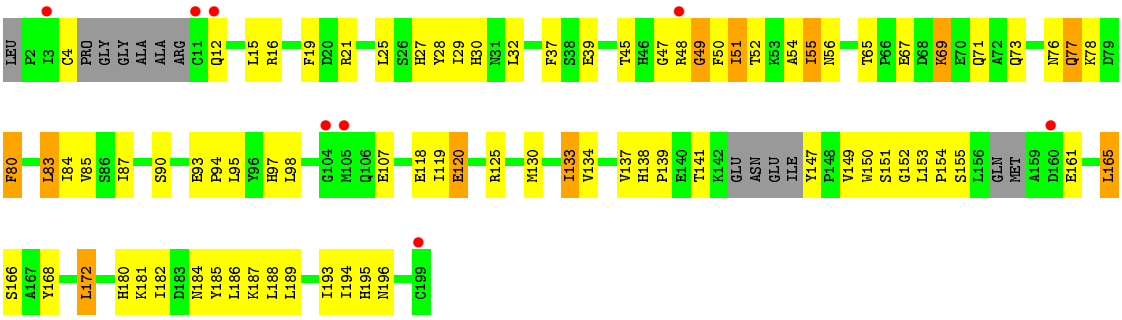
Chain	Residue	Modelled	Actual	Comment	Reference
C	219	HIS	-	EXPRESSION TAG	UNP P05710
C	220	HIS	-	EXPRESSION TAG	UNP P05710

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.

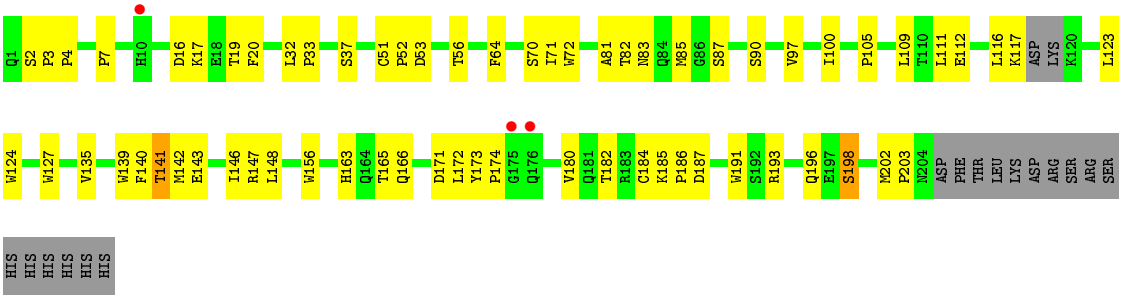
- Molecule 1: Prolactin

Chain A:



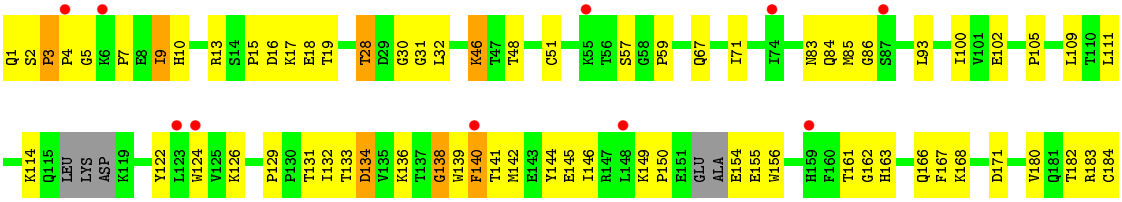
- Molecule 2: Prolactin receptor

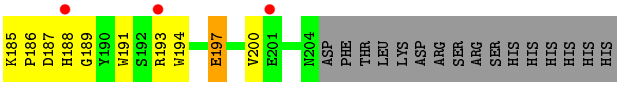
Chain B:



- Molecule 2: Prolactin receptor

Chain C:




K185
P186
D187
H188
G189
Y190
W191
S192
R193
W194
E197
V200
E201
N204
ASP
PHE
THR
LEU
LYS
ASP
ARG
SER
ARG
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.17Å 92.17Å 216.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.78 – 3.35 84.78 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (84.78-3.35) 97.0 (84.78-3.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.234 , 0.292 0.228 , 0.219	Depositor DCC
R_{free} test set	683 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 13682 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.52	0/1535	0.70	0/2071
2	B	0.52	0/1724	0.67	0/2351
2	C	0.49	0/1701	0.64	0/2318
All	All	0.51	0/4960	0.67	0/6740

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
2	C	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
2	C	138	GLY	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	A	1507	0	1485	72	0
2	B	1666	0	1581	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1644	0	1558	61	0
All	All	4817	0	4624	174	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 18.

The worst 5 of 174 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)
2:B:146:ILE:HG22	2:B:182:THR:HG22	1.24	1.10
2:B:82:THR:HG22	2:B:87:SER:HB3	1.26	1.10
1:A:15:LEU:HD11	1:A:133:ILE:CD1	1.90	1.02
1:A:15:LEU:HD11	1:A:133:ILE:HD13	1.40	1.00
2:C:154:GLU:HG2	2:C:155:GLU:H	1.34	0.93

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	178/199 (89%)	154 (86%)	19 (11%)	5 (3%)	6 37
2	B	198/220 (90%)	182 (92%)	16 (8%)	0	100 100
2	C	193/220 (88%)	151 (78%)	30 (16%)	12 (6%)	2 15
All	All	569/639 (89%)	487 (86%)	65 (11%)	17 (3%)	5 36

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	155	SER

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Mol	Chain	Res	Type
2	C	10	HIS
2	C	140	PHE
1	A	141	THR

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	171/181 (94%)	158 (92%)	13 (8%)	16	53
2	B	189/207 (91%)	183 (97%)	6 (3%)	46	80
2	C	187/207 (90%)	180 (96%)	7 (4%)	41	76
All	All	547/595 (92%)	521 (95%)	26 (5%)	31	70

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	LEU
2	B	124	TRP
2	C	134	ASP
1	A	172	LEU
2	B	37	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	195	HIS
2	B	159	HIS
1	A	106	GLN
2	B	163	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 carbohydrates 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	A	186/199 (93%)	0.51	8 (4%)	39	38	17, 49, 117, 173	0
2	B	202/220 (91%)	0.59	3 (1%)	76	77	18, 48, 96, 128	0
2	C	199/220 (90%)	0.86	13 (6%)	22	23	37, 65, 125, 188	0
All	All	587/639 (91%)	0.66	24 (4%)	41	40	17, 55, 120, 188	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	4	PRO	4.1
1	A	12	GLN	3.5
2	C	188	HIS	3.4
2	C	140	PHE	3.1
2	C	123	LEU	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 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.