W O R L D W I D E
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P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 10:49 PM GMT

PDB ID : 1XB7
Title : X-ray structure of ERRalpha LBD in complex with a PGC-1alpha peptide at 2.5A resolution
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Deposited on : 2004-08-30
Resolution : 2.50 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.50 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.
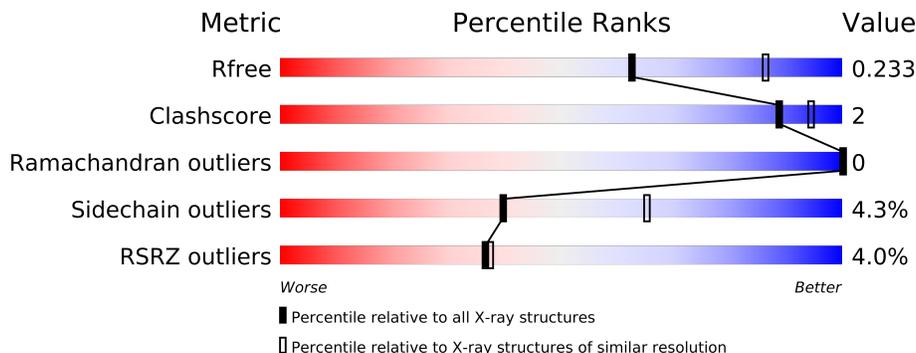
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	247	
2	P	12	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1826 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Steroid hormone receptor ERR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total 1667	C 1071	N 284	O 306	S 6	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	-	EXPRESSION TAG	UNP P11474
A	274	SER	-	EXPRESSION TAG	UNP P11474
A	275	SER	-	EXPRESSION TAG	UNP P11474
A	276	HIS	-	EXPRESSION TAG	UNP P11474
A	277	HIS	-	EXPRESSION TAG	UNP P11474
A	278	HIS	-	EXPRESSION TAG	UNP P11474
A	279	HIS	-	EXPRESSION TAG	UNP P11474
A	280	HIS	-	EXPRESSION TAG	UNP P11474
A	281	HIS	-	EXPRESSION TAG	UNP P11474
A	282	LEU	-	EXPRESSION TAG	UNP P11474
A	283	GLU	-	EXPRESSION TAG	UNP P11474
A	284	VAL	-	EXPRESSION TAG	UNP P11474
A	285	LEU	-	EXPRESSION TAG	UNP P11474
A	286	PHE	-	EXPRESSION TAG	UNP P11474
A	287	GLN	-	EXPRESSION TAG	UNP P11474
A	288	GLY	-	EXPRESSION TAG	UNP P11474
A	289	PRO	-	EXPRESSION TAG	UNP P11474

- Molecule 2 is a protein called Peroxisome proliferator activated receptor gamma coactivator 1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total 74	C 49	N 10	O 15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	207	ALA	CYS	ENGINEERED	UNP Q9UBK2

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total I		0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total O		0	0
			82	82		
4	P	2	Total O		0	0
			2	2		

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 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: Steroid hormone receptor ERR1

Chain A:
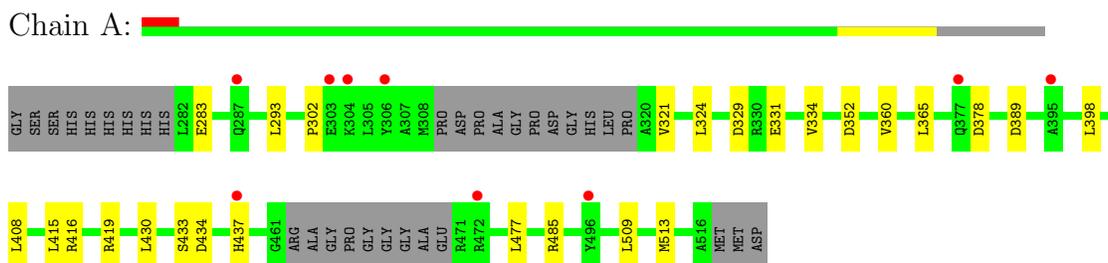
• Molecule 2: Peroxisome proliferator activated receptor gamma coactivator 1 alpha

Chain P:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.00Å 110.00Å 104.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.50) 94.8 (19.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.247 0.210 , 0.233	Depositor DCC
R_{free} test set	625 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 12686 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1826	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
IOD

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	0.65	0/1689	0.80	4/2285 (0.2%)
2	P	0.60	0/74	0.80	0/99
All	All	0.64	0/1763	0.80	4/2384 (0.2%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	329	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	389	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	378	ASP	CB-CG-OD2	5.45	123.21	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens
added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,
and the number in parentheses is this value normalized per 1000 atoms of the molecule in the
chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the
Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1667	0	1726	8	0
2	P	74	0	79	0	0
3	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	82	0	0	0	0
4	P	2	0	0	0	0
All	All	1826	0	1805	8	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (8) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:VAL:HG21	1:A:430:LEU:HD12	1.80	0.64
1:A:324:LEU:HD12	1:A:398:LEU:HD21	1.83	0.61
1:A:415:LEU:HD13	1:A:477:LEU:HD23	1.85	0.58
1:A:433:SER:O	1:A:434:ASP:HB2	2.11	0.51
1:A:302:PRO:HB3	1:A:334:VAL:CG1	2.41	0.50
1:A:302:PRO:HB3	1:A:334:VAL:HG13	1.97	0.45
1:A:331:GLU:HB3	1:A:365:LEU:HD22	2.03	0.41
1:A:509:LEU:O	1:A:513:MET:HG2	2.21	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	209/247 (85%)	206 (99%)	3 (1%)	0	100	100
2	P	7/12 (58%)	7 (100%)	0	0	100	100
All	All	216/259 (83%)	213 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	176/199 (88%)	168 (96%)	8 (4%)	38	63
2	P	9/11 (82%)	9 (100%)	0	100	100
All	All	185/210 (88%)	177 (96%)	8 (4%)	40	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	GLU
1	A	293	LEU
1	A	321	VAL
1	A	408	LEU
1	A	416	ARG
1	A	419	ARG
1	A	437	HIS
1	A	485	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	215/247 (87%)	0.03	9 (4%)	35	36	21, 37, 70, 74	0
2	P	9/12 (75%)	0.08	0	100	100	39, 44, 48, 53	0
All	All	224/259 (86%)	0.03	9 (4%)	36	37	21, 38, 69, 74	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	GLN	3.6
1	A	304	LYS	3.5
1	A	306	TYR	3.2
1	A	395	ALA	2.8
1	A	377	GLN	2.4
1	A	496	TYR	2.3
1	A	303	GLU	2.1
1	A	472	ARG	2.1
1	A	437	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	IOD	P	101	1/1	0.04	-11.47	45,45,45,45	1

6.5 Other polymers ⓘ

There are no such residues in this entry.