



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2018 – 12:37 am GMT

PDB ID : 3D24
Title : Crystal structure of ligand-binding domain of estrogen-related receptor alpha (ERRalpha) in complex with the peroxisome proliferators-activated receptor coactivator-1alpha box3 peptide (PGC-1alpha)
Authors : Moras, D.; Greschik, H.; Flaig, R.; Sato, Y.; Rochel, N.; Structural Proteomics in Europe (SPINE)
Deposited on : 2008-05-07
Resolution : 2.11 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

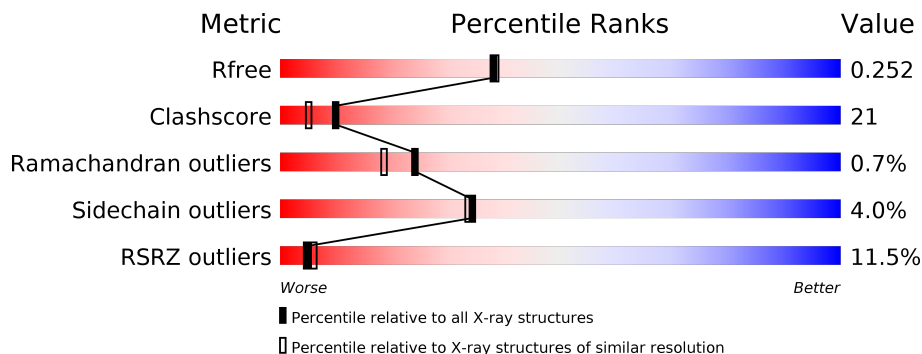
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	111664	5449 (2.14-2.10)
Clashscore	122126	5972 (2.14-2.10)
Ramachandran outliers	120053	5914 (2.14-2.10)
Sidechain outliers	120020	5915 (2.14-2.10)
RSRZ outliers	108989	5321 (2.14-2.10)

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 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	253	<div> <div>9%</div> <div>53%</div> <div>28%</div> <div>•</div> <div>17%</div> </div>
1	C	253	<div> <div>8%</div> <div>61%</div> <div>23%</div> <div>•</div> <div>15%</div> </div>
2	B	22	<div> <div>23%</div> <div>18%</div> <div>36%</div> <div>5%</div> <div>41%</div> </div>
2	D	22	<div> <div>18%</div> <div>32%</div> <div>32%</div> <div>36%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3794 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 Steroid hormone receptor ERR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1624	1040	277	301	6			
1	C	216	Total	C	N	O	S	0	1	0
			1678	1072	287	311	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	MET	-	EXPRESSION TAG	UNP P11474
A	172	ARG	-	EXPRESSION TAG	UNP P11474
A	173	SER	-	EXPRESSION TAG	UNP P11474
A	174	HIS	-	EXPRESSION TAG	UNP P11474
A	175	HIS	-	EXPRESSION TAG	UNP P11474
A	176	HIS	-	EXPRESSION TAG	UNP P11474
A	177	HIS	-	EXPRESSION TAG	UNP P11474
A	178	HIS	-	EXPRESSION TAG	UNP P11474
A	179	HIS	-	EXPRESSION TAG	UNP P11474
A	180	GLY	-	EXPRESSION TAG	UNP P11474
A	181	PRO	-	EXPRESSION TAG	UNP P11474
A	182	GLY	-	EXPRESSION TAG	UNP P11474
A	183	LEU	-	EXPRESSION TAG	UNP P11474
A	184	VAL	-	EXPRESSION TAG	UNP P11474
A	185	PRO	-	EXPRESSION TAG	UNP P11474
A	186	ARG	-	EXPRESSION TAG	UNP P11474
A	187	GLY	-	EXPRESSION TAG	UNP P11474
A	188	SER	-	EXPRESSION TAG	UNP P11474
A	189	LYS	-	EXPRESSION TAG	UNP P11474
A	190	THR	-	EXPRESSION TAG	UNP P11474
A	191	ALA	-	EXPRESSION TAG	UNP P11474
C	171	MET	-	EXPRESSION TAG	UNP P11474
C	172	ARG	-	EXPRESSION TAG	UNP P11474
C	173	SER	-	EXPRESSION TAG	UNP P11474
C	174	HIS	-	EXPRESSION TAG	UNP P11474

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Chain	Residue	Modelled	Actual	Comment	Reference
C	175	HIS	-	EXPRESSION TAG	UNP P11474
C	176	HIS	-	EXPRESSION TAG	UNP P11474
C	177	HIS	-	EXPRESSION TAG	UNP P11474
C	178	HIS	-	EXPRESSION TAG	UNP P11474
C	179	HIS	-	EXPRESSION TAG	UNP P11474
C	180	GLY	-	EXPRESSION TAG	UNP P11474
C	181	PRO	-	EXPRESSION TAG	UNP P11474
C	182	GLY	-	EXPRESSION TAG	UNP P11474
C	183	LEU	-	EXPRESSION TAG	UNP P11474
C	184	VAL	-	EXPRESSION TAG	UNP P11474
C	185	PRO	-	EXPRESSION TAG	UNP P11474
C	186	ARG	-	EXPRESSION TAG	UNP P11474
C	187	GLY	-	EXPRESSION TAG	UNP P11474
C	188	SER	-	EXPRESSION TAG	UNP P11474
C	189	LYS	-	EXPRESSION TAG	UNP P11474
C	190	THR	-	EXPRESSION TAG	UNP P11474
C	191	ALA	-	EXPRESSION TAG	UNP P11474

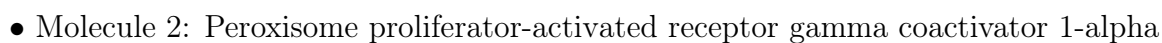
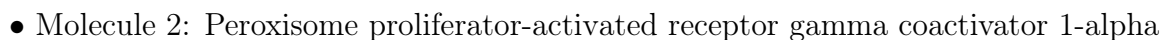
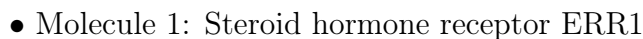
- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma coactivator 1-alpha.

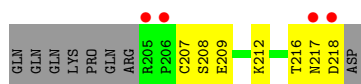
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total 106	C 67	N 18	O 20	S 1	0	0	0
2	D	14	Total 114	C 71	N 19	O 23	S 1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	2	Total	O	0	0
			2	2		
3	C	163	Total	O	0	0
			163	163		
3	D	7	Total	O	0	0
			7	7		

- Molecule 1: Steroid hormone receptor ERR1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.40Å 56.00Å 96.20Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.11 17.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.4 (50.00-2.11) 88.9 (17.17-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.68 (at 2.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.255 0.212 , 0.252	Depositor DCC
R_{free} test set	1584 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3794	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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	A	0.27	0/1645	0.49	0/2224
1	C	0.32	0/1706	0.54	0/2305
2	B	0.34	0/107	0.49	0/144
2	D	0.35	0/115	0.59	0/155
All	All	0.30	0/3573	0.52	0/4828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1624	0	1680	85	0
1	C	1678	0	1731	71	0
2	B	106	0	110	12	0
2	D	114	0	114	7	0
3	A	100	0	0	2	0
3	B	2	0	0	0	0
3	C	163	0	0	9	1
3	D	7	0	0	0	0
All	All	3794	0	3635	147	1

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 21.

The worst 5 of 147 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:216:THR:HG22	2:B:217:ASN:H	1.17	1.04
1:A:375:ARG:HE	1:C:376:ARG:HG3	1.31	0.94
1:C:212:MET:HB3	1:C:213:PRO:CA	2.05	0.87
1:A:376:ARG:H	1:A:376:ARG:HD3	1.40	0.86
1:C:195:ASN:HD22	1:C:198:VAL:H	1.25	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:529:HOH:O	3:C:529:HOH:O[2_657]	2.01	0.19

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	203/253 (80%)	192 (95%)	11 (5%)	0	100	100
1	C	211/253 (83%)	201 (95%)	8 (4%)	2 (1%)	19	13
2	B	11/22 (50%)	7 (64%)	4 (36%)	0	100	100
2	D	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	0
All	All	437/550 (80%)	410 (94%)	24 (6%)	3 (1%)	24	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	MET
1	C	224	ALA
2	D	217	ASN

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	172/202 (85%)	165 (96%)	7 (4%)	33	32
1	C	178/202 (88%)	172 (97%)	6 (3%)	40	40
2	B	13/22 (59%)	11 (85%)	2 (15%)	3	1
2	D	14/22 (64%)	14 (100%)	0	100	100
All	All	377/448 (84%)	362 (96%)	15 (4%)	34	33

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
2	B	205	ARG
1	C	312	LEU
1	A	376	ARG
1	C	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	C	195	ASN
1	C	275	GLN
1	C	350	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 [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	209/253 (82%)	0.60	24 (11%) 5 6	17, 45, 82, 95	0
1	C	216/253 (85%)	0.35	19 (8%) 10 13	15, 30, 72, 82	0
2	B	13/22 (59%)	2.20	5 (38%) 0 0	48, 57, 80, 83	0
2	D	14/22 (63%)	1.41	4 (28%) 0 0	19, 34, 70, 78	0
All	All	452/550 (82%)	0.55	52 (11%) 5 6	15, 38, 77, 95	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	PRO	9.6
1	C	213	PRO	9.2
2	B	205	ARG	7.5
1	A	365	GLY	7.1
2	D	217	ASN	7.1

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.