



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:43 PM GMT

PDB ID : 4AA6
Title : THE OESTROGEN RECEPTOR RECOGNIZES AN IMPERFECTLY
PALINDROMIC RESPONSE ELEMENT THROUGH AN ALTERNATIVE
SIDE-CHAIN CONFORMATION
Authors : Schwabe, J.W.; Chapman, L.; Rhodes, D.
Deposited on : 2011-11-30
Resolution : 2.60 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 ⓘ 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

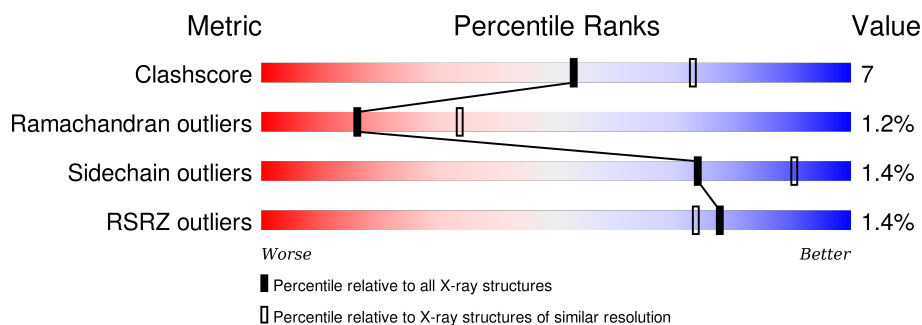
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



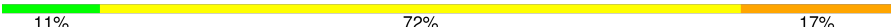
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	71	<div> <div>3%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	B	71	<div> <div>3%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
1	E	71	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	F	71	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	C	18	<div> <div>17%</div> <div>56%</div> <div>28%</div> </div>
2	G	18	<div> <div>11%</div> <div>83%</div> <div>6%</div> </div>
3	D	18	<div> <div>6%</div> <div>72%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	18	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment on the left labeled '11%', a yellow segment in the middle labeled '72%', and an orange segment on the right labeled '17%'.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4615 atoms, of which 886 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 ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	69	Total	C	H	N	O	S	0	0	0
			675	335	129	103	97	11			
1	B	70	Total	C	H	N	O	S	0	0	0
			678	338	127	103	98	12			
1	E	68	Total	C	H	N	O	S	0	0	0
			609	306	108	92	92	11			
1	F	69	Total	C	H	N	O	S	0	0	0
			649	326	120	97	94	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*AP*GP*TP*CP*AP*CP*AP*GP*TP*GP*AP *CP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	H	N	O	P	0	0	0
			403	175	38	68	105	17			
2	G	18	Total	C	H	N	O	P	0	0	0
			403	175	38	68	105	17			

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*AP*GP*GP*TP*CP*AP*CP*TP*GP*TP*GP*AP *CP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	18	Total	C	H	N	O	P	0	0	0
			401	176	36	64	108	17			
3	H	18	Total	C	H	N	O	P	0	0	0
			401	176	36	64	108	17			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Zn 2	0	0
4	F	2	Total 2	Zn 2	0	0
4	E	2	Total 2	Zn 2	0	0

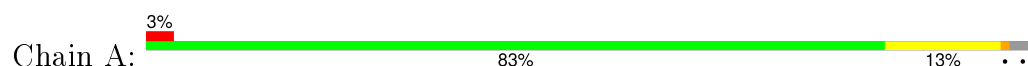
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	35	Total 103	H 68	O 35	0	0
5	B	18	Total 52	H 34	O 18	0	0
5	C	9	Total 25	H 16	O 9	0	0
5	D	10	Total 28	H 18	O 10	0	0
5	E	25	Total 69	H 44	O 25	0	0
5	F	19	Total 57	H 38	O 19	0	0
5	G	12	Total 36	H 24	O 12	0	0
5	H	6	Total 18	H 12	O 6	0	0

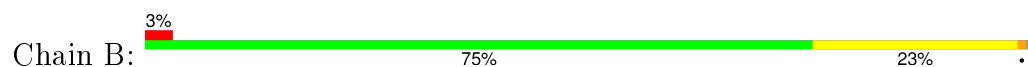
3 Residue-property plots [i](#)

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: ESTROGEN RECEPTOR



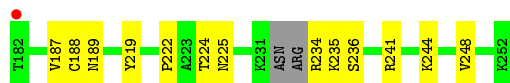
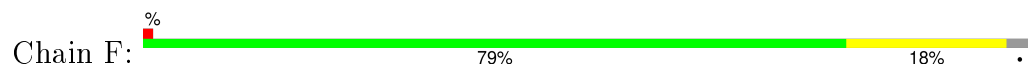
- Molecule 1: ESTROGEN RECEPTOR



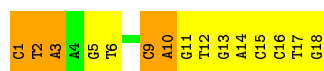
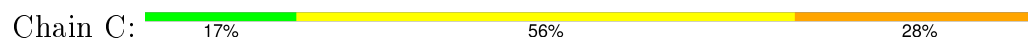
- Molecule 1: ESTROGEN RECEPTOR



- Molecule 1: ESTROGEN RECEPTOR



- Molecule 2: 5'-D(*CP*TP*AP*AP*GP*TP*CP*AP*CP*AP*GP*TP*GP*AP*CP*CP*TP*G)-3'




- Molecule 2: 5'-D(*CP*TP*AP*AP*GP*TP*CP*AP*CP*AP*GP*TP*GP*AP*CP*CP*TP*G)-3'

Chain G:  11% 83% 6%



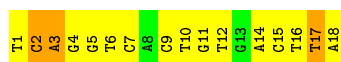
● Molecule 3: 5'-D(*TP*CP*AP*GP*GP*TP*CP*AP*CP*TP*GP*TP*GP*AP *CP*TP*TP*A)-3'

Chain D:  6% 72% 22%



● Molecule 3: 5'-D(*TP*CP*AP*GP*GP*TP*CP*AP*CP*TP*GP*TP*GP*AP *CP*TP*TP*A)-3'

Chain H:  11% 72% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.68Å 113.09Å 62.36Å 90.00° 117.45° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60 15.85 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (7.00-2.60) 99.2 (15.85-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.52Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 25463 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4615	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.27 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4214e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

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

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	0.37	0/557	0.54	0/744
1	B	0.36	0/562	0.56	0/751
1	E	0.34	0/509	0.55	0/676
1	F	0.38	0/539	0.57	0/718
2	C	1.80	5/409 (1.2%)	2.53	34/629 (5.4%)
2	G	1.80	7/409 (1.7%)	2.40	36/629 (5.7%)
3	D	1.82	4/408 (1.0%)	2.74	44/628 (7.0%)
3	H	1.72	5/408 (1.2%)	2.67	43/628 (6.8%)
All	All	1.20	21/3801 (0.6%)	1.81	157/5403 (2.9%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	17	DT	C5-C7	7.28	1.54	1.50
3	D	12	DT	O3'-P	-7.27	1.52	1.61
3	D	5	DG	C5'-C4'	-7.24	1.43	1.51
2	C	5	DG	C5'-C4'	-6.98	1.43	1.51
2	C	17	DT	C5-C7	6.87	1.54	1.50

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	16	DT	C6-C5-C7	-12.42	115.45	122.90
3	D	6	DT	C6-C5-C7	-11.70	115.88	122.90
3	H	12	DT	O4'-C1'-C2'	-10.18	97.76	105.90
3	D	1	DT	P-O3'-C3'	10.12	131.84	119.70
3	H	10	DT	O4'-C1'-C2'	-10.11	97.81	105.90

There are no chirality outliers.

There are no planarity outliers.

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	546	129	503	8	0
1	B	551	127	505	11	0
1	E	501	108	451	3	0
1	F	529	120	487	8	0
2	C	365	38	204	4	0
2	G	365	38	204	1	0
3	D	365	36	206	3	0
3	H	365	36	206	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	35	68	0	0	0
5	B	18	34	0	0	0
5	C	9	16	0	0	0
5	D	10	18	0	1	0
5	E	25	44	0	1	0
5	F	19	38	0	1	0
5	G	12	24	0	0	0
5	H	6	12	0	1	0
All	All	3729	886	2766	40	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 7.

The worst 5 of 40 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:240:CYS:SG	1:A:243:ARG:NH1	2.62	0.72
1:E:203:GLU:HG3	5:E:2007:HOH:O	1.90	0.70
1:B:192:ALA:HB3	1:B:200:TRP:CD1	2.32	0.65
1:F:234:ARG:HD2	1:F:241:ARG:NH2	2.12	0.63
1:B:234:ARG:HD2	1:B:241:ARG:NH2	2.14	0.63

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	65/71 (92%)	63 (97%)	2 (3%)	0	100	100
1	B	66/71 (93%)	60 (91%)	5 (8%)	1 (2%)	13	26
1	E	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
1	F	65/71 (92%)	56 (86%)	7 (11%)	2 (3%)	5	8
All	All	260/284 (92%)	240 (92%)	17 (6%)	3 (1%)	16	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	219	TYR
1	B	183	ARG
1	F	236	SER

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	58/61 (95%)	57 (98%)	1 (2%)	68	88
1	B	58/61 (95%)	57 (98%)	1 (2%)	68	88
1	E	51/61 (84%)	51 (100%)	0	100	100
1	F	55/61 (90%)	54 (98%)	1 (2%)	66	87
All	All	222/244 (91%)	219 (99%)	3 (1%)	74	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	B	214	GLN
1	F	189	ASN

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

Mol	Chain	Res	Type
1	B	214	GLN
1	E	189	ASN

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](#)

Of 8 ligands modelled in this entry, 8 are 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.

No monomer is involved in short contacts.

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	69/71 (97%)	-0.18	2 (2%) 55 48	5, 16, 39, 63	0
1	B	70/71 (98%)	0.02	2 (2%) 55 48	7, 22, 51, 64	0
1	E	68/71 (95%)	-0.15	0 100 100	8, 25, 47, 59	0
1	F	69/71 (97%)	0.07	1 (1%) 78 74	7, 20, 52, 59	0
2	C	18/18 (100%)	-0.86	0 100 100	10, 22, 30, 33	0
2	G	18/18 (100%)	-0.64	0 100 100	11, 27, 36, 47	0
3	D	18/18 (100%)	-0.77	0 100 100	4, 23, 29, 36	0
3	H	18/18 (100%)	-0.81	0 100 100	9, 25, 35, 46	0
All	All	348/356 (97%)	-0.21	5 (1%) 78 74	4, 22, 48, 64	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	THR	4.2
1	A	218	ASP	2.3
1	B	200	TRP	2.2
1	A	216	HIS	2.2
1	F	182	THR	2.1

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 [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	B	254	1/1	0.99	0.11	-0.95	16,16,16,16	0
4	ZN	A	254	1/1	1.00	0.08	-1.92	15,15,15,15	0
4	ZN	F	253	1/1	0.98	0.09	-1.99	21,21,21,21	0
4	ZN	E	253	1/1	0.99	0.09	-2.00	22,22,22,22	0
4	ZN	A	253	1/1	0.99	0.09	-2.34	15,15,15,15	0
4	ZN	F	254	1/1	1.00	0.09	-2.83	16,16,16,16	0
4	ZN	B	253	1/1	0.99	0.06	-3.06	22,22,22,22	0
4	ZN	E	254	1/1	1.00	0.06	-3.73	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.