



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:48 PM GMT

PDB ID : 4Q13
Title : Apo Estrogen Receptor Alpha Ligand Binding Domain D538G Mutant with a glucocorticoid receptor-interacting protein 1 NR box II peptide
Authors : Fanning, S.W.; Panchamukhi, S.; Greene, G.L.
Deposited on : 2014-04-02
Resolution : 2.24 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

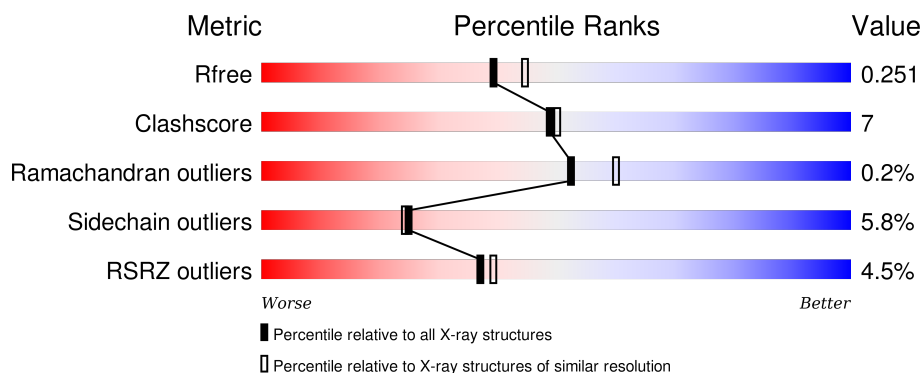
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	261	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	261	<div> <div></div> <div> <div></div> <div>73%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
2	C	13	<div> <div>8%</div> <div> <div></div> <div>38%</div> <div>8%</div> <div></div> <div>54%</div> </div> </div>
2	D	13	<div> <div></div> <div> <div></div> <div>31%</div> <div>31%</div> <div></div> <div>38%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3784 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	1	0
			1807	1155	313	319	20			
1	B	226	Total	C	N	O	S	0	2	0
			1821	1167	315	319	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLN	-	EXPRESSION TAG	UNP P03372
A	295	SER	-	EXPRESSION TAG	UNP P03372
A	296	ASN	-	EXPRESSION TAG	UNP P03372
A	297	ALA	-	EXPRESSION TAG	UNP P03372
A	298	MET	-	EXPRESSION TAG	UNP P03372
A	538	GLY	ASP	ENGINEERED MUTATION	UNP P03372
B	294	GLN	-	EXPRESSION TAG	UNP P03372
B	295	SER	-	EXPRESSION TAG	UNP P03372
B	296	ASN	-	EXPRESSION TAG	UNP P03372
B	297	ALA	-	EXPRESSION TAG	UNP P03372
B	298	MET	-	EXPRESSION TAG	UNP P03372
B	538	GLY	ASP	ENGINEERED MUTATION	UNP P03372

- Molecule 2 is a protein called Clucocorticoid receptor-interacting protein 1 NR box II peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			53	36	11	6			
2	D	8	Total	C	N	O	0	0	0
			71	47	15	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	28	Total 32	O 32	0	4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.14Å 82.66Å 59.11Å 90.00° 111.05° 90.00°	Depositor
Resolution (Å)	55.17 – 2.24 33.08 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (55.17-2.24) 98.8 (33.08-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.198 , 0.249 0.201 , 0.251	Depositor DCC
R_{free} test set	1227 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 23992 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3784	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 [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	0.80	0/1837	0.90	1/2476 (0.0%)
1	B	0.83	0/1852	0.90	3/2495 (0.1%)
2	C	0.79	0/53	0.98	0/70
2	D	0.85	0/71	0.81	0/93
All	All	0.82	0/3813	0.90	4/5134 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	LYS	N-CA-CB	-9.76	93.03	110.60
1	B	436	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	394	ARG	CG-CD-NE	5.57	123.49	111.80
1	B	394	ARG	CB-CA-C	-5.53	99.34	110.40

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	1807	0	1853	27	0
1	B	1821	0	1872	23	0
2	C	53	0	63	2	0
2	D	71	0	84	4	0
3	B	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3784	0	3872	55	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.

All (55) 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:B:363[A]:ARG:HH11	1:B:363[A]:ARG:HG2	1.00	1.15
1:A:536:LEU:HD11	1:A:541:LEU:HD13	1.50	0.93
1:A:536:LEU:CD1	1:A:541:LEU:HD13	2.01	0.90
1:B:363[A]:ARG:HG2	1:B:363[A]:ARG:NH1	1.81	0.89
1:A:377:HIS:NE2	1:A:460:THR:HG22	1.91	0.85
1:A:536:LEU:HD12	1:A:541:LEU:HB2	1.62	0.81
1:A:529:LYS:HB2	1:A:536:LEU:HD21	1.62	0.81
2:D:688:LYS:N	2:D:691:HIS:HD2	1.89	0.69
2:C:692:ARG:HG2	2:C:692:ARG:HH11	1.56	0.69
1:A:501:HIS:HB3	3:B:620:HOH:O	1.95	0.67
1:B:339:GLU:HG3	1:B:418:VAL:HA	1.78	0.66
1:A:377:HIS:NE2	1:A:460:THR:CG2	2.61	0.64
1:B:396:MET:CE	1:B:436:ARG:HA	2.28	0.63
1:A:536:LEU:HD12	1:A:541:LEU:HD13	1.83	0.59
1:B:403:LEU:HD12	1:B:409:LEU:HD13	1.84	0.59
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.86	0.57
1:B:396:MET:O	1:B:436:ARG:HD3	2.05	0.57
2:C:692:ARG:HG2	2:C:692:ARG:NH1	2.18	0.56
1:A:498:GLN:HA	1:A:501:HIS:CE1	2.40	0.56
1:B:529:LYS:HB2	1:B:536:LEU:HD12	1.87	0.56
1:A:536:LEU:HD12	1:A:541:LEU:CB	2.33	0.55
1:B:348:ASN:ND2	1:B:352:ARG:HH21	2.05	0.55
1:B:396:MET:HE3	1:B:436:ARG:HA	1.89	0.54
1:B:396:MET:HE2	1:B:436:ARG:HA	1.90	0.53
1:A:396:MET:CE	1:A:436:ARG:HA	2.39	0.52
1:B:532:ASN:C	1:B:534:VAL:N	2.63	0.52
1:A:310:LEU:HD22	1:A:314:GLN:HB3	1.89	0.52
1:B:402:LEU:HD12	1:B:425:PHE:CE1	2.45	0.51
1:A:496:THR:OG1	1:A:499:GLN:HG3	2.12	0.49
1:B:363[A]:ARG:CG	1:B:363[A]:ARG:NH1	2.62	0.49
1:B:542:GLU:OE2	2:D:689:ILE:HG13	2.13	0.49
2:D:688:LYS:O	2:D:691:HIS:HB2	2.13	0.48
1:A:528:MET:CE	1:A:528:MET:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:MET:HE1	1:A:436:ARG:HA	1.97	0.47
1:B:348:ASN:HD22	1:B:352:ARG:HH21	1.63	0.47
1:A:377:HIS:CE1	1:A:460:THR:CG2	2.98	0.46
1:B:348:ASN:ND2	1:B:352:ARG:HE	2.14	0.46
1:B:363[A]:ARG:CG	1:B:363[A]:ARG:HH11	1.91	0.44
1:B:547:HIS:O	1:B:548:ARG:C	2.56	0.44
1:B:474:HIS:O	1:B:478:VAL:HG23	2.18	0.44
1:B:536:LEU:O	1:B:541:LEU:HG	2.18	0.43
1:B:348:ASN:HD21	1:B:352:ARG:HE	1.66	0.43
1:A:536:LEU:CD1	1:A:541:LEU:CD1	2.85	0.43
1:A:506:GLN:O	1:A:510:ILE:HG13	2.19	0.43
1:A:335:ARG:NH2	1:A:341:SER:HB3	2.34	0.42
1:B:525:LEU:HA	1:B:525:LEU:HD12	1.75	0.42
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.01	0.42
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.90	0.42
1:B:496:THR:O	1:B:500:GLN:HG3	2.19	0.42
1:A:423:GLU:HG3	1:A:423:GLU:H	1.54	0.42
1:A:380:GLU:O	1:A:547:HIS:NE2	2.41	0.42
1:A:429:LEU:HA	1:A:429:LEU:HD23	1.89	0.42
2:D:688:LYS:HA	2:D:691:HIS:CD2	2.55	0.41
1:A:367:PHE:CE2	1:A:375:GLN:HG2	2.55	0.41
1:A:531:LYS:O	1:A:531:LYS:CG	2.70	0.41

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	217/261 (83%)	209 (96%)	8 (4%)	0	100	100
1	B	220/261 (84%)	214 (97%)	5 (2%)	1 (0%)	34	34
2	C	4/13 (31%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	6/13 (46%)	6 (100%)	0	0	100	100
All	All	447/548 (82%)	433 (97%)	13 (3%)	1 (0%)	52	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	531	LYS

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	202/234 (86%)	192 (95%)	10 (5%)	30	31
1	B	203/234 (87%)	189 (93%)	14 (7%)	19	17
2	C	6/13 (46%)	6 (100%)	0	100	100
2	D	8/13 (62%)	7 (88%)	1 (12%)	6	3
All	All	419/494 (85%)	394 (94%)	25 (6%)	25	22

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	317	SER
1	A	334	THR
1	A	397	GLU
1	A	423	GLU
1	A	460	THR
1	A	497	LEU
1	A	528	MET
1	A	529	LYS
1	A	536	LEU
1	B	321	ASP
1	B	324	PRO
1	B	341	SER

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Mol	Chain	Res	Type
1	B	363[A]	ARG
1	B	363[B]	ARG
1	B	368	VAL
1	B	403	LEU
1	B	412	ARG
1	B	425	PHE
1	B	472	LYS
1	B	473	ASP
1	B	497	LEU
1	B	528	MET
1	B	541	LEU
2	D	695	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	ASN
1	B	348	ASN
2	D	691	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

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	226/261 (86%)	0.33	19 (8%) 14 14	20, 44, 77, 104	1 (0%)
1	B	226/261 (86%)	0.04	1 (0%) 93 94	18, 39, 67, 89	0
2	C	6/13 (46%)	0.37	1 (16%) 2 2	43, 51, 68, 68	0
2	D	8/13 (61%)	-0.24	0 100 100	35, 43, 56, 61	0
All	All	466/548 (85%)	0.18	21 (4%) 37 39	18, 42, 75, 104	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	537	TYR	4.3
1	A	306	LEU	3.8
1	A	528	MET	3.8
1	A	526	TYR	3.6
1	A	541	LEU	3.5
1	A	373	HIS	3.4
1	A	417	CYS	2.7
1	A	369	ASP	2.6
1	A	368	VAL	2.6
1	A	511	LEU	2.6
1	A	307	ALA	2.6
2	C	691	HIS	2.5
1	A	545	ASP	2.5
1	A	321	ASP	2.5
1	A	548	ARG	2.3
1	A	527	SER	2.3
1	B	306	LEU	2.2
1	A	532	ASN	2.2
1	A	372	LEU	2.0
1	A	411	ASP	2.0
1	A	509	LEU	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.