



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 02:03 pm GMT

PDB ID : 2QW4
Title : Human NR4A1 ligand-binding domain
Authors : Min, J.R.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2007-08-09
Resolution : 2.80 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	:	trunk31020
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)	:	trunk31020

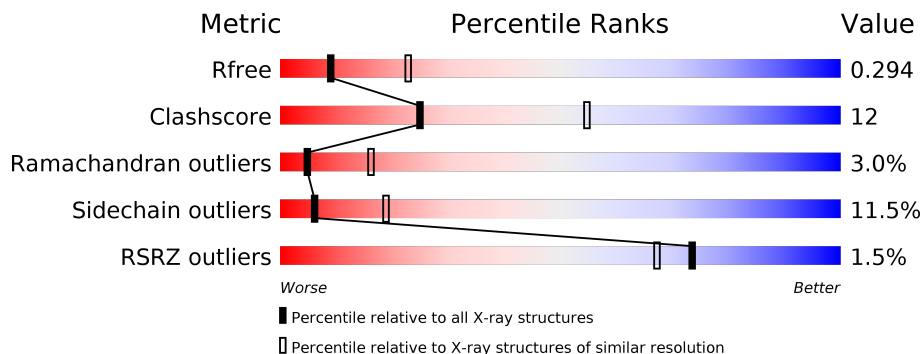
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	273	<div> <div>58%</div> <div>22%</div> <div>• •</div> <div>16%</div> </div>
1	B	273	<div> <div>56%</div> <div>23%</div> <div>5%</div> <div>16%</div> </div>
1	C	273	<div> <div>61%</div> <div>19%</div> <div>• •</div> <div>17%</div> </div>
1	D	273	<div> <div>54%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7147 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 Orphan nuclear receptor NR4A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1781	1145	307	323	6			
1	B	230	Total	C	N	O	S	0	0	0
			1793	1155	307	324	7			
1	C	227	Total	C	N	O	S	0	0	0
			1777	1149	302	319	7			
1	D	227	Total	C	N	O	S	0	0	0
			1786	1152	305	322	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP P22736
A	-4	GLY	-	EXPRESSION TAG	UNP P22736
A	-3	SER	-	EXPRESSION TAG	UNP P22736
A	-2	SER	-	EXPRESSION TAG	UNP P22736
A	-1	HIS	-	EXPRESSION TAG	UNP P22736
A	0	HIS	-	EXPRESSION TAG	UNP P22736
A	1	HIS	-	EXPRESSION TAG	UNP P22736
A	2	HIS	-	EXPRESSION TAG	UNP P22736
A	3	HIS	-	EXPRESSION TAG	UNP P22736
A	4	HIS	-	EXPRESSION TAG	UNP P22736
A	5	SER	-	EXPRESSION TAG	UNP P22736
A	6	SER	-	EXPRESSION TAG	UNP P22736
A	7	GLY	-	EXPRESSION TAG	UNP P22736
A	8	LEU	-	EXPRESSION TAG	UNP P22736
A	9	VAL	-	EXPRESSION TAG	UNP P22736
A	10	PRO	-	EXPRESSION TAG	UNP P22736
A	11	ARG	-	EXPRESSION TAG	UNP P22736
A	12	GLY	-	EXPRESSION TAG	UNP P22736
A	13	SER	-	EXPRESSION TAG	UNP P22736
A	14	HIS	-	EXPRESSION TAG	UNP P22736
A	15	MET	-	EXPRESSION TAG	UNP P22736

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	EXPRESSION TAG	UNP P22736
B	-4	GLY	-	EXPRESSION TAG	UNP P22736
B	-3	SER	-	EXPRESSION TAG	UNP P22736
B	-2	SER	-	EXPRESSION TAG	UNP P22736
B	-1	HIS	-	EXPRESSION TAG	UNP P22736
B	0	HIS	-	EXPRESSION TAG	UNP P22736
B	1	HIS	-	EXPRESSION TAG	UNP P22736
B	2	HIS	-	EXPRESSION TAG	UNP P22736
B	3	HIS	-	EXPRESSION TAG	UNP P22736
B	4	HIS	-	EXPRESSION TAG	UNP P22736
B	5	SER	-	EXPRESSION TAG	UNP P22736
B	6	SER	-	EXPRESSION TAG	UNP P22736
B	7	GLY	-	EXPRESSION TAG	UNP P22736
B	8	LEU	-	EXPRESSION TAG	UNP P22736
B	9	VAL	-	EXPRESSION TAG	UNP P22736
B	10	PRO	-	EXPRESSION TAG	UNP P22736
B	11	ARG	-	EXPRESSION TAG	UNP P22736
B	12	GLY	-	EXPRESSION TAG	UNP P22736
B	13	SER	-	EXPRESSION TAG	UNP P22736
B	14	HIS	-	EXPRESSION TAG	UNP P22736
B	15	MET	-	EXPRESSION TAG	UNP P22736
C	-5	MET	-	EXPRESSION TAG	UNP P22736
C	-4	GLY	-	EXPRESSION TAG	UNP P22736
C	-3	SER	-	EXPRESSION TAG	UNP P22736
C	-2	SER	-	EXPRESSION TAG	UNP P22736
C	-1	HIS	-	EXPRESSION TAG	UNP P22736
C	0	HIS	-	EXPRESSION TAG	UNP P22736
C	1	HIS	-	EXPRESSION TAG	UNP P22736
C	2	HIS	-	EXPRESSION TAG	UNP P22736
C	3	HIS	-	EXPRESSION TAG	UNP P22736
C	4	HIS	-	EXPRESSION TAG	UNP P22736
C	5	SER	-	EXPRESSION TAG	UNP P22736
C	6	SER	-	EXPRESSION TAG	UNP P22736
C	7	GLY	-	EXPRESSION TAG	UNP P22736
C	8	LEU	-	EXPRESSION TAG	UNP P22736
C	9	VAL	-	EXPRESSION TAG	UNP P22736
C	10	PRO	-	EXPRESSION TAG	UNP P22736
C	11	ARG	-	EXPRESSION TAG	UNP P22736
C	12	GLY	-	EXPRESSION TAG	UNP P22736
C	13	SER	-	EXPRESSION TAG	UNP P22736
C	14	HIS	-	EXPRESSION TAG	UNP P22736
C	15	MET	-	EXPRESSION TAG	UNP P22736

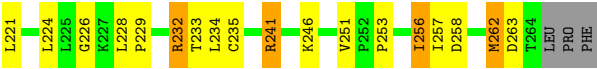
Continued on next page...

Continued from previous page...

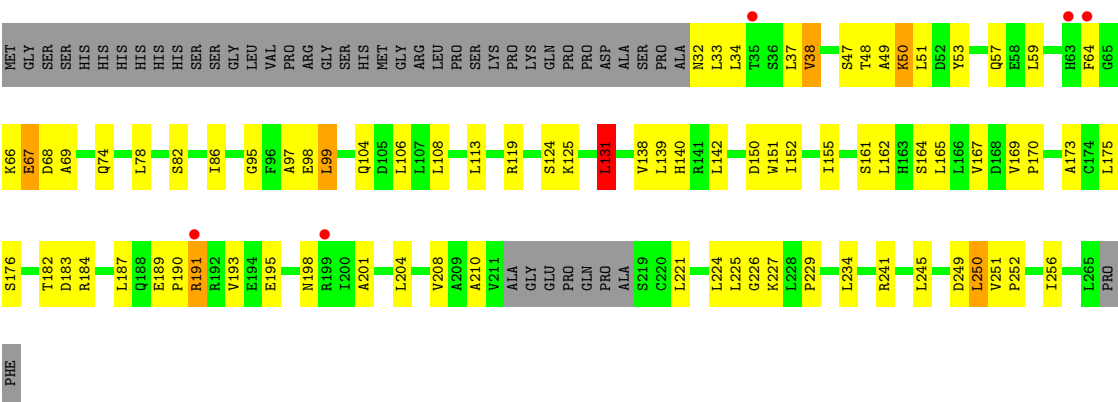
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	EXPRESSION TAG	UNP P22736
D	-4	GLY	-	EXPRESSION TAG	UNP P22736
D	-3	SER	-	EXPRESSION TAG	UNP P22736
D	-2	SER	-	EXPRESSION TAG	UNP P22736
D	-1	HIS	-	EXPRESSION TAG	UNP P22736
D	0	HIS	-	EXPRESSION TAG	UNP P22736
D	1	HIS	-	EXPRESSION TAG	UNP P22736
D	2	HIS	-	EXPRESSION TAG	UNP P22736
D	3	HIS	-	EXPRESSION TAG	UNP P22736
D	4	HIS	-	EXPRESSION TAG	UNP P22736
D	5	SER	-	EXPRESSION TAG	UNP P22736
D	6	SER	-	EXPRESSION TAG	UNP P22736
D	7	GLY	-	EXPRESSION TAG	UNP P22736
D	8	LEU	-	EXPRESSION TAG	UNP P22736
D	9	VAL	-	EXPRESSION TAG	UNP P22736
D	10	PRO	-	EXPRESSION TAG	UNP P22736
D	11	ARG	-	EXPRESSION TAG	UNP P22736
D	12	GLY	-	EXPRESSION TAG	UNP P22736
D	13	SER	-	EXPRESSION TAG	UNP P22736
D	14	HIS	-	EXPRESSION TAG	UNP P22736
D	15	MET	-	EXPRESSION TAG	UNP P22736

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0



● Molecule 1: Orphan nuclear receptor NR4A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.53Å 96.36Å 144.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.80 48.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.17-2.80) 98.5 (48.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.292 0.227 , 0.294	Depositor DCC
R_{free} test set	1566 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.76	5/1816 (0.3%)	0.93	5/2457 (0.2%)
1	B	0.78	2/1829 (0.1%)	0.89	2/2475 (0.1%)
1	C	0.73	2/1814 (0.1%)	0.79	1/2455 (0.0%)
1	D	0.63	0/1822	0.73	1/2465 (0.0%)
All	All	0.73	9/7281 (0.1%)	0.84	9/9852 (0.1%)

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
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	PRO	N-CA	11.82	1.67	1.47
1	A	217	PRO	CA-CB	-8.18	1.37	1.53
1	A	191	ARG	CZ-NH2	-7.26	1.23	1.33
1	C	74	GLN	CB-CG	7.17	1.71	1.52
1	A	217	PRO	CA-C	-6.39	1.40	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	PRO	N-CA-CB	18.06	124.97	103.30
1	A	191	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	A	191	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	217	PRO	N-CA-C	-6.64	94.83	112.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	CYS	N-CA-C	6.32	128.06	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	SER	Peptide
1	B	50	LYS	Peptide
1	C	30	PRO	Peptide

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	1781	0	1805	45	0
1	B	1793	0	1821	53	0
1	C	1777	0	1819	30	0
1	D	1786	0	1827	40	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	7147	0	7272	167	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 12.

The worst 5 of 167 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:C:117:ILE:HD12	1:C:235:CYS:SG	1.91	1.10
1:B:221:LEU:H	1:B:221:LEU:HD23	1.20	1.05
1:C:184:ARG:HH12	1:C:232:ARG:HH12	1.05	1.02
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.26	0.98
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.37	0.90

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	226/273 (83%)	204 (90%)	17 (8%)	5 (2%)	7	25
1	B	226/273 (83%)	201 (89%)	15 (7%)	10 (4%)	3	9
1	C	223/273 (82%)	190 (85%)	27 (12%)	6 (3%)	5	19
1	D	223/273 (82%)	205 (92%)	12 (5%)	6 (3%)	5	19
All	All	898/1092 (82%)	800 (89%)	71 (8%)	27 (3%)	5	16

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ALA
1	A	212	ALA
1	A	250	LEU
1	B	211	VAL
1	C	31	ALA

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	193/235 (82%)	172 (89%)	21 (11%)	7	21
1	B	195/235 (83%)	172 (88%)	23 (12%)	6	17
1	C	195/235 (83%)	171 (88%)	24 (12%)	5	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	197/235 (84%)	175 (89%)	22 (11%)	6	20
All	All	780/940 (83%)	690 (88%)	90 (12%)	6	19

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	ARG
1	C	99	LEU
1	D	176	SER
1	B	232	ARG
1	C	50	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	63	HIS
1	C	74	GLN
1	D	140	HIS
1	C	57	GLN
1	C	240	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	230/273 (84%)	0.01	3 (1%) 77 71	30, 52, 72, 77	0
1	B	230/273 (84%)	0.07	4 (1%) 70 63	31, 51, 65, 74	0
1	C	227/273 (83%)	0.08	2 (0%) 84 79	38, 54, 72, 81	0
1	D	227/273 (83%)	0.14	5 (2%) 62 52	46, 62, 81, 85	0
All	All	914/1092 (83%)	0.08	14 (1%) 73 67	30, 54, 77, 85	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	HIS	4.0
1	B	62	PRO	3.7
1	B	217	PRO	3.4
1	D	64	PHE	3.4
1	D	63	HIS	3.2

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.