



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 02:23 PM EDT

PDB ID : 3F5C  
Title : Structure of Dax-1:LRH-1 complex  
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Deposited on : 2008-11-03  
Resolution : 3.00 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](mailto: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.

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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	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

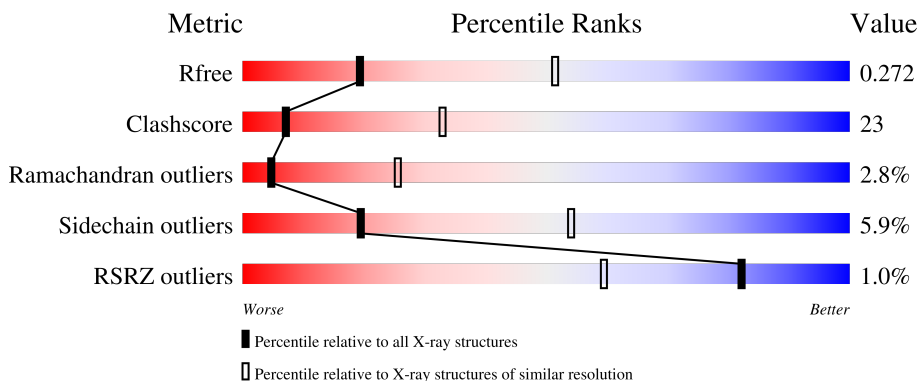
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	248	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>43%</div> <div>7%</div> </div> </div>
2	B	268	<div> <div></div> <div> <div>39%</div> <div>27%</div> <div>32%</div> </div> </div>
2	C	268	<div> <div>%</div> <div> <div>38%</div> <div>27%</div> <div>32%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4936 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 Nuclear receptor subfamily 5 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1983	1270	337	367	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	LEU	ILE	engineered mutation	UNP P45448

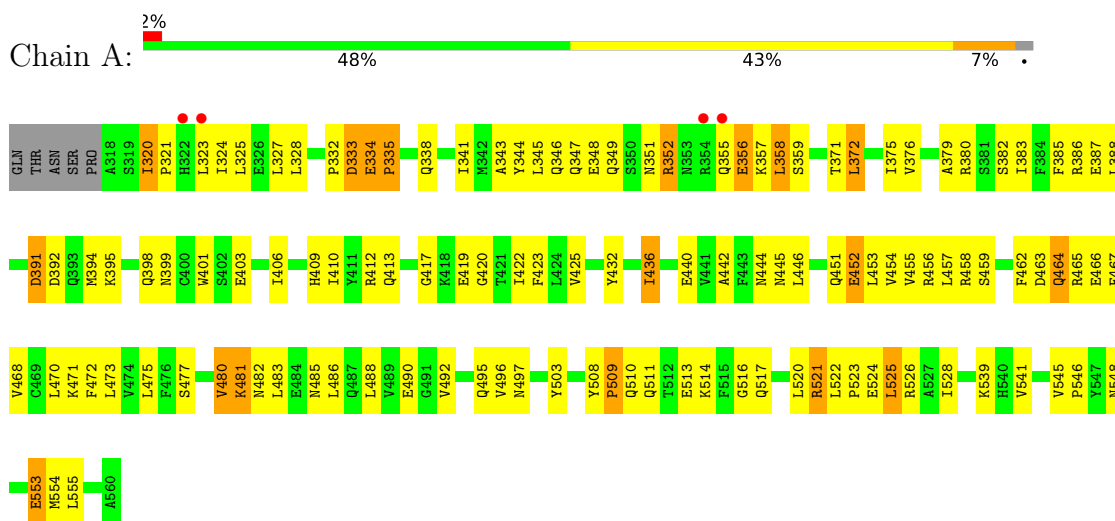
- Molecule 2 is a protein called Nuclear receptor subfamily 0 group B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1485	970	243	257	15			
2	C	181	Total	C	N	O	S	0	0	0
			1468	958	240	255	15			

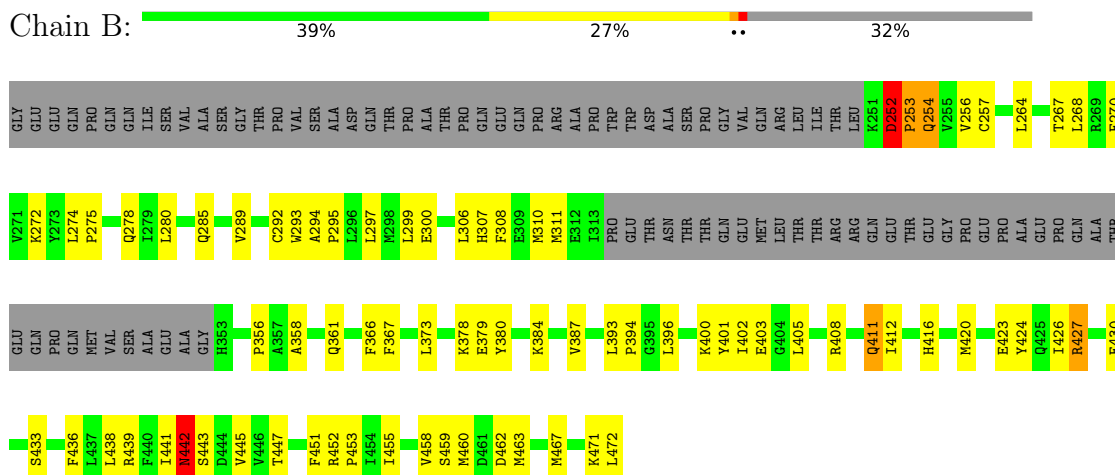
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Nuclear receptor subfamily 5 group A member 2



- Molecule 2: Nuclear receptor subfamily 0 group B member 1



- Molecule 2: Nuclear receptor subfamily 0 group B member 1



R427	E430	L435	F436	L437	L438	R439	F440	I441	N442	S443	D444	V445	E448	L449	F450	F451	R452	P453	I454	I455	G456	A457	V458	S459	M460	D461	L465	K471	L472																												
GLN	MET	VAL	SER	ALA	GLU	ALA	GLY	R353	L354	L355	P356	A359	I363	F366	F367	L373	Y380	L383	K384	V387	L388	F389	R390	P391	D392	L393	P394	G395	L396	V399	I402	E403	Q406	R407	R408	I412	L413	T414	E415	R418	M419	M420	Q421	R422	E423	I426											
GLY	GLU	GLN	PRO	GLN	GLN	ILE	SER	VAL	ALA	SER	GLY	THR	PRO	VAL	SER	ALA	ASP	GLN	THR	PRO	ALA	THR	PRO	GLN	GLN	PRO	ARG	ALA	TRP	TRP	ASP	ALA	SER	PRO	GLY	VAL	GLN	ARG	LEU	ILE	THR	LEU	LYS	D252	P253	Q254	V255	V256	C257	E258	A262	K266	T267				
F270	V271	K272	Y273	L274	F277	Q278	L279	P281	L280	L282	D283	Q284	Q285	L286	V287	W293	A294	P295	L296	L297	M298	Q303	E312	ILE	PRO	PRO	GLU	THR	ASN	THR	THR	THR	GLN	GLU	MET	LEU	THR	THR	ARG	ARG	GLN	GLU	THR	GLU	GLY	PRO	GLU	PRO	GLU	ALA	PRO	GLN	ALA	THR	GLU	GLN	PRO

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.36Å 103.36Å 117.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 3.00 47.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.79-3.00) 98.3 (47.30-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX, CNS	Depositor
R, $R_{free}$	0.222 , 0.279 0.219 , 0.272	Depositor DCC
$R_{free}$ test set	703 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/2019	0.63	1/2731 (0.0%)
2	B	0.56	0/1517	0.65	0/2050
2	C	0.51	0/1500	0.62	1/2028 (0.0%)
All	All	0.52	0/5036	0.63	2/6809 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLU	N-CA-C	5.79	126.62	111.00
2	C	389	PHE	CB-CA-C	-5.63	99.15	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	1983	0	1997	100	0
2	B	1485	0	1523	65	0
2	C	1468	0	1499	64	0
All	All	4936	0	5019	226	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 23.

The worst 5 of 226 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:358:LEU:HB2	1:A:359:SER:HA	1.44	0.99
1:A:356:GLU:O	1:A:356:GLU:HG2	1.64	0.98
1:A:333:ASP:O	1:A:334:GLU:HB2	1.65	0.94
2:C:282:LEU:HA	2:C:285:GLN:HB3	1.52	0.91
1:A:358:LEU:CB	1:A:359:SER:HA	2.00	0.86

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	241/248 (97%)	205 (85%)	26 (11%)	10 (4%)	3	16
2	B	179/268 (67%)	154 (86%)	20 (11%)	5 (3%)	5	25
2	C	177/268 (66%)	144 (81%)	31 (18%)	2 (1%)	14	50
All	All	597/784 (76%)	503 (84%)	77 (13%)	17 (3%)	5	25

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	ASP
1	A	334	GLU
1	A	358	LEU
2	B	423	GLU
1	A	480	VAL

### 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	221/226 (98%)	208 (94%)	13 (6%)	19	54
2	B	164/235 (70%)	154 (94%)	10 (6%)	18	53
2	C	162/235 (69%)	153 (94%)	9 (6%)	21	56
All	All	547/696 (79%)	515 (94%)	32 (6%)	19	54

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	402	ILE
2	C	418	ARG
1	A	553	GLU
1	A	525	LEU
2	C	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	425	GLN
2	C	278	GLN
2	C	410	GLN
2	C	285	GLN
2	C	254	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	243/248 (97%)	-0.34	4 (1%) 72 44	68, 121, 197, 256	0
2	B	183/268 (68%)	-0.53	0 100 100	64, 97, 156, 190	0
2	C	181/268 (67%)	-0.41	2 (1%) 80 56	75, 105, 180, 207	0
All	All	607/784 (77%)	-0.42	6 (0%) 82 59	64, 108, 182, 256	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	457	ALA	4.3
1	A	355	GLN	4.0
1	A	354	ARG	3.2
1	A	323	LEU	3.1
1	A	322	HIS	2.9

### 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 monosaccharides 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.