



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 18, 2019 – 04:13 AM EDT

PDB ID : 3F5C
Title : Structure of Dax-1:LRH-1 complex
Authors : Fletterick, R.J.; Sablin, E.P.
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

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 : 2.3.2
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) : 2.3.2

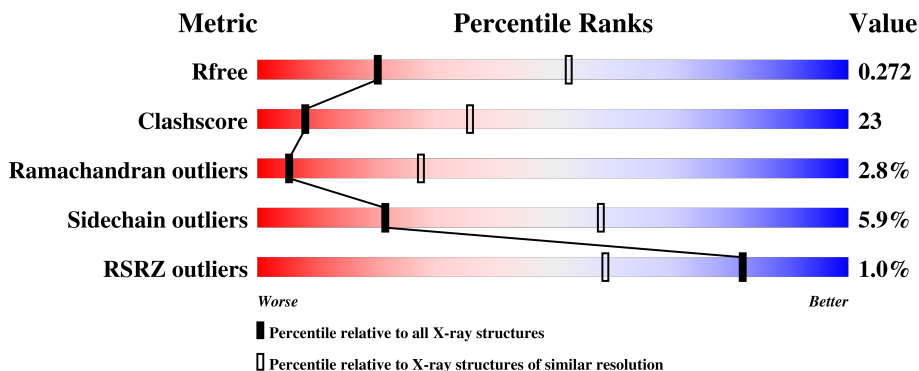
1 Overall quality at a glance

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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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 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	248	<div> <div>2%</div> <div>48%</div> <div>43%</div> <div>7%</div> <div>.</div> </div>
2	B	268	<div> <div>39%</div> <div>27%</div> <div>..</div> <div>32%</div> </div>
2	C	268	<div> <div>%</div> <div>38%</div> <div>27%</div> <div>.</div> <div>32%</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.

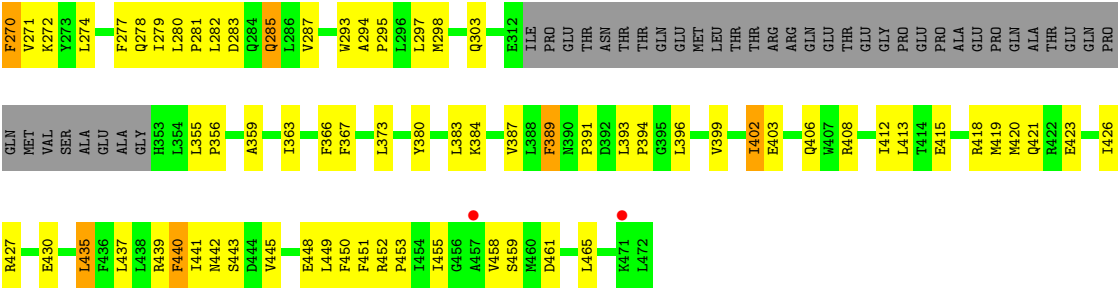
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1983	1270	337	367	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	LEU	ILE	ENGINEERED	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			



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	79.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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	0.49	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	18
2	B	179/268 (67%)	154 (86%)	20 (11%)	5 (3%)	5	28
2	C	177/268 (66%)	144 (81%)	31 (18%)	2 (1%)	16	53
All	All	597/784 (76%)	503 (84%)	77 (13%)	17 (3%)	5	28

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%)	21	58
2	B	164/235 (70%)	154 (94%)	10 (6%)	20	57
2	C	162/235 (69%)	153 (94%)	9 (6%)	23	60
All	All	547/696 (79%)	515 (94%)	32 (6%)	21	58

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

Mol	Chain	Res	Type
2	B	254	GLN
2	B	299	LEU
2	C	418	ARG
2	B	297	LEU
2	B	310	MET

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

Mol	Chain	Res	Type
1	A	510	GLN
2	B	361	GLN
2	C	278	GLN
1	A	497	ASN
2	C	285	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 [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	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 55	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 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.