



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:25 PM GMT

PDB ID : 1OVL
Title : Crystal Structure of Nurr1 LBD
Authors : Wang, Z.; Liu, J.; Walker, N.
Deposited on : 2003-03-26
Resolution : 2.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

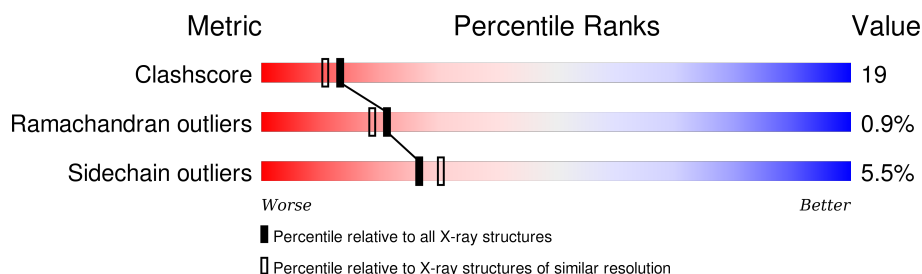
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	271	
1	D	271	
2	B	271	
2	C	271	
2	E	271	
2	F	271	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	E	815	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11703 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 NURR1 (MSE 414, 496, 511).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	Se	0	0	0
			1819	1169	310	331	7	2			
1	D	230	Total	C	N	O	S	Se	0	0	0
			1834	1178	312	335	7	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
A	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
D	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
D	511	MSE	MET	MODIFIED RESIDUE	UNP P43354

- Molecule 2 is a protein called Orphan nuclear receptor NURR1 (MSE 496, 511).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	Se	0	0	0
			1881	1206	319	346	7	3			
2	C	226	Total	C	N	O	S	Se	0	0	0
			1803	1160	304	330	6	3			
2	E	250	Total	C	N	O	S	Se	0	0	0
			1992	1271	346	365	7	3			
2	F	223	Total	C	N	O	S	Se	0	0	0
			1784	1149	301	325	6	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
B	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
B	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
C	414	MSE	MET	MODIFIED RESIDUE	UNP P43354

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
C	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
E	511	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	414	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	496	MSE	MET	MODIFIED RESIDUE	UNP P43354
F	511	MSE	MET	MODIFIED RESIDUE	UNP P43354

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total K 3 3	0	0
3	A	1	Total K 1 1	0	0
3	D	2	Total K 2 2	0	0
3	F	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total Br 4 4	0	0
4	E	7	Total Br 7 7	0	0
4	B	1	Total Br 1 1	0	0
4	C	1	Total Br 1 1	0	0
4	A	4	Total Br 4 4	0	0
4	F	2	Total Br 2 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total I 1 1	0	0

- Molecule 6 is water.

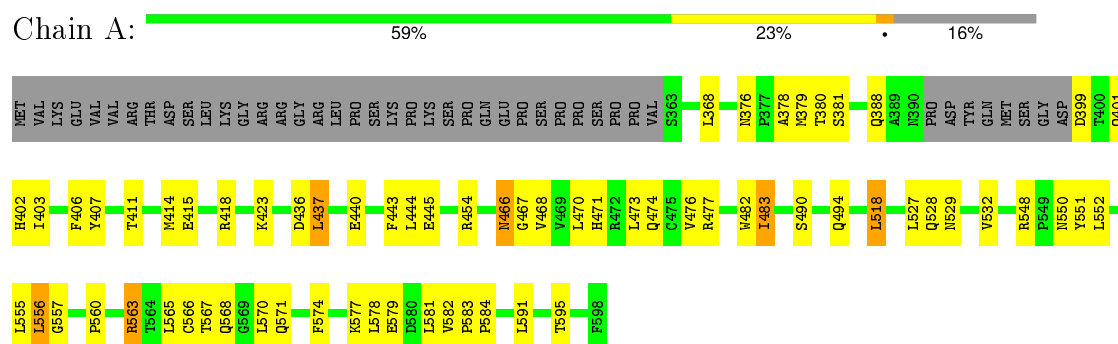
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	88	Total O 88 88	0	0
6	B	100	Total O 100 100	0	0
6	C	68	Total O 68 68	0	0
6	D	107	Total O 107 107	0	0
6	E	114	Total O 114 114	0	0
6	F	85	Total O 85 85	0	0

3 Residue-property plots

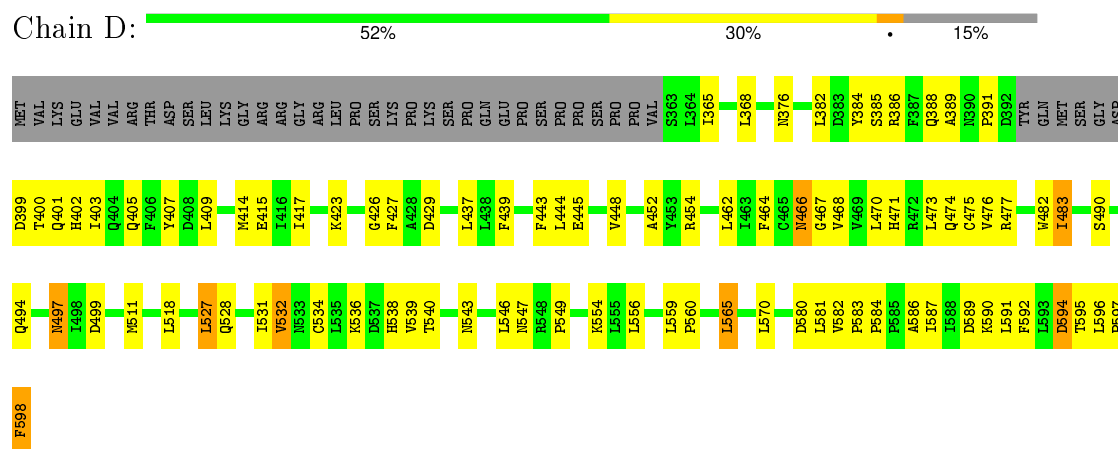
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

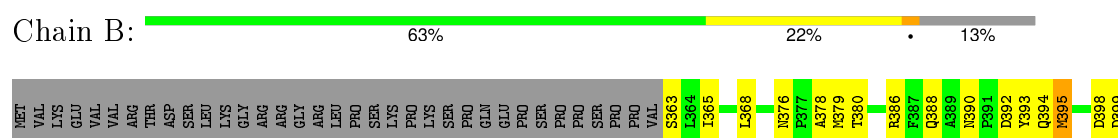
- Molecule 1: Orphan nuclear receptor NURR1 (MSE 414, 496, 511)

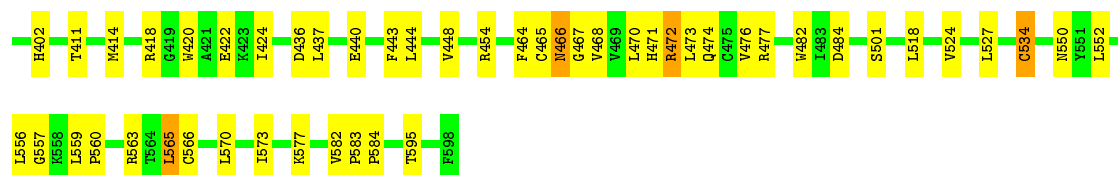


- Molecule 1: Orphan nuclear receptor NURR1 (MSE 414, 496, 511)



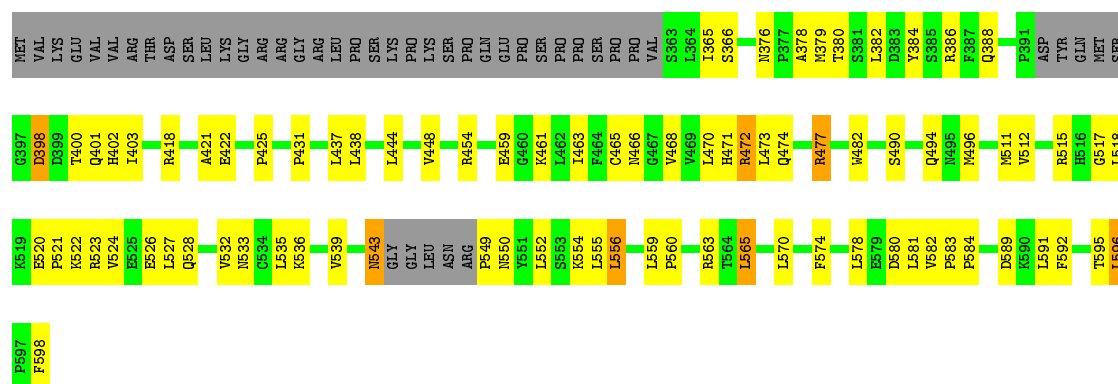
- Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)





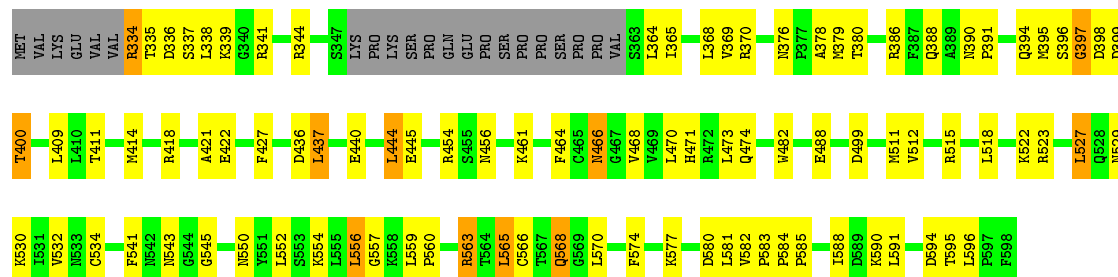
- Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain C: 52% 28% 17%



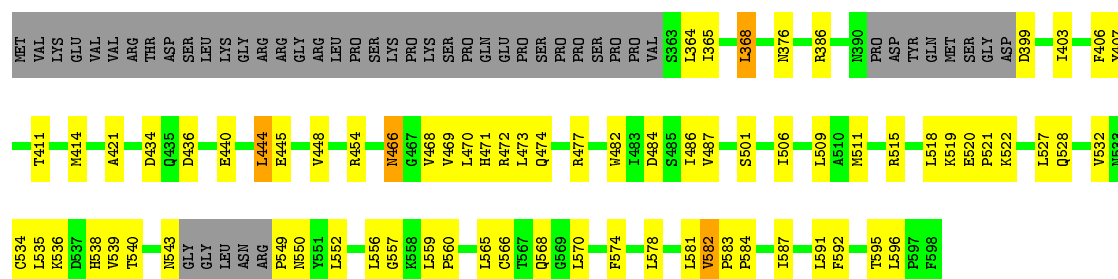
- Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain E: 58% 30% 8%



- Molecule 2: Orphan nuclear receptor NURR1 (MSE 496, 511)

Chain F: 55% 26% 18%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	80.38 Å 80.38 Å 227.37 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.7 (500.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.217 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11703	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, BR

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	0.35	0/1854	0.54	0/2505
1	D	0.34	0/1870	0.56	0/2528
2	B	0.36	0/1918	0.56	0/2592
2	C	0.34	1/1837 (0.1%)	0.53	0/2480
2	E	0.35	0/2029	0.55	0/2737
2	F	0.33	0/1817	0.51	0/2452
All	All	0.35	1/11325 (0.0%)	0.54	0/15294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	465	CYS	CB-SG	5.29	1.91	1.82

There are no bond angle outliers.

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	1819	0	1837	70	0
1	D	1834	0	1848	80	0
2	B	1881	0	1887	57	0
2	C	1803	0	1815	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1992	0	2007	82	0
2	F	1784	0	1801	61	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	1	0
4	E	7	0	0	2	0
4	F	2	0	0	0	0
5	B	1	0	0	1	0
6	A	88	0	0	11	0
6	B	100	0	0	4	0
6	C	68	0	0	2	0
6	D	107	0	0	4	0
6	E	114	0	0	4	0
6	F	85	0	0	5	0
All	All	11703	0	11195	420	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 19.

The worst 5 of 420 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)
2:F:471:HIS:H	2:F:474:GLN:HE21	0.98	0.95
2:E:365:ILE:HG13	2:E:534:CYS:SG	2.10	0.91
2:B:388:GLN:HE21	2:B:390:ASN:H	1.21	0.89
2:C:472:ARG:HH11	2:C:472:ARG:HG3	1.40	0.87
2:E:563:ARG:HH11	2:E:563:ARG:HB2	1.38	0.87

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	224/271 (83%)	216 (96%)	7 (3%)	1 (0%)	39	42
1	D	226/271 (83%)	215 (95%)	8 (4%)	3 (1%)	15	11
2	B	234/271 (86%)	225 (96%)	5 (2%)	4 (2%)	11	7
2	C	220/271 (81%)	209 (95%)	11 (5%)	0	100	100
2	E	246/271 (91%)	236 (96%)	6 (2%)	4 (2%)	12	8
2	F	217/271 (80%)	209 (96%)	8 (4%)	0	100	100
All	All	1367/1626 (84%)	1310 (96%)	45 (3%)	12 (1%)	21	19

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	MET
2	B	465	CYS
2	E	395	MET
2	E	396	SER
2	B	379	MET

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	202/240 (84%)	191 (95%)	11 (5%)	27	31
1	D	204/240 (85%)	192 (94%)	12 (6%)	24	27
2	B	209/239 (87%)	198 (95%)	11 (5%)	28	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	201/239 (84%)	190 (94%)	11 (6%)	27	30
2	E	221/239 (92%)	206 (93%)	15 (7%)	20	21
2	F	199/239 (83%)	191 (96%)	8 (4%)	38	47
All	All	1236/1436 (86%)	1168 (94%)	68 (6%)	27	30

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	565	LEU
1	D	518	LEU
2	F	466	ASN
2	C	596	LEU
1	D	415	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	542	ASN
1	D	404	GLN
2	F	474	GLN
2	C	543	ASN
1	D	376	ASN

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

Of 28 ligands modelled in this entry, 28 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.