



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:57 am GMT

PDB ID : 1PDU
Title : Ligand-binding domain of Drosophila orphan nuclear receptor DHR38
Authors : Baker, K.D.; Shewchuk, L.M.; Korlova, T.; Makishima, M.; Hassell, A.M.; Wisely, B.; Caravella, J.A.; Lambert, M.H.; Wilson, T.M.; Mangelsdorf, D.J.
Deposited on : 2003-05-20
Resolution : 2.30 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

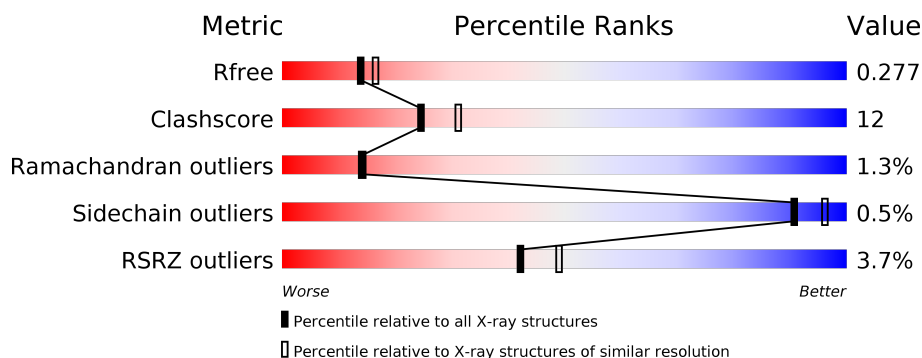
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	244	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• 6%</div> </div> </div>
1	B	244	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3803 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 hormone receptor HR38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1823	1172	306	336	9			
1	B	228	Total	C	N	O	S	0	0	0
			1809	1164	303	333	9			

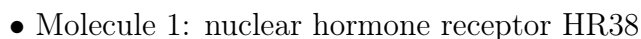
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	MET	-	EXPRESSION TAG	UNP P49869
A	309	LYS	-	EXPRESSION TAG	UNP P49869
A	310	LYS	-	EXPRESSION TAG	UNP P49869
A	311	GLY	-	EXPRESSION TAG	UNP P49869
A	312	HIS	-	EXPRESSION TAG	UNP P49869
A	313	HIS	-	EXPRESSION TAG	UNP P49869
A	314	HIS	-	EXPRESSION TAG	UNP P49869
A	315	HIS	-	EXPRESSION TAG	UNP P49869
A	316	HIS	-	EXPRESSION TAG	UNP P49869
A	317	HIS	-	EXPRESSION TAG	UNP P49869
A	318	GLY	-	EXPRESSION TAG	UNP P49869
A	319	ALA	-	EXPRESSION TAG	UNP P49869
B	308	MET	-	EXPRESSION TAG	UNP P49869
B	309	LYS	-	EXPRESSION TAG	UNP P49869
B	310	LYS	-	EXPRESSION TAG	UNP P49869
B	311	GLY	-	EXPRESSION TAG	UNP P49869
B	312	HIS	-	EXPRESSION TAG	UNP P49869
B	313	HIS	-	EXPRESSION TAG	UNP P49869
B	314	HIS	-	EXPRESSION TAG	UNP P49869
B	315	HIS	-	EXPRESSION TAG	UNP P49869
B	316	HIS	-	EXPRESSION TAG	UNP P49869
B	317	HIS	-	EXPRESSION TAG	UNP P49869
B	318	GLY	-	EXPRESSION TAG	UNP P49869
B	319	ALA	-	EXPRESSION TAG	UNP P49869

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total 85	O 85	0	0
2	B	86	Total 86	O 86	0	0

- Molecule 1: nuclear hormone receptor HR38



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.38Å 82.23Å 84.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.95 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.30) 89.5 (19.95-2.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.270 0.223 , 0.277	Depositor DCC
R_{free} test set	2342 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3803	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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

5.1 Standard geometry

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	0.38	0/1859	0.55	0/2520
1	B	0.38	0/1845	0.55	0/2501
All	All	0.38	0/3704	0.55	0/5021

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1823	0	1808	42	0
1	B	1809	0	1795	47	0
2	A	85	0	0	4	0
2	B	86	0	0	8	0
All	All	3803	0	3603	89	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.

All (89) 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:459:LEU:HD11	1:B:508:LEU:HD11	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LEU:HD21	1:B:508:LEU:HG	1.55	0.86
1:B:472:ARG:HG3	1:B:472:ARG:HH11	1.45	0.81
1:B:350:MET:HE2	1:B:354:ASP:HB3	1.65	0.78
1:B:398:GLU:HG3	2:B:22:HOH:O	1.82	0.78
1:B:459:LEU:HD11	1:B:508:LEU:CD1	2.15	0.73
1:B:350:MET:CE	1:B:354:ASP:HB3	2.19	0.72
1:A:362:LEU:HD11	1:A:417:PHE:CG	2.26	0.71
1:A:466:THR:HA	1:A:481:GLN:NE2	2.08	0.68
1:A:350:MET:HE3	1:A:354:ASP:HB3	1.76	0.68
1:A:323:ILE:HD11	1:A:454:SER:HB3	1.77	0.67
1:A:413:THR:O	1:A:425:ARG:HG3	1.95	0.67
1:A:459:LEU:HD21	1:A:508:LEU:HG	1.77	0.66
1:A:530:LYS:HE2	1:A:542:GLU:OE2	1.96	0.65
1:B:327:VAL:HG22	1:B:454:SER:HA	1.79	0.64
1:A:412:ASP:OD1	1:A:414:LYS:HG2	2.00	0.61
1:A:350:MET:CE	1:A:354:ASP:HB3	2.30	0.61
1:A:362:LEU:HD21	1:A:417:PHE:CE2	2.35	0.61
1:B:386:GLU:CD	1:B:386:GLU:H	2.05	0.61
1:B:322:LEU:HD13	1:B:378:PRO:HG2	1.85	0.59
1:B:472:ARG:CG	1:B:472:ARG:HH11	2.17	0.57
1:A:407:ARG:HD2	2:A:53:HOH:O	2.03	0.56
1:A:416:ILE:HG12	1:A:422:VAL:HG22	1.88	0.56
1:A:412:ASP:HB3	1:A:425:ARG:NH2	2.22	0.55
1:A:432:PHE:O	1:A:525:ARG:HG3	2.07	0.55
1:B:512:LEU:HB2	1:B:513:PRO:HD3	1.87	0.55
1:B:368:ASP:O	1:B:371:LYS:HB3	2.07	0.55
1:B:327:VAL:CG2	1:B:454:SER:HA	2.38	0.54
1:A:466:THR:HA	1:A:481:GLN:HE21	1.73	0.53
1:A:459:LEU:HD11	1:A:508:LEU:HD11	1.90	0.53
1:A:361:GLN:NE2	2:A:109:HOH:O	2.41	0.53
1:B:337:PRO:HG3	2:B:100:HOH:O	2.07	0.53
1:A:362:LEU:HD21	1:A:417:PHE:CZ	2.44	0.52
1:B:440:MET:O	1:B:443:SER:HB3	2.09	0.52
1:A:322:LEU:CD1	1:A:378:PRO:HG2	2.40	0.52
1:A:322:LEU:HD13	1:A:378:PRO:HG2	1.92	0.52
1:B:472:ARG:HG3	1:B:472:ARG:NH1	2.20	0.51
1:A:415:LEU:HD13	1:A:440:MET:HE1	1.94	0.50
1:B:468:ARG:NH1	1:B:516:ARG:CZ	2.74	0.50
1:B:468:ARG:NH1	1:B:516:ARG:NH2	2.60	0.50
1:B:335:PRO:HG3	2:B:97:HOH:O	2.12	0.49
1:A:395:ALA:HB2	1:A:468:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:C	1:A:548:THR:H	2.16	0.49
1:B:322:LEU:CD1	1:B:378:PRO:HG2	2.42	0.48
1:A:407:ARG:HH11	1:A:407:ARG:HG2	1.78	0.48
1:A:327:VAL:HG22	1:A:454:SER:HA	1.96	0.48
1:A:503:HIS:CE1	1:A:505:PHE:HB3	2.49	0.47
1:B:322:LEU:O	1:B:326:LEU:HG	2.13	0.47
1:B:407:ARG:NH1	2:B:99:HOH:O	2.48	0.47
1:B:350:MET:HE2	1:B:354:ASP:CB	2.41	0.46
1:A:459:LEU:HD11	1:A:508:LEU:CD1	2.46	0.46
1:B:467:GLU:C	1:B:468:ARG:HG2	2.35	0.46
1:B:434:GLU:OE1	1:B:437:ASN:ND2	2.48	0.46
1:B:415:LEU:HD13	1:B:440:MET:HE3	1.97	0.45
1:A:502:GLN:O	1:A:503:HIS:C	2.54	0.45
1:B:432:PHE:O	1:B:525:ARG:HG3	2.16	0.45
1:B:538:PRO:HD2	1:B:541:ILE:HG13	1.99	0.44
1:B:362:LEU:HD11	1:B:417:PHE:CG	2.52	0.44
1:A:364:THR:HA	1:A:540:LEU:HD23	1.99	0.44
1:B:350:MET:HE2	1:B:354:ASP:C	2.38	0.44
1:B:386:GLU:N	1:B:386:GLU:CD	2.70	0.44
1:B:468:ARG:HH12	1:B:516:ARG:NE	2.14	0.44
1:B:416:ILE:HG12	1:B:422:VAL:HG22	1.99	0.44
1:A:404:LEU:HD11	1:A:415:LEU:HG	2.00	0.43
1:A:415:LEU:HD21	1:A:436:LEU:HD11	2.00	0.43
1:B:472:ARG:CG	1:B:472:ARG:NH1	2.76	0.43
1:A:407:ARG:NH1	2:A:94:HOH:O	2.52	0.43
1:B:412:ASP:OD2	1:B:414:LYS:HG2	2.18	0.43
1:A:406:TYR:O	1:A:447:HIS:CE1	2.71	0.43
1:A:364:THR:HG22	1:A:540:LEU:HB3	2.00	0.43
1:B:410:ILE:O	1:B:411:ASP:O	2.37	0.43
1:B:468:ARG:HH12	1:B:516:ARG:CZ	2.31	0.43
1:B:433:GLY:C	1:B:435:TRP:H	2.23	0.42
1:A:497:GLU:HA	1:A:500:LYS:HE3	2.00	0.41
1:A:482:MET:CE	1:A:485:ILE:HD12	2.51	0.41
1:B:407:ARG:HD2	2:B:26:HOH:O	2.18	0.41
1:B:476:LYS:HG2	2:B:140:HOH:O	2.19	0.41
1:A:330:HIS:HD2	1:A:453:ILE:HD11	1.86	0.41
1:A:345:TYR:CZ	1:A:424:HIS:CE1	3.09	0.41
1:B:376:LYS:HD3	2:B:117:HOH:O	2.20	0.41
1:B:403:ARG:HG2	2:B:98:HOH:O	2.19	0.41
1:B:435:TRP:CE2	1:B:439:ILE:HD11	2.56	0.41
1:A:403:ARG:NH1	2:A:52:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HA	1:A:415:LEU:HD12	1.85	0.41
1:B:323:ILE:HD11	1:B:454:SER:HB3	2.02	0.41
1:A:537:ALA:HA	1:A:538:PRO:HD3	1.90	0.40
1:B:488:LEU:O	1:B:492:VAL:HG23	2.21	0.40
1:B:546:VAL:HG12	1:B:546:VAL:O	2.20	0.40
1:A:368:ASP:O	1:A:371:LYS:HB3	2.22	0.40

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	228/244 (93%)	223 (98%)	2 (1%)	3 (1%)	14	14
1	B	226/244 (93%)	217 (96%)	6 (3%)	3 (1%)	14	14
All	All	454/488 (93%)	440 (97%)	8 (2%)	6 (1%)	14	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411	ASP
1	B	450	GLU
1	A	450	GLU
1	A	503	HIS
1	A	547	THR
1	B	337	PRO

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	198/221 (90%)	197 (100%)	1 (0%)	91	96
1	B	197/221 (89%)	196 (100%)	1 (0%)	91	96
All	All	395/442 (89%)	393 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	ARG
1	B	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	479	GLN
1	A	481	GLN
1	B	330	HIS
1	B	358	GLN
1	B	372	GLN
1	B	393	GLN
1	B	479	GLN
1	B	481	GLN
1	B	524	GLN

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

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 [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	230/244 (94%)	0.23	8 (3%) 44 51	27, 40, 59, 71	0
1	B	228/244 (93%)	0.24	9 (3%) 40 47	28, 41, 58, 68	0
All	All	458/488 (93%)	0.24	17 (3%) 42 49	27, 41, 59, 71	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	HIS	7.6
1	A	319	ALA	6.6
1	B	339	CYS	4.2
1	A	349	SER	4.0
1	A	411	ASP	4.0
1	B	410	ILE	3.8
1	A	410	ILE	3.6
1	B	349	SER	3.1
1	B	546	VAL	3.1
1	B	336	ASP	3.0
1	A	345	TYR	2.7
1	A	348	GLN	2.7
1	B	434	GLU	2.3
1	B	350	MET	2.1
1	A	434	GLU	2.1
1	B	429	LEU	2.1
1	A	459	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.