



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:45 PM GMT

PDB ID : 1YJE
Title : Crystal structure of the rNGFI-B ligand-binding domain
Authors : Flaig, R.; Greschik, H.; Peluso-Iltis, C.; Moras, D.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-01-14
Resolution : 2.40 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

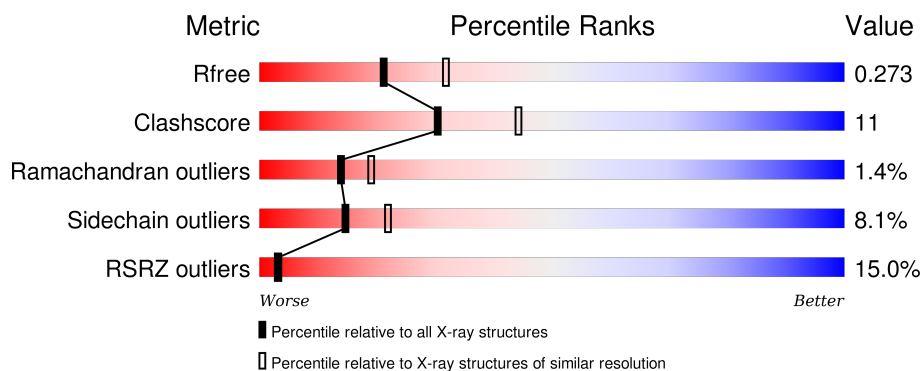
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	264	<div> <div>13%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1795 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	226	Total	C	N	O	S	0	0	0
			1726	1113	291	313	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	EXPRESSION TAG	UNP P22829
A	335	SER	-	EXPRESSION TAG	UNP P22829
A	336	SER	-	EXPRESSION TAG	UNP P22829
A	337	HIS	-	EXPRESSION TAG	UNP P22829
A	338	HIS	-	EXPRESSION TAG	UNP P22829
A	339	HIS	-	EXPRESSION TAG	UNP P22829
A	340	HIS	-	EXPRESSION TAG	UNP P22829
A	341	HIS	-	EXPRESSION TAG	UNP P22829
A	342	HIS	-	EXPRESSION TAG	UNP P22829
A	343	SER	-	EXPRESSION TAG	UNP P22829
A	344	SER	-	EXPRESSION TAG	UNP P22829
A	345	GLY	-	EXPRESSION TAG	UNP P22829
A	346	LEU	-	EXPRESSION TAG	UNP P22829
A	347	VAL	-	EXPRESSION TAG	UNP P22829
A	348	PRO	-	EXPRESSION TAG	UNP P22829
A	349	ARG	-	EXPRESSION TAG	UNP P22829
A	350	GLY	-	EXPRESSION TAG	UNP P22829
A	351	SER	-	EXPRESSION TAG	UNP P22829
A	352	HIS	-	EXPRESSION TAG	UNP P22829
A	353	MET	-	EXPRESSION TAG	UNP P22829

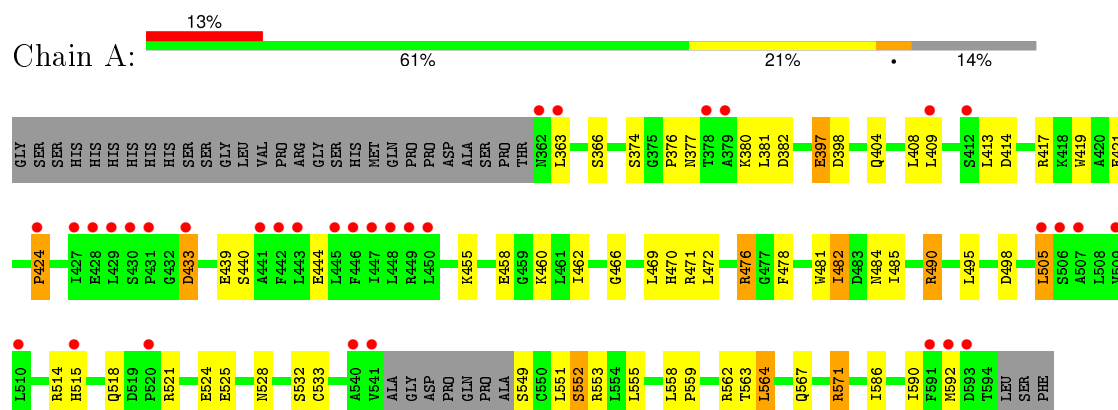
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	69	Total	O	0	0
			69	69		

3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Orphan nuclear receptor NR4A1



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.42Å 90.42Å 140.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 30.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.40) 99.2 (30.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.243 , 0.278 0.239 , 0.273	Depositor DCC
R_{free} test set	583 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 11676 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1795	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.67	0/1760	0.87	5/2388 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	382	ASP	CB-CG-OD2	9.46	126.82	118.30
1	A	414	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	398	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	505	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	498	ASP	CB-CG-OD2	5.38	123.14	118.30

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	1726	0	1727	38	0
2	A	69	0	0	6	0
All	All	1795	0	1727	38	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 11.

All (38) 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:417:ARG:O	1:A:421:GLU:HG2	1.83	0.79
1:A:397:GLU:HG2	1:A:476:ARG:O	1.90	0.71
1:A:563:THR:O	1:A:567:GLN:HG3	1.93	0.68
1:A:470:HIS:HD2	1:A:472:LEU:H	1.46	0.63
1:A:381:LEU:HD11	2:A:32:HOH:O	2.00	0.61
1:A:374:SER:CB	1:A:419:TRP:HB2	2.32	0.60
1:A:374:SER:HB3	1:A:419:TRP:HB2	1.86	0.57
1:A:458:GLU:OE1	1:A:460:LYS:HE3	2.05	0.57
1:A:471:ARG:HD2	2:A:58:HOH:O	2.03	0.57
1:A:470:HIS:CD2	1:A:472:LEU:H	2.23	0.57
1:A:363:LEU:HD12	1:A:424:PRO:HG2	1.87	0.56
1:A:490:ARG:NH1	2:A:13:HOH:O	2.39	0.55
1:A:549:SER:HB3	1:A:552:SER:HB3	1.90	0.54
1:A:413:LEU:HD22	1:A:586:ILE:HD13	1.90	0.53
1:A:478:PHE:O	1:A:571:ARG:HG3	2.11	0.50
1:A:439:GLU:O	1:A:590:ILE:HD11	2.11	0.50
1:A:563:THR:HG22	1:A:567:GLN:HE21	1.78	0.48
1:A:551:LEU:O	1:A:555:LEU:HG	2.13	0.47
1:A:440:SER:CB	1:A:514:ARG:HD2	2.44	0.47
1:A:417:ARG:CD	2:A:19:HOH:O	2.62	0.47
1:A:495:LEU:HD11	1:A:553:ARG:HB3	1.96	0.46
1:A:482:ILE:HA	1:A:482:ILE:HD13	1.83	0.45
1:A:521:ARG:O	1:A:525:GLU:HB2	2.16	0.45
1:A:440:SER:HB2	1:A:514:ARG:HD2	1.98	0.45
1:A:376:PRO:HB3	1:A:466:GLY:N	2.32	0.45
1:A:484:ASN:ND2	1:A:567:GLN:OE1	2.49	0.44
1:A:558:LEU:N	1:A:559:PRO:CD	2.81	0.44
1:A:433:ASP:OD1	1:A:433:ASP:N	2.48	0.44
1:A:397:GLU:HB3	1:A:476:ARG:HB3	1.99	0.44
1:A:404:GLN:HG3	2:A:71:HOH:O	2.19	0.43
1:A:481:TRP:CE2	1:A:485:ILE:HD11	2.54	0.42
1:A:444:GLU:OE1	1:A:562:ARG:NH1	2.48	0.42
1:A:363:LEU:HD23	1:A:533:CYS:SG	2.60	0.42
1:A:377:ASN:O	1:A:380:LYS:C	2.58	0.42
1:A:455:LYS:HD2	1:A:462:ILE:HD11	2.02	0.41
1:A:524:GLU:O	1:A:528:ASN:ND2	2.52	0.41
1:A:444:GLU:OE1	2:A:18:HOH:O	2.21	0.41
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.91	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	222/264 (84%)	208 (94%)	11 (5%)	3 (1%)	14 19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	GLN
1	A	424	PRO
1	A	515	HIS

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	185/228 (81%)	170 (92%)	15 (8%)	15 22

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	SER
1	A	397	GLU
1	A	408	LEU
1	A	409	LEU
1	A	433	ASP
1	A	469	LEU
1	A	476	ARG
1	A	482	ILE

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Mol	Chain	Res	Type
1	A	490	ARG
1	A	505	LEU
1	A	532	SER
1	A	552	SER
1	A	564	LEU
1	A	571	ARG
1	A	592	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	470	HIS
1	A	484	ASN
1	A	493	HIS
1	A	527	GLN
1	A	528	ASN
1	A	567	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 ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	226/264 (85%)	0.61	34 (15%) 3 3	39, 66, 99, 105	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	PHE	6.6
1	A	445	LEU	4.1
1	A	505	LEU	3.9
1	A	430	SER	3.9
1	A	446	PHE	3.5
1	A	428	GLU	3.5
1	A	433	ASP	3.5
1	A	592	MET	3.4
1	A	509	VAL	3.4
1	A	447	ILE	3.3
1	A	520	PRO	3.3
1	A	443	LEU	3.2
1	A	507	ALA	3.1
1	A	363	LEU	3.0
1	A	506	SER	2.9
1	A	515	HIS	2.8
1	A	540	ALA	2.7
1	A	429	LEU	2.6
1	A	431	PRO	2.6
1	A	378	THR	2.5
1	A	448	LEU	2.5
1	A	412	SER	2.5
1	A	409	LEU	2.4
1	A	541	VAL	2.3
1	A	442	PHE	2.3
1	A	450	LEU	2.3
1	A	424	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	441	ALA	2.2
1	A	593	ASP	2.1
1	A	427	ILE	2.1
1	A	379	ALA	2.1
1	A	362	ASN	2.1
1	A	449	ARG	2.0
1	A	510	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.