Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 06:33 pm GMT

PDB ID	:	6F5N
Title	:	Nickel-Bound Crystal Structure of a GB1 Variant
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Deposited on	:	2017-12-01
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

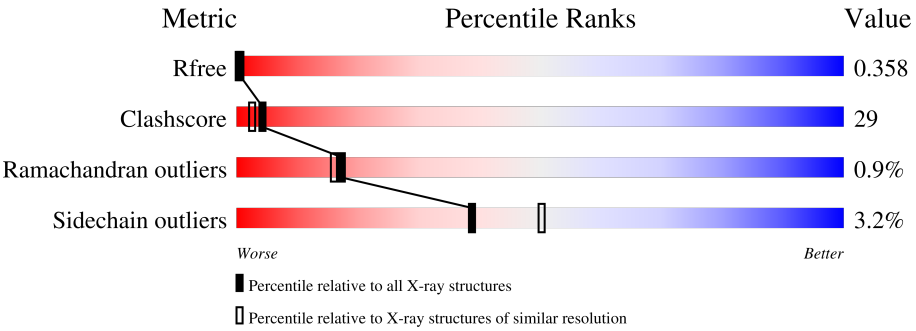
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	56	57% 38% 5%
1	B	56	45% 52% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 974 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 Nickel-Binding Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	1	0
			459	293	73	92	1			
1	B	56	Total	C	N	O	S	0	0	0
			450	287	71	91	1			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

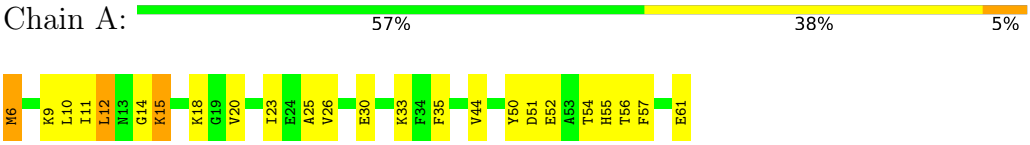
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	37	Total	O	0	0
			37	37		

3 Residue-property plots (i)

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. 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. 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.

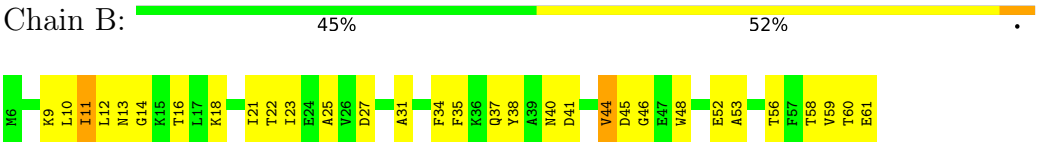
• Molecule 1: Nickel-Binding Protein

Chain A:



• Molecule 1: Nickel-Binding Protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	26.68Å 59.33Å 75.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.20 46.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	79.2 (46.70-2.20) 74.1 (46.70-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.257 , 0.356 0.258 , 0.358	Depositor DCC
R_{free} test set	520 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	2.851	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 89.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	974	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1608e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.47	0/468	0.74	1/630 (0.2%)
1	B	0.44	0/459	0.69	0/619
All	All	0.45	0/927	0.72	1/1249 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	LEU	CA-CB-CG	5.68	128.36	115.30

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	459	0	437	23	0
1	B	450	0	425	29	0
2	A	1	0	0	0	0
3	A	27	0	0	4	0
3	B	37	0	0	7	0
All	All	974	0	862	52	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 29.

All (52) 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:12:LEU:HD11	1:B:44:VAL:HG21	1.57	0.86
1:B:27:ASP:OD2	3:B:101:HOH:O	2.01	0.78
1:B:14:GLY:O	1:B:18:LYS:NZ	2.17	0.76
1:A:55:HIS:O	3:A:201:HOH:O	2.04	0.75
1:A:26:VAL:HG23	1:A:30:GLU:OE1	1.88	0.73
1:A:11:ILE:HG12	1:A:20:VAL:HG22	1.70	0.72
1:B:16:THR:O	3:B:102:HOH:O	2.11	0.66
1:B:9:LYS:HE2	1:B:22:THR:HG22	1.78	0.65
1:B:37:GLN:HA	1:B:40:ASN:OD1	1.97	0.64
1:A:52:GLU:OE1	3:A:202:HOH:O	2.14	0.64
1:A:9:LYS:N	3:A:201:HOH:O	2.30	0.63
1:A:44:VAL:HG23	1:A:61:GLU:HG3	1.81	0.60
1:B:45:ASP:O	1:B:61:GLU:HG2	2.02	0.59
1:A:6:MET:N	1:A:25:ALA:O	2.35	0.58
1:B:61:GLU:OXT	3:B:103:HOH:O	2.17	0.58
1:B:21:ILE:HD11	1:B:38:TYR:CZ	2.41	0.55
1:B:53:ALA:N	3:B:108:HOH:O	2.40	0.54
1:B:12:LEU:CD1	1:B:44:VAL:HG21	2.34	0.54
1:A:10:LEU:HD23	1:A:57:PHE:HB2	1.91	0.53
1:A:10:LEU:HA	1:A:57:PHE:O	2.09	0.52
1:B:10:LEU:HD22	1:B:35:PHE:CD1	2.46	0.51
1:B:40:ASN:ND2	3:B:109:HOH:O	2.41	0.50
1:B:12:LEU:HD11	1:B:44:VAL:HG11	1.94	0.49
1:B:34:PHE:O	1:B:37:GLN:NE2	2.46	0.48
1:B:25:ALA:HB3	1:B:31:ALA:HB2	1.95	0.47
1:B:52:GLU:O	1:B:52:GLU:HG3	2.15	0.47
1:B:48:TRP:CE2	1:B:59:VAL:HB	2.50	0.47
1:A:50:TYR:CE2	1:A:52:GLU:HB2	2.51	0.46
1:A:15[A]:LYS:O	1:A:18:LYS:NZ	2.48	0.46
1:A:26:VAL:N	1:A:30:GLU:OE1	2.33	0.46
1:A:9:LYS:HE3	1:A:9:LYS:HB2	1.57	0.46
1:A:14:GLY:O	1:A:18:LYS:NZ	2.32	0.45
1:A:51:ASP:HB3	1:A:54:THR:OG1	2.17	0.45
1:B:12:LEU:HD21	1:B:44:VAL:HG11	1.97	0.45
1:B:34:PHE:O	1:B:38:TYR:HB2	2.17	0.44
1:A:10:LEU:HB2	1:A:35:PHE:CD2	2.52	0.44
1:B:11:ILE:HD13	1:B:56:THR:HG23	1.98	0.44
1:B:23:ILE:HD13	1:B:34:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	3:B:104:HOH:O	2.18	0.43
1:B:13:ASN:CG	1:B:60:THR:HG23	2.39	0.43
1:B:46:GLY:HA3	1:B:61:GLU:HA	2.00	0.43
1:A:15[B]:LYS:O	1:A:18:LYS:NZ	2.51	0.43
1:B:44:VAL:HA	1:B:61:GLU:OE2	2.17	0.43
1:A:33:LYS:HD3	1:A:33:LYS:C	2.39	0.43
1:A:23:ILE:HD12	1:A:25:ALA:HB2	2.01	0.43
1:A:12:LEU:HD22	1:A:44:VAL:HG11	2.01	0.42
1:A:51:ASP:HB3	1:A:54:THR:HG1	1.85	0.42
1:B:56:THR:O	3:B:104:HOH:O	2.22	0.41
1:B:37:GLN:O	1:B:41:ASP:HB2	2.20	0.41
1:A:54:THR:HB	1:A:56:THR:OG1	2.20	0.41
1:A:56:THR:O	3:A:203:HOH:O	2.22	0.41
1:B:34:PHE:HA	1:B:37:GLN:HE21	1.86	0.41

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	55/56 (98%)	52 (94%)	1 (2%)	2 (4%)	3 1
1	B	54/56 (96%)	50 (93%)	4 (7%)	0	100 100
All	All	109/112 (97%)	102 (94%)	5 (5%)	2 (2%)	17 5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15[A]	LYS
1	A	15[B]	LYS

5.3.2 Protein sidechains

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	48/47 (102%)	47 (98%)	1 (2%)	53 67
1	B	47/47 (100%)	45 (96%)	2 (4%)	29 36
All	All	95/94 (101%)	92 (97%)	3 (3%)	39 50

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	B	11	ILE
1	B	44	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	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

Of 1 ligands modelled in this entry, 1 is 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

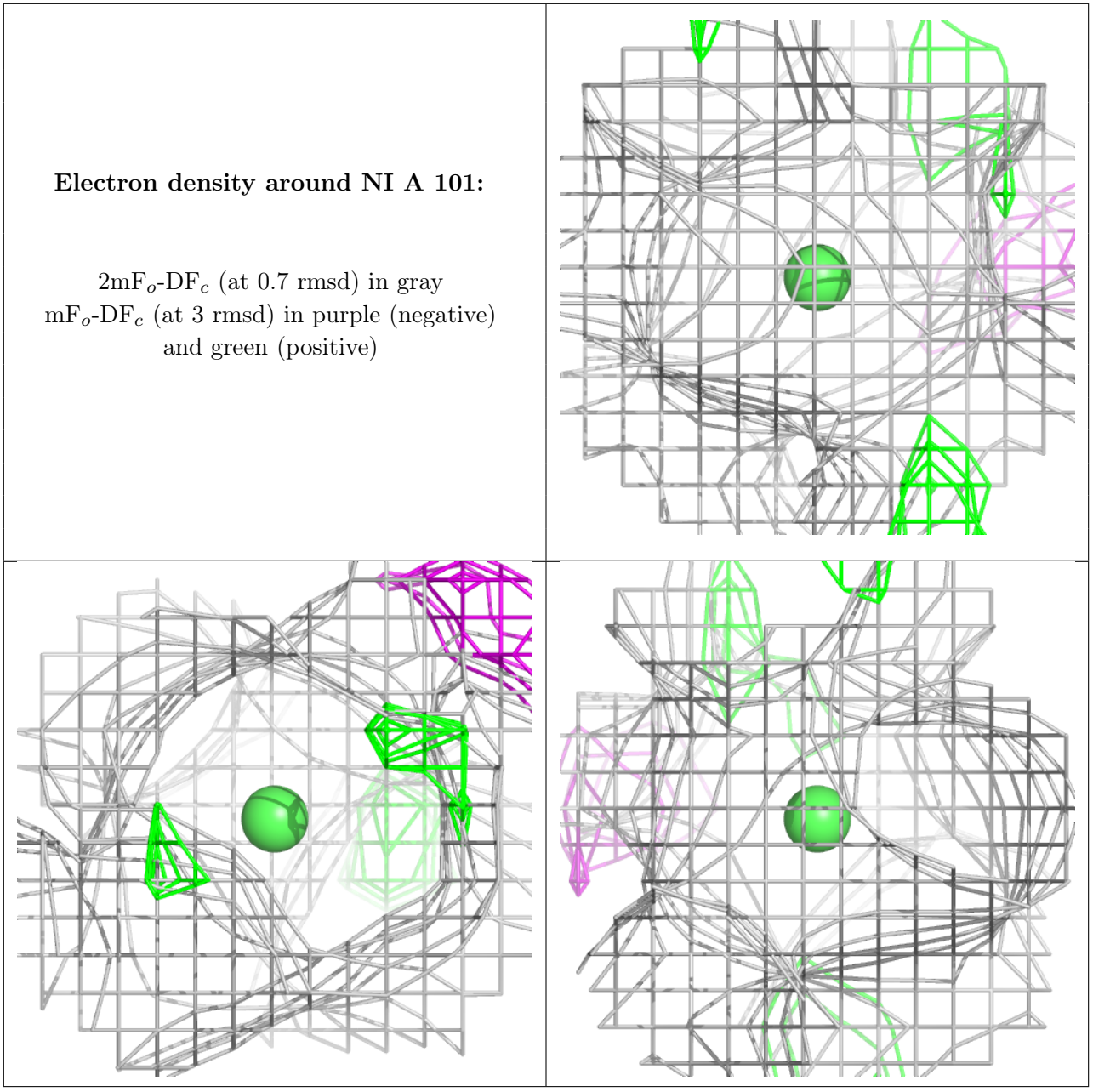
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NI A 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.