



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:13 AM GMT

PDB ID : 3LCN
Title : Nab2:Gfd1 complex
Authors : Stewart, M.
Deposited on : 2010-01-11
Resolution : 2.00 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

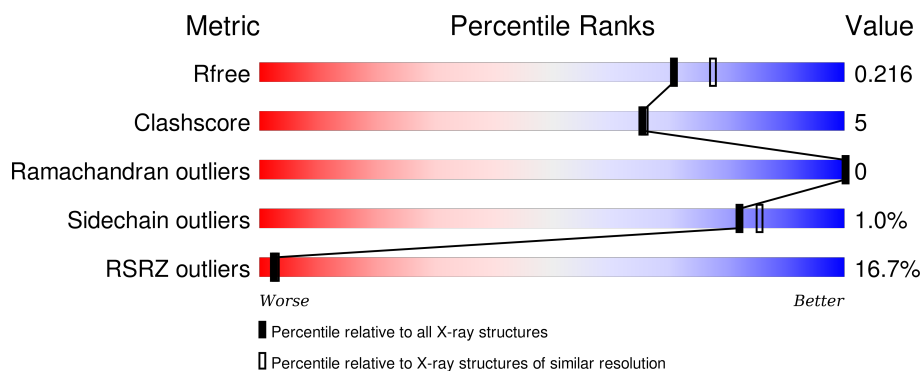
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	105	<div> <div>11%</div> <div>83%</div> <div>9%</div> <div>9%</div> </div>
1	B	105	<div> <div>12%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
2	C	29	<div> <div>17%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>
2	D	29	<div> <div>34%</div> <div>48%</div> <div>24%</div> <div>24%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3920 atoms, of which 1943 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 polyadenylated RNA-binding protein NAB2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	96	Total	C	H	N	O	S	0	0	0
			1475	467	740	118	148	2			
1	B	97	Total	C	H	N	O	S	0	0	0
			1490	472	746	119	151	2			

- Molecule 2 is a protein called mRNA transport factor GFD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	25	Total	C	H	N	O	S	0	0	0
			449	134	237	41	36	1			
2	D	22	Total	C	H	N	O	S	0	0	0
			414	124	220	38	31	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	2	Total	Zn	0	0
			2	2		

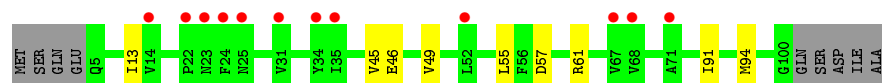
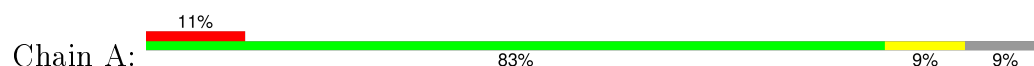
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	32	Total	O	0	0
			32	32		
4	C	12	Total	O	0	0
			12	12		
4	D	5	Total	O	0	0
			5	5		

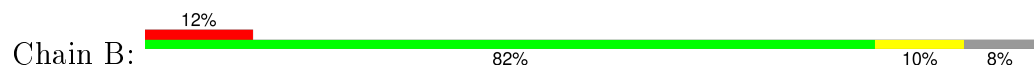
3 Residue-property plots [i](#)

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.

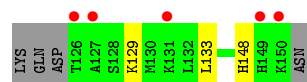
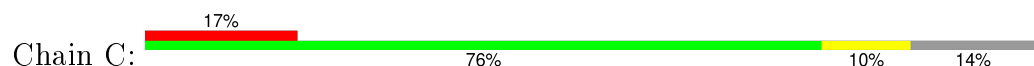
- Molecule 1: Nuclear polyadenylated RNA-binding protein NAB2



- Molecule 1: Nuclear polyadenylated RNA-binding protein NAB2



- Molecule 2: mRNA transport factor GFD1



- Molecule 2: mRNA transport factor GFD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	55.83Å 121.76Å 37.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.07 – 2.00 19.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.07-2.00) 98.9 (19.59-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_249)	Depositor
R, R_{free}	0.187 , 0.226 0.178 , 0.216	Depositor DCC
R_{free} test set	1578 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17715 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3920	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% 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

5.1 Standard geometry

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

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	0.37	0/742	0.46	0/1006
1	B	0.37	0/751	0.44	0/1018
2	C	0.35	0/213	0.40	0/278
2	D	0.25	0/195	0.57	1/253 (0.4%)
All	All	0.36	0/1901	0.46	1/2555 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	145	GLN	OE1-CD-NE2	-6.06	107.97	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	145	GLN	Sidechain

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	735	740	740	7	0
1	B	744	746	746	8	0
2	C	212	237	239	4	0
2	D	194	220	222	4	1
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	40	0	0	0	0
4	B	32	0	0	0	0
4	C	12	0	0	1	0
4	D	5	0	0	0	0
All	All	1977	1943	1947	19	1

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 5.

All (19) 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:D:129:LYS:N	2:D:133:LEU:H	1.93	0.66
1:B:4:GLU:HG2	1:B:5:GLN:N	2.18	0.58
1:A:46:GLU:OE2	1:A:61:ARG:NH2	2.38	0.57
1:A:55:LEU:O	2:C:129:LYS:HE3	2.06	0.56
1:B:13:ILE:HG23	1:B:91:ILE:CD1	2.38	0.52
1:B:4:GLU:CG	1:B:5:GLN:N	2.72	0.52
2:D:129:LYS:N	2:D:132:LEU:N	2.59	0.50
2:C:148:HIS:NE2	4:C:75:HOH:O	2.35	0.49
1:B:21:ILE:HG22	1:B:24:PHE:HB2	1.97	0.47
1:B:55:LEU:HD13	2:D:136:LYS:HE3	1.97	0.46
1:A:45:VAL:O	1:A:49:VAL:HG23	2.16	0.46
1:A:13:ILE:HG23	1:A:91:ILE:CD1	2.46	0.45
1:B:4:GLU:CG	1:B:5:GLN:H	2.29	0.45
2:D:144:LEU:O	2:D:144:LEU:HD12	2.17	0.44
1:B:96:ALA:O	1:B:97:GLN:HB2	2.18	0.44
1:A:55:LEU:O	2:C:129:LYS:CE	2.66	0.42
1:B:46:GLU:OE2	1:B:61:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD21	2:C:133:LEU:HD13	2.01	0.41
1:A:91:ILE:HA	1:A:94:MET:HE2	2.02	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:GLU:OE1	2:D:145:GLN:OE1[2_755]	2.14	0.06

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	94/105 (90%)	94 (100%)	0	0	100	100
1	B	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
2	C	23/29 (79%)	23 (100%)	0	0	100	100
2	D	20/29 (69%)	20 (100%)	0	0	100	100
All	All	232/268 (87%)	228 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	81/89 (91%)	80 (99%)	1 (1%)	78	81
1	B	82/89 (92%)	82 (100%)	0	100	100
2	C	24/28 (86%)	24 (100%)	0	100	100
2	D	22/28 (79%)	21 (96%)	1 (4%)	34	29
All	All	209/234 (89%)	207 (99%)	2 (1%)	82	85

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

Mol	Chain	Res	Type
1	A	57	ASP
2	D	149	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 3 ligands modelled in this entry, 3 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 ⓘ

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	96/105 (91%)	0.66	12 (12%) 5 5	25, 45, 85, 131	0
1	B	97/105 (92%)	0.92	13 (13%) 4 5	31, 45, 94, 130	0
2	C	25/29 (86%)	0.94	5 (20%) 1 2	30, 56, 88, 102	0
2	D	22/29 (75%)	2.07	10 (45%) 0 1	44, 80, 133, 172	0
All	All	240/268 (89%)	0.92	40 (16%) 2 3	25, 49, 103, 172	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ASN	7.1
1	B	25	ASN	7.1
2	D	148	HIS	7.0
2	D	149	HIS	6.5
1	B	22	PRO	5.7
1	B	5	GLN	5.6
2	D	145	GLN	5.5
1	A	22	PRO	5.4
2	C	127	ALA	5.3
1	A	25	ASN	5.1
1	A	23	ASN	4.5
2	D	150	LYS	4.3
1	B	14	VAL	4.2
2	C	149	HIS	4.1
1	A	67	VAL	3.4
2	C	126	THR	3.3
2	D	131	LYS	3.2
2	D	130	MET	3.2
1	A	68	VAL	3.2
1	B	35	ILE	3.1
2	D	146	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	30	TYR	2.9
2	D	144	LEU	2.8
2	D	147	THR	2.8
1	B	85	GLU	2.8
1	B	13	ILE	2.8
1	B	24	PHE	2.7
2	C	131	LYS	2.7
2	C	150	LYS	2.6
2	D	143	ILE	2.6
1	B	27	ASP	2.6
1	A	24	PHE	2.6
1	A	35	ILE	2.6
1	A	52	LEU	2.5
1	A	14	VAL	2.5
1	A	34	TYR	2.3
1	B	67	VAL	2.3
1	A	71	ALA	2.2
1	A	31	VAL	2.1
1	B	18	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	A	106	1/1	0.99	0.09	-1.30	37,37,37,37	0
3	ZN	A	107	1/1	0.99	0.04	-4.83	42,42,42,42	0
3	ZN	B	106	1/1	0.98	0.04	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.