



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 07:04 am GMT

PDB ID : 2V4H
Title : NEMO CC2-LZ domain - 1D5 DARPin complex
Authors : Grubisha, O.; Duquerroy, S.; Cordier, F.; Haouz, A.; Delepierre, M.; Veron, M.; Agou, F.
Deposited on : 2008-09-22
Resolution : 2.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Xtrriage (Phenix) : 1.13
EDS : 2.36
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

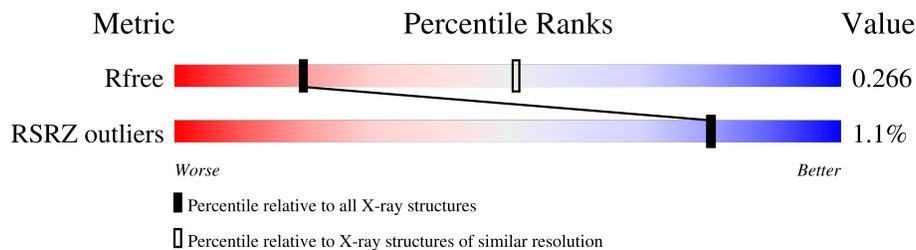
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3542 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 NF-KAPPA-B ESSENTIAL MODULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	98	808	505	144	156	3	0	0	0
1	B	91	761	476	134	148	3	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	MET	-	expression tag	UNP O88522
A	229	GLY	-	expression tag	UNP O88522
A	230	SER	-	expression tag	UNP O88522
A	231	SER	-	expression tag	UNP O88522
A	232	HIS	-	expression tag	UNP O88522
A	233	HIS	-	expression tag	UNP O88522
A	234	HIS	-	expression tag	UNP O88522
A	235	HIS	-	expression tag	UNP O88522
A	236	HIS	-	expression tag	UNP O88522
A	237	HIS	-	expression tag	UNP O88522
A	238	SER	-	expression tag	UNP O88522
A	239	SER	-	expression tag	UNP O88522
A	240	GLY	-	expression tag	UNP O88522
A	241	LEU	-	expression tag	UNP O88522
A	242	VAL	-	expression tag	UNP O88522
A	243	PRO	-	expression tag	UNP O88522
A	244	ARG	-	expression tag	UNP O88522
A	245	GLY	-	expression tag	UNP O88522
A	246	SER	-	expression tag	UNP O88522
A	247	HIS	-	expression tag	UNP O88522
A	248	MET	-	expression tag	UNP O88522
A	249	ALA	-	expression tag	UNP O88522
A	250	SER	-	expression tag	UNP O88522
B	228	MET	-	expression tag	UNP O88522
B	229	GLY	-	expression tag	UNP O88522

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	SER	-	expression tag	UNP O88522
B	231	SER	-	expression tag	UNP O88522
B	232	HIS	-	expression tag	UNP O88522
B	233	HIS	-	expression tag	UNP O88522
B	234	HIS	-	expression tag	UNP O88522
B	235	HIS	-	expression tag	UNP O88522
B	236	HIS	-	expression tag	UNP O88522
B	237	HIS	-	expression tag	UNP O88522
B	238	SER	-	expression tag	UNP O88522
B	239	SER	-	expression tag	UNP O88522
B	240	GLY	-	expression tag	UNP O88522
B	241	LEU	-	expression tag	UNP O88522
B	242	VAL	-	expression tag	UNP O88522
B	243	PRO	-	expression tag	UNP O88522
B	244	ARG	-	expression tag	UNP O88522
B	245	GLY	-	expression tag	UNP O88522
B	246	SER	-	expression tag	UNP O88522
B	247	HIS	-	expression tag	UNP O88522
B	248	MET	-	expression tag	UNP O88522
B	249	ALA	-	expression tag	UNP O88522
B	250	SER	-	expression tag	UNP O88522

- Molecule 2 is a protein called 1D5 DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			949	587	169	192	1			
2	D	128	Total	C	N	O	S	0	0	0
			973	601	176	195	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	8	Total	O	0	0
			8	8		
3	C	14	Total	O	0	0
			14	14		
3	D	19	Total	O	0	0
			19	19		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.02Å 63.02Å 436.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.90 47.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	86.5 (47.67-2.90) 86.5 (47.65-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.208 , 0.268 0.206 , 0.266	Depositor DCC
R_{free} test set	883 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3542	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	98/110 (89%)	0.01	3 (3%) 49 44	38, 54, 70, 80	0
1	B	91/110 (82%)	-0.10	1 (1%) 80 80	36, 54, 68, 76	0
2	C	125/136 (91%)	-0.18	1 (0%) 86 86	35, 51, 63, 74	0
2	D	128/136 (94%)	-0.24	0 100 100	39, 50, 62, 82	0
All	All	442/492 (89%)	-0.14	5 (1%) 80 80	35, 52, 66, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	HIS	3.6
1	A	336	LEU	3.5
2	C	12	SER	2.6
1	A	337	LYS	2.3
1	A	241	LEU	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.