wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 07:04 am GMT

PDB ID	:	2V4H
Title	:	NEMO CC2-LZ domain - 1D5 DARPin complex
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Deposited on	:	2008-09-22
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	FAILED
Xtriage (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

PERCENTILES INFOmissingINFO

1 Entry composition (i)

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
1	A	98	Total	C	N	O	S	0	0	0
			808	505	144	156	3			
1	B	91	Total	C	N	O	S	0	0	0
			761	476	134	148	3			

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		

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.61 (at 2.91Å)	Xtriage
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	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[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.

3 Model quality

3.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

3.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

3.3 Torsion angles

3.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

3.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

3.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

3.5 Carbohydrates

There are no monosaccharides in this entry.

3.6 Ligand geometry

There are no ligands in this entry.

3.7 Other polymers

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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, 95^{th} 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

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

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

4.3 Carbohydrates

There are no monosaccharides in this entry.

4.4 Ligands

There are no ligands in this entry.

4.5 Other polymers (i)

There are no such residues in this entry.