



Full wwPDB X-ray Structure Validation Report i

Nov 1, 2023 – 02:32 PM JST

PDB ID : 5ITR
Title : Crystal Structure of Human NEIL1(P2G) bound to duplex DNA containing THF
Authors : Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.
Deposited on : 2016-03-17
Resolution : 2.46 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
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

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.31 Å 109.04 Å 169.84 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.75 – 2.46 44.81 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.75-2.46) 99.4 (44.81-2.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ ¹	2.59 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R , R_{free}	0.211 , 0.263 0.242 , 0.282	Depositor DCC
R_{free} test set	2488 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.4	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HB3	1:C:96:HIS:CD2	2.54	0.42
1:B:262:CYS:SG	1:B:281:PHE:HA	2.60	0.42
1:A:148:VAL:HG22	1:A:170:PHE:HB3	2.02	0.41
3:F:3:DT:H2'	3:F:4:DC:C6	2.55	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:C:224:ASP:C	1:C:224:ASP:OD1	2.59	0.41
1:A:29:LYS:HE2	1:A:35:ASN:O	2.20	0.41
1:A:32:VAL:O	1:A:32:VAL:HG13	2.21	0.41
2:E:26:DC:H2"	2:E:27:DG:C8	2.56	0.41
1:B:52:ARG:HG3	1:B:136:CYS:HB2	2.02	0.40
1:B:95:ARG:HG3	1:B:96:HIS:CD2	2.56	0.40
1:B:189:PRO:HB2	1:B:192:GLU:CG	2.51	0.40
1:A:238:GLN:HE21	1:A:238:GLN:HB3	1.66	0.40
1:B:161:ILE:HA	1:B:194:ALA:HB2	2.03	0.40
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.94	0.40
1:B:130:GLN:NE2	1:B:133:ARG:HH11	2.18	0.40
1:C:76:VAL:HG21	1:C:128:LYS:O	2.21	0.40
1:A:95:ARG:HG3	1:A:96:HIS:CG	2.56	0.40
1:B:130:GLN:HB3	1:B:133:ARG:HD2	2.02	0.40
1:A:251:GLU:H	1:A:251:GLU:HG3	1.53	0.40
1:C:269:SER:HB3	1:C:281:PHE:CE1	2.56	0.40

All (2) 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)
4:A:551:HOH:O	4:B:525:HOH:O[3_555]	1.81	0.39
4:A:558:HOH:O	4:B:537:HOH:O[3_555]	1.99	0.21

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.

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Mol	Chain	Res	Type
1	A	96	HIS
1	A	100	ARG
1	A	105	PRO
1	A	125	LEU
1	A	143	GLN
1	A	144	PHE
1	A	155	LYS
1	A	159	ARG
1	A	201	LEU
1	A	238	GLN
1	A	248	SER
1	A	251	GLU
1	A	272	GLN
1	A	279	ILE
1	B	63	LEU
1	B	81	MET
1	B	95	ARG
1	B	100	ARG
1	B	144	PHE
1	B	155	LYS
1	B	177	TYR
1	B	187	LYS
1	B	191	PHE
1	B	192	GLU
1	B	201	LEU
1	B	269	SER
1	B	272	GLN
1	B	273	ASP
1	B	282	GLN
1	C	46	ARG
1	C	69	GLN
1	C	92	GLU
1	C	95	ARG
1	C	113	CYS
1	C	122	ARG
1	C	124	ASP
1	C	150	ARG
1	C	192	GLU
1	C	195	ARG
1	C	198	LEU
1	C	199	GLU
1	C	219	LYS

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Mol	Chain	Res	Type
1	C	239	LEU
1	C	257	ARG
1	C	261	ARG
1	C	282	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	70	GLN
1	A	96	HIS
1	A	130	GLN
1	A	143	GLN
1	A	238	GLN
1	B	12	GLN
1	B	130	GLN
1	B	143	GLN
1	C	12	GLN
1	C	98	HIS
1	C	139	GLN
1	C	151	ASN
1	C	282	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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Mol	Chain	Res	Type	RSRZ
1	C	147	ASN	4.7
1	C	220	LEU	4.6
1	C	92	GLU	4.6
1	C	47	ILE	4.4
1	C	19	ARG	4.4
1	A	247	GLU	4.3
1	C	122	ARG	4.3
1	C	126	GLY	4.2
1	C	40	PHE	4.2
1	C	71	GLU	4.1
1	C	155	LYS	4.0
1	A	291	LYS	3.9
1	C	90	ARG	3.9
3	F	28	DG	3.8
1	C	91	GLU	3.7
1	C	280	TRP	3.7
1	A	245	GLY	3.7
1	C	21	LEU	3.7
1	C	20	ALA	3.7
2	D	16	DT	3.7
1	C	48	SER	3.7
1	A	249	GLY	3.7
1	C	58	LEU	3.7
3	F	2	DG	3.6
1	C	63	LEU	3.6
1	C	18	CYS	3.6
1	C	64	PRO	3.6
1	C	27	VAL	3.5
1	A	32	VAL	3.5
1	A	274	ARG	3.5
1	A	94	PRO	3.5
1	A	248	SER	3.4
1	C	165	LEU	3.4
1	A	246	SER	3.4
2	D	13	DC	3.4
1	C	287	PRO	3.3
1	C	149	LEU	3.3
1	C	152	LEU	3.3
1	C	69	GLN	3.2
3	F	1	DC	3.2
1	C	34	ARG	3.2
1	A	34	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	289	ALA	2.0
1	C	263	TYR	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 monosaccharides 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.