wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 10:24 pm GMT

PDB ID	:	4CT4
Title	:	CNOT1 MIF4G domain - DDX6 complex
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Deposited on	:	2014-03-12
Resolution	:	2.30 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:

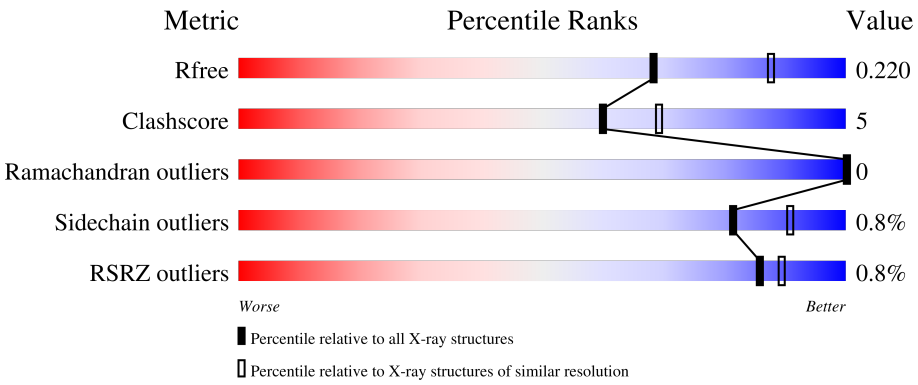
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	258	2% 83% 9% 9%
1	C	258	% 85% 9% 6%
2	B	378	87% 13%
2	D	378	83% 13% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9926 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 CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	1872	1211	311	342	8	0	0	0
1	C	242	1919	1238	316	357	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	GLN	-	expression tag	UNP A5YKK6
A	1053	GLY	-	expression tag	UNP A5YKK6
A	1054	PRO	-	expression tag	UNP A5YKK6
A	1055	ASP	-	expression tag	UNP A5YKK6
A	1056	SER	-	expression tag	UNP A5YKK6
A	1057	MET	-	expression tag	UNP A5YKK6
C	1052	GLN	-	expression tag	UNP A5YKK6
C	1053	GLY	-	expression tag	UNP A5YKK6
C	1054	PRO	-	expression tag	UNP A5YKK6
C	1055	ASP	-	expression tag	UNP A5YKK6
C	1056	SER	-	expression tag	UNP A5YKK6
C	1057	MET	-	expression tag	UNP A5YKK6

- Molecule 2 is a protein called PROBABLE ATP-DEPENDENT RNA HELICASE DDX6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	378	2995	1908	523	545	19	0	0	0
2	D	364	2867	1829	502	518	18	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	ARG	-	expression tag	UNP P26196
B	93	SER	-	expression tag	UNP P26196
B	94	MET	-	expression tag	UNP P26196
D	92	ARG	-	expression tag	UNP P26196
D	93	SER	-	expression tag	UNP P26196
D	94	MET	-	expression tag	UNP P26196

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

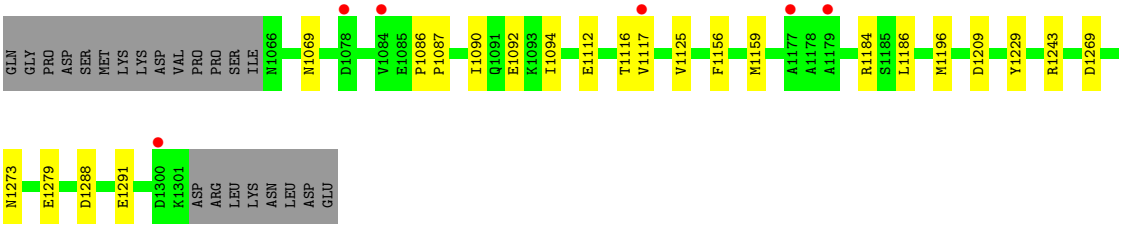
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	110	Total O 110 110	0	0
5	C	40	Total O 40 40	0	0
5	D	78	Total O 78 78	0	0

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 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.

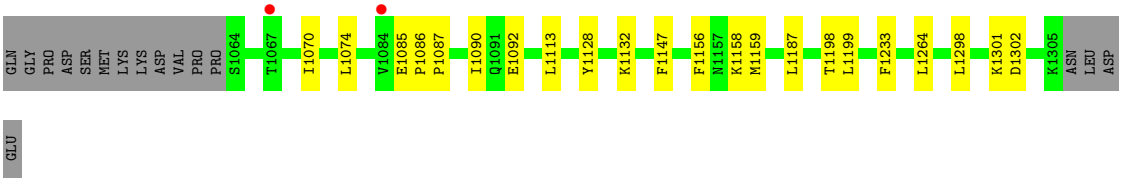
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

Chain A: 2% 83% 9% 9%



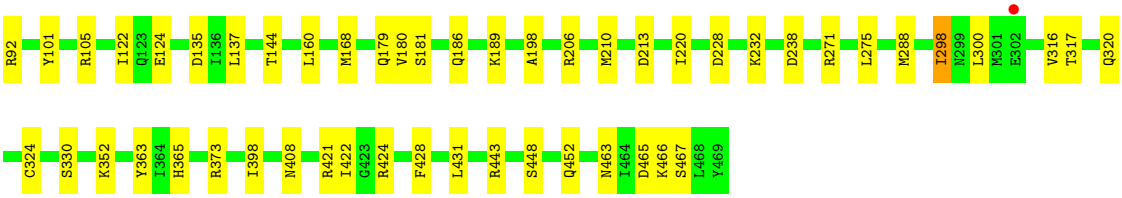
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

Chain C: % 85% 9% 6%



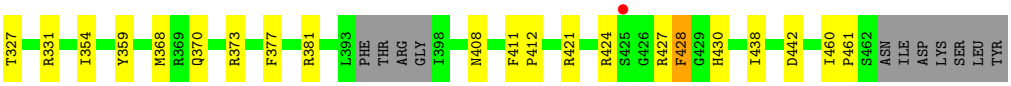
• Molecule 2: PROBABLE ATP-DEPENDENT RNA HELICASE DDX6

Chain B: 87% 13%



• Molecule 2: PROBABLE ATP-DEPENDENT RNA HELICASE DDX6

Chain D: 83% 13%


T327
R331
I354
Y359
M368
R369
Q370
R373
F377
R381
L393
PHE
THR
ARG
GLY
I398
N408
F411
P412
R421
R424
S425
G426
R427
F428
G429
H430
I438
D442
I460
P461
S462
ASN
ILE
ASP
LYS
SER
LEU
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.53Å 120.01Å 78.47Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	64.29 – 2.30 64.29 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.29-2.30) 98.2 (64.29-2.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.220 0.165 , 0.220	Depositor DCC
R_{free} test set	3322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9926	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.41	0/1908	0.52	0/2592
1	C	0.36	0/1955	0.51	0/2657
2	B	0.42	0/3045	0.62	0/4112
2	D	0.42	0/2914	0.60	0/3936
All	All	0.41	0/9822	0.57	0/13297

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	299	ASN	Mainchain
2	D	307	LYS	Peptide

5.2 Too-close contacts (i)

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	1872	0	1905	16	0
1	C	1919	0	1945	14	0
2	B	2995	0	3051	33	0
2	D	2867	0	2918	30	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	1	0
5	A	40	0	0	3	0
5	B	110	0	0	6	1
5	C	40	0	0	2	0
5	D	78	0	0	3	0
All	All	9926	0	9819	89	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.

The worst 5 of 89 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:B:122:ILE:HG13	2:B:300:LEU:HD13	1.60	0.83
1:C:1156:PHE:HA	1:C:1159:MET:HE2	1.65	0.76
1:A:1273:ASN:OD1	5:A:2036:HOH:O	2.05	0.75
2:D:370:GLN:OE1	2:D:373:ARG:NH2	2.22	0.73
2:B:135:ASP:OD2	5:B:2019:HOH:O	2.09	0.70

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)
5:B:2006:HOH:O	5:B:2065:HOH:O[2_645]	1.74	0.46

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	234/258 (91%)	228 (97%)	6 (3%)	0	100	100
1	C	240/258 (93%)	233 (97%)	7 (3%)	0	100	100
2	B	376/378 (100%)	367 (98%)	9 (2%)	0	100	100
2	D	360/378 (95%)	352 (98%)	8 (2%)	0	100	100
All	All	1210/1272 (95%)	1180 (98%)	30 (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	210/242 (87%)	210 (100%)	0	100	100
1	C	217/242 (90%)	217 (100%)	0	100	100
2	B	330/338 (98%)	325 (98%)	5 (2%)	65	79
2	D	313/338 (93%)	309 (99%)	4 (1%)	69	82
All	All	1070/1160 (92%)	1061 (99%)	9 (1%)	81	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	377	PHE
2	D	428	PHE
2	B	428	PHE
2	B	443	ARG
2	D	174	ARG

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

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)

Of 5 ligands modelled in this entry, 5 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 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	236/258 (91%)	-0.15	6 (2%)	57	64	30, 60, 108, 131	0
1	C	242/258 (93%)	-0.18	2 (0%)	86	89	34, 64, 105, 136	0
2	B	378/378 (100%)	-0.38	1 (0%)	94	96	28, 48, 83, 117	0
2	D	364/378 (96%)	-0.38	1 (0%)	94	96	28, 52, 80, 124	0
All	All	1220/1272 (95%)	-0.29	10 (0%)	86	89	28, 54, 97, 136	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1177	ALA	6.1
1	C	1067	THR	3.1
1	C	1084	VAL	2.7
1	A	1084	VAL	2.6
1	A	1300	ASP	2.6

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)

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. 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	B-factors(Å^2)	Q<0.9
3	MG	B	1472	1/1	0.90	0.10	65,65,65,65	0
3	MG	B	1471	1/1	0.94	0.12	63,63,63,63	0
3	MG	D	1463	1/1	0.96	0.10	49,49,49,49	0
4	CL	D	1464	1/1	0.96	0.07	66,66,66,66	0
3	MG	B	1470	1/1	0.97	0.14	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.