wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 10:16 am BST

PDB ID	:	4CV5
Title	:	yeast NOT1 CN9BD-CAF40 complex
Authors	:	Basquin, J.; Conti, E.
Deposited on	:	2014-03-23
Resolution	:	3.81 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 (i)) were used in the production of this report:

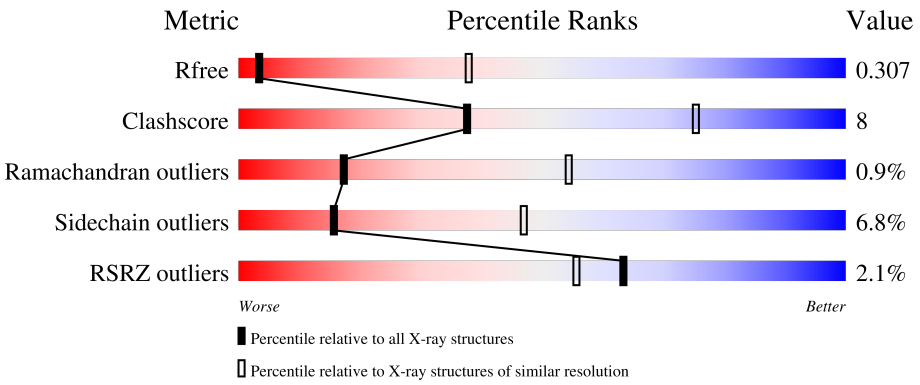
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.81 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	212	.% 71% 14% • 13%
1	C	212	3% 71% 14% • 13%
2	B	320	.% 65% 16% 19%
2	D	320	2% 66% 13% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	A	2273	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6172 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.

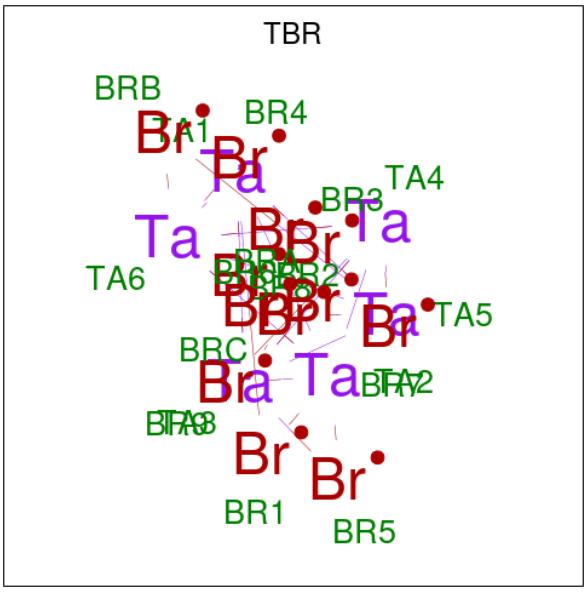
- Molecule 1 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1248	792	219	232	5	0	0	0
1	C	185	1248	792	219	232	5	0	0	0

- Molecule 2 is a protein called PROTEIN CAF40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	1820	1174	306	330	10	0	0	0
2	D	261	1802	1155	309	327	11	0	0	0

- Molecule 3 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



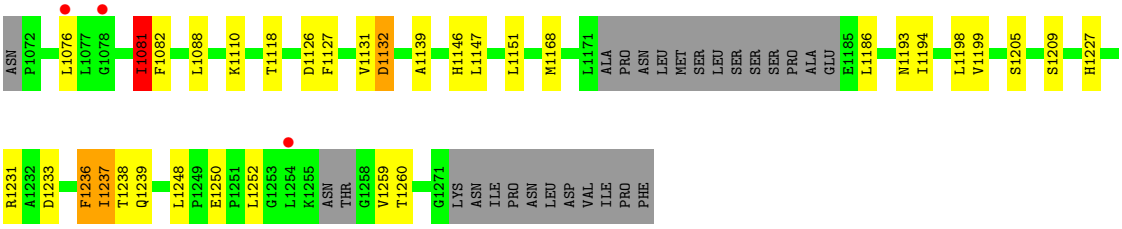
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Br	Ta		
3	A	1	18	12	6	0	0
			Total	Br	Ta		
3	A	1	18	12	6	0	0
			Total	Br	Ta		
3	B	1	18	12	6	0	0

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.

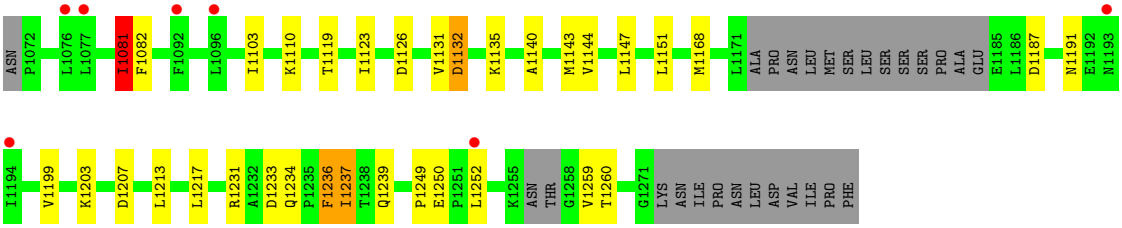
• Molecule 1: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain A:



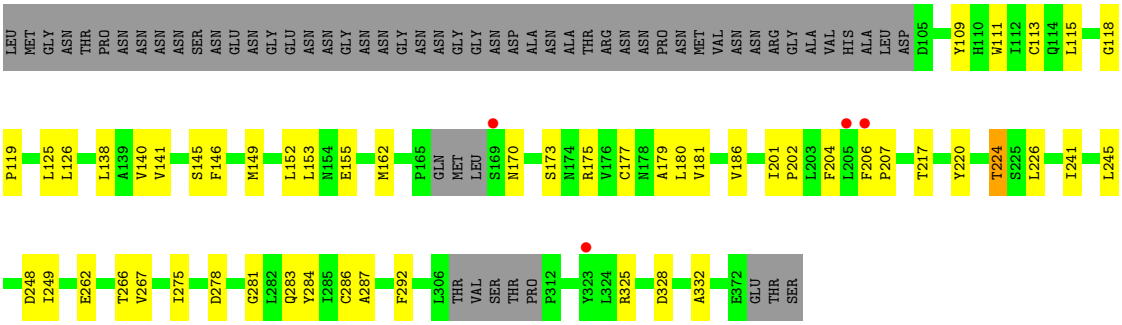
• Molecule 1: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain C:



• Molecule 2: PROTEIN CAF40

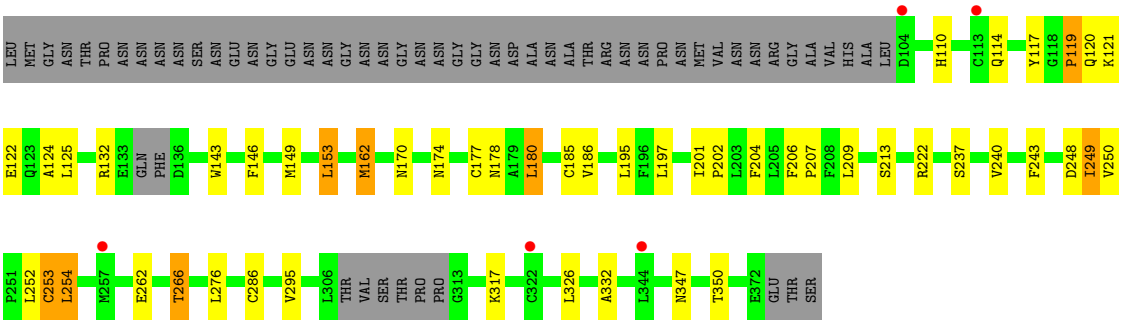
Chain B:



• Molecule 2: PROTEIN CAF40

Chain D:

2%
66%
13%
18%


LEU MET GLY ASN THR PRO ASN ASN ASN ASN SER ASN GLU ASN GLY GLU ASN ASN GLY ASN ASN GLY ASN ASN GLY GLY ASN ASP ALA ASN ALA THR ARG ASN ASN PRO ASN MET VAL ASN ASN ARG GLY ALA VAL HIS ALA LEU D104 H110 C113 Q114 Y117 G118 P119 Q120 K121
E122 Q123 A124 L125 R132 E133 GLN PHE D136 W143 F146 M149 L153 M162 N170 N174 C177 N178 A179 L180 C185 V186 L195 F196 L197 I201 P202 L203 F204 L205 F206 P207 F208 L209 S213 R222 S237 V240 F243 D248 I249 V250
P251 L252 C253 L254 M257 E262 T266 L276 C286 V295 L306 THR VAL SER THR PRO PRO G313 K317 C322 L326 A332 L344 N347 T350 E372 GLU THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.34Å 188.34Å 126.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 3.81 48.29 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.29-3.81) 99.9 (48.29-3.81)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.276 , 0.295 0.296 , 0.307	Depositor DCC
R_{free} test set	1143 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	148.8	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 101.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: TBR

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	0.23	0/1261	0.47	0/1722
1	C	0.22	0/1261	0.46	0/1722
2	B	0.22	0/1851	0.42	0/2542
2	D	0.22	0/1831	0.44	0/2512
All	All	0.22	0/6204	0.45	0/8498

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
1	A	0	1
2	D	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1248	LEU	Peptide
2	D	119	PRO	Peptide
2	D	248	ASP	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	1248	0	1163	24	0
1	C	1248	0	1164	19	0
2	B	1820	0	1648	26	0
2	D	1802	0	1613	29	0
3	A	36	0	0	6	0
3	B	18	0	0	1	0
All	All	6172	0	5588	91	0

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 8.

The worst 5 of 91 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)
1:A:1238:THR:HB	3:A:2273:TBR:BR7	2.02	1.15
2:B:278:ASP:OD1	3:B:1373:TBR:BRB	2.59	0.76
2:D:249:ILE:HG23	2:D:250:VAL:H	1.54	0.72
1:A:1081:ILE:HG23	1:A:1082:PHE:H	1.55	0.71
1:A:1238:THR:CB	3:A:2273:TBR:BR7	2.88	0.71

There are no symmetry-related clashes.

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	179/212 (84%)	163 (91%)	14 (8%)	2 (1%)	14 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	179/212 (84%)	165 (92%)	11 (6%)	3 (2%)	9	43
2	B	254/320 (79%)	240 (94%)	14 (6%)	0	100	100
2	D	255/320 (80%)	242 (95%)	10 (4%)	3 (1%)	13	50
All	All	867/1064 (82%)	810 (93%)	49 (6%)	8 (1%)	17	54

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	120	GLN
2	D	249	ILE
1	A	1081	ILE
1	A	1237	ILE
1	C	1081	ILE

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	110/187 (59%)	100 (91%)	10 (9%)	9	36
1	C	110/187 (59%)	103 (94%)	7 (6%)	17	48
2	B	166/289 (57%)	154 (93%)	12 (7%)	14	45
2	D	162/289 (56%)	154 (95%)	8 (5%)	25	55
All	All	548/952 (58%)	511 (93%)	37 (7%)	16	47

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1236	PHE
2	D	266	THR
2	D	117	TYR
2	D	180	LEU
2	B	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1193	ASN
2	D	178	ASN

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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TBR	A	2272	-	0,36,36	-	-	-		
3	TBR	B	1373	-	0,36,36	-	-	-		
3	TBR	A	2273	-	0,36,36	-	-	-		

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2272	TBR	1	0
3	B	1373	TBR	1	0
3	A	2273	TBR	5	0

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	185/212 (87%)	-0.16	3 (1%)	72	64	32, 87, 163, 241	0
1	C	185/212 (87%)	-0.20	7 (3%)	40	33	35, 93, 166, 261	0
2	B	260/320 (81%)	-0.12	4 (1%)	73	66	37, 83, 167, 239	0
2	D	261/320 (81%)	-0.17	5 (1%)	66	59	43, 85, 156, 198	0
All	All	891/1064 (83%)	-0.16	19 (2%)	63	55	32, 87, 165, 261	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	SER	3.7
1	A	1078	GLY	3.3
1	A	1076	LEU	3.3
1	C	1076	LEU	3.1
1	C	1194	ILE	3.0

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)

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	TBR	A	2272	18/18	0.91	0.19	147,189,220,228	18
3	TBR	B	1373	18/18	0.94	0.21	104,146,178,185	18
3	TBR	A	2273	18/18	0.96	0.21	121,162,194,201	18

6.5 Other polymers (i)

There are no such residues in this entry.