



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:09 PM UTC

PDB ID : 7CVQ / pdb_00007cvq
Title : crystal structure of Arabidopsis CO CCT domain in complex with NF-YB2/YC3 and FT CORE1 DNA
Authors : Lv, X.; Du, J.
Deposited on : 2020-08-26
Resolution : 3.30 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

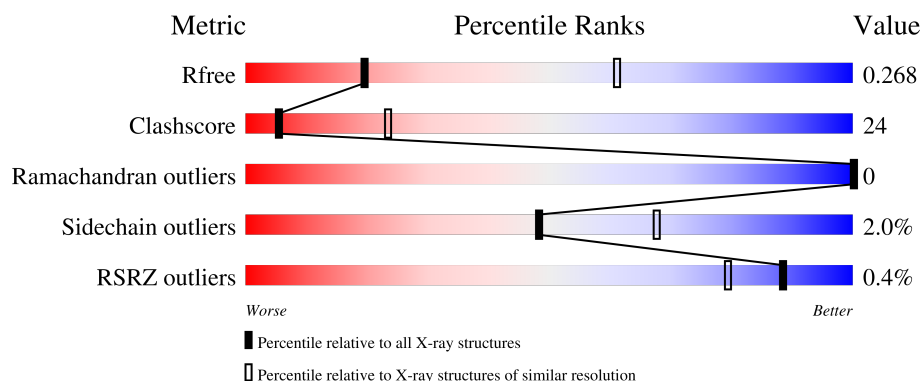
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	174	44% 28% 28%
1	F	174	% 43% 29% 28%
1	K	174	% 40% 24% .. 33%
1	P	174	37% 30% . 30%
2	B	97	53% 34% . 12%

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Mol	Chain	Length	Quality of chain
2	G	97	
2	L	97	
2	Q	97	
3	D	25	
3	I	25	
3	N	25	
3	T	25	
4	E	25	
4	J	25	
4	O	25	
4	U	25	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10910 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 Chimera of Nuclear transcription factor Y subunit C-3 and Zinc finger protein CONSTANS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1050	662	204	179	5			
1	F	125	Total	C	N	O	S	0	0	0
			1050	662	204	179	5			
1	K	117	Total	C	N	O	S	0	0	0
			978	615	188	170	5			
1	P	121	Total	C	N	O	S	0	0	0
			1011	637	195	174	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	GLY	-	linker	UNP Q9ZVL3
A	279	SER	-	linker	UNP Q9ZVL3
A	280	GLY	-	linker	UNP Q9ZVL3
A	281	SER	-	linker	UNP Q9ZVL3
A	282	GLY	-	linker	UNP Q9ZVL3
A	283	SER	-	linker	UNP Q9ZVL3
A	284	GLY	-	linker	UNP Q9ZVL3
A	285	SER	-	linker	UNP Q9ZVL3
A	286	GLY	-	linker	UNP Q9ZVL3
A	287	SER	-	linker	UNP Q9ZVL3
A	288	GLY	-	linker	UNP Q9ZVL3
A	289	SER	-	linker	UNP Q9ZVL3
F	278	GLY	-	linker	UNP Q9ZVL3
F	279	SER	-	linker	UNP Q9ZVL3
F	280	GLY	-	linker	UNP Q9ZVL3
F	281	SER	-	linker	UNP Q9ZVL3
F	282	GLY	-	linker	UNP Q9ZVL3
F	283	SER	-	linker	UNP Q9ZVL3
F	284	GLY	-	linker	UNP Q9ZVL3
F	285	SER	-	linker	UNP Q9ZVL3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	GLY	-	linker	UNP Q9ZVL3
F	287	SER	-	linker	UNP Q9ZVL3
F	288	GLY	-	linker	UNP Q9ZVL3
F	289	SER	-	linker	UNP Q9ZVL3
K	278	GLY	-	linker	UNP Q9ZVL3
K	279	SER	-	linker	UNP Q9ZVL3
K	280	GLY	-	linker	UNP Q9ZVL3
K	281	SER	-	linker	UNP Q9ZVL3
K	282	GLY	-	linker	UNP Q9ZVL3
K	283	SER	-	linker	UNP Q9ZVL3
K	284	GLY	-	linker	UNP Q9ZVL3
K	285	SER	-	linker	UNP Q9ZVL3
K	286	GLY	-	linker	UNP Q9ZVL3
K	287	SER	-	linker	UNP Q9ZVL3
K	288	GLY	-	linker	UNP Q9ZVL3
K	289	SER	-	linker	UNP Q9ZVL3
P	278	GLY	-	linker	UNP Q9ZVL3
P	279	SER	-	linker	UNP Q9ZVL3
P	280	GLY	-	linker	UNP Q9ZVL3
P	281	SER	-	linker	UNP Q9ZVL3
P	282	GLY	-	linker	UNP Q9ZVL3
P	283	SER	-	linker	UNP Q9ZVL3
P	284	GLY	-	linker	UNP Q9ZVL3
P	285	SER	-	linker	UNP Q9ZVL3
P	286	GLY	-	linker	UNP Q9ZVL3
P	287	SER	-	linker	UNP Q9ZVL3
P	288	GLY	-	linker	UNP Q9ZVL3
P	289	SER	-	linker	UNP Q9ZVL3

- Molecule 2 is a protein called Nuclear transcription factor Y subunit B-2.

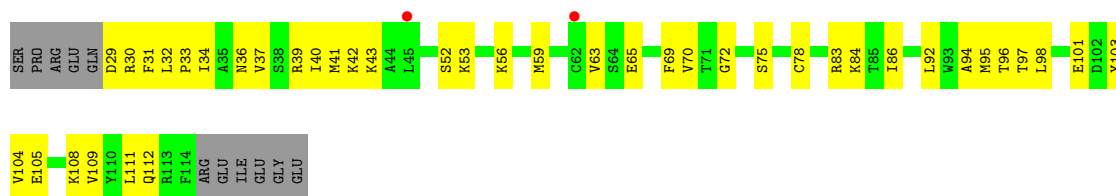
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	0	0
			678	430	114	129	5			
2	G	86	Total	C	N	O	S	0	0	0
			689	439	115	130	5			
2	L	86	Total	C	N	O	S	0	0	0
			689	439	115	130	5			
2	Q	86	Total	C	N	O	S	0	0	0
			689	439	115	130	5			

- Molecule 3 is a DNA chain called FT CORE1 DNA forward strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	25	Total 516	C 247	N 98	O 147	P 24	0	0	0
3	I	25	Total 516	C 247	N 98	O 147	P 24	0	0	0
3	N	25	Total 516	C 247	N 98	O 147	P 24	0	0	0
3	T	25	Total 516	C 247	N 98	O 147	P 24	0	0	0

- Molecule 4 is a DNA chain called FT CORE1 DNA reverse strand.

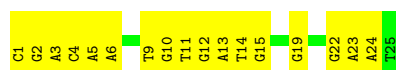
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	25	Total 503	C 243	N 87	O 149	P 24	0	0	0
4	J	25	Total 503	C 243	N 87	O 149	P 24	0	0	0
4	O	25	Total 503	C 243	N 87	O 149	P 24	0	0	0
4	U	25	Total 503	C 243	N 87	O 149	P 24	0	0	0



- Molecule 3: FT CORE1 DNA forward strand



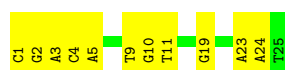
- Molecule 3: FT CORE1 DNA forward strand



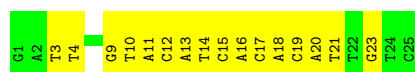
- Molecule 3: FT CORE1 DNA forward strand



- Molecule 3: FT CORE1 DNA forward strand



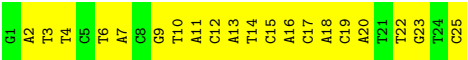
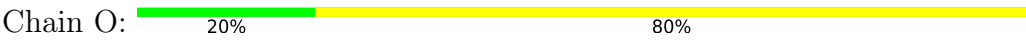
- Molecule 4: FT CORE1 DNA reverse strand



- Molecule 4: FT CORE1 DNA reverse strand



- Molecule 4: FT CORE1 DNA reverse strand



● Molecule 4: FT CORE1 DNA reverse strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.24Å 65.27Å 138.28Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	35.18 – 3.30 35.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.18-3.30) 99.1 (35.18-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.241 , 0.264 0.247 , 0.268	Depositor DCC
R_{free} test set	1423 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10910	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/1066	0.48	0/1425
1	F	0.32	0/1066	0.62	1/1425 (0.1%)
1	K	0.41	1/992 (0.1%)	0.75	1/1328 (0.1%)
1	P	0.32	0/1026	0.62	0/1373
2	B	0.28	0/688	0.47	0/923
2	G	0.24	0/700	0.52	0/939
2	L	0.19	0/700	0.48	0/939
2	Q	0.19	0/700	0.46	0/939
3	D	0.24	0/580	0.48	0/895
3	I	0.25	0/580	0.49	0/895
3	N	0.23	0/580	0.46	0/895
3	T	0.22	0/580	0.45	0/895
4	E	0.24	0/562	0.50	0/864
4	J	0.24	0/562	0.51	0/864
4	O	0.26	0/562	0.55	0/864
4	U	0.26	0/562	0.51	0/864
All	All	0.27	1/11506 (0.0%)	0.54	2/16327 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	139	PHE	C-N	-6.46	1.24	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	336	GLU	N-CA-C	-9.94	100.26	112.38
1	K	145	ILE	N-CA-C	5.37	116.10	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1050	0	1093	52	0
1	F	1050	0	1093	58	0
1	K	978	0	1018	81	0
1	P	1011	0	1052	79	0
2	B	678	0	692	36	0
2	G	689	0	701	42	0
2	L	689	0	701	44	0
2	Q	689	0	701	46	0
3	D	516	0	284	14	0
3	I	516	0	284	18	0
3	N	516	0	284	19	0
3	T	516	0	284	9	0
4	E	503	0	285	20	0
4	J	503	0	285	24	0
4	O	503	0	285	27	0
4	U	503	0	285	22	0
All	All	10910	0	9327	462	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 24.

The worst 5 of 462 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:K:335:ALA:HA	1:K:338:ARG:CD	1.72	1.20
1:K:140:ASP:HB2	1:K:306:ARG:HH12	1.07	1.17
1:P:139:PHE:HB3	1:P:142:LEU:HD12	1.27	1.13
1:P:84:GLU:OE2	1:P:321:LYS:HD2	1.50	1.11
2:L:98:LEU:HD22	2:L:100:PHE:CZ	1.89	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	121/174 (70%)	116 (96%)	5 (4%)	0	100	100
1	F	121/174 (70%)	117 (97%)	4 (3%)	0	100	100
1	K	113/174 (65%)	107 (95%)	6 (5%)	0	100	100
1	P	117/174 (67%)	113 (97%)	4 (3%)	0	100	100
2	B	83/97 (86%)	81 (98%)	2 (2%)	0	100	100
2	G	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
2	L	84/97 (87%)	84 (100%)	0	0	100	100
2	Q	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
All	All	807/1084 (74%)	783 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	111/150 (74%)	111 (100%)	0	100	100
1	F	111/150 (74%)	110 (99%)	1 (1%)	70	78
1	K	104/150 (69%)	100 (96%)	4 (4%)	29	57
1	P	107/150 (71%)	101 (94%)	6 (6%)	19	47
2	B	75/86 (87%)	73 (97%)	2 (3%)	39	63
2	G	76/86 (88%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	76/86 (88%)	75 (99%)	1 (1%)	61	74
2	Q	76/86 (88%)	75 (99%)	1 (1%)	61	74
All	All	736/944 (78%)	721 (98%)	15 (2%)	48	68

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	136	THR
2	L	98	LEU
1	P	138	ILE
2	Q	95	MET
1	P	312	ARG

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

Mol	Chain	Res	Type
2	B	112	GLN
1	K	115	HIS

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 oligosaccharides 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.

6 Fit of model and data ⓘ

6.1 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, 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	125/174 (71%)	-0.06	0 100 100	70, 103, 134, 162	0
1	F	125/174 (71%)	-0.14	1 (0%) 82 68	57, 87, 120, 143	0
1	K	117/174 (67%)	0.09	1 (0%) 81 65	103, 141, 212, 234	0
1	P	121/174 (69%)	0.02	0 100 100	102, 155, 205, 226	0
2	B	85/97 (87%)	-0.30	0 100 100	66, 86, 111, 127	0
2	G	86/97 (88%)	-0.38	0 100 100	55, 77, 98, 110	0
2	L	86/97 (88%)	-0.04	0 100 100	105, 134, 157, 178	0
2	Q	86/97 (88%)	0.23	2 (2%) 61 42	105, 165, 188, 194	0
3	D	25/25 (100%)	-0.25	0 100 100	89, 116, 136, 148	0
3	I	25/25 (100%)	-0.22	0 100 100	86, 108, 137, 146	0
3	N	25/25 (100%)	0.08	0 100 100	154, 176, 210, 230	0
3	T	25/25 (100%)	-0.20	0 100 100	107, 136, 171, 193	0
4	E	25/25 (100%)	-0.21	0 100 100	91, 108, 152, 156	0
4	J	25/25 (100%)	0.10	0 100 100	87, 107, 130, 135	0
4	O	25/25 (100%)	0.12	0 100 100	161, 183, 209, 219	0
4	U	25/25 (100%)	-0.05	0 100 100	115, 137, 165, 196	0
All	All	1031/1284 (80%)	-0.07	4 (0%) 88 79	55, 121, 191, 234	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	45	LEU	2.9
2	Q	62	CYS	2.3
1	K	142	LEU	2.2
1	F	91	ALA	2.1

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 oligosaccharides 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.