



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:30 am GMT

PDB ID : 4C8H
Title : Crystal structure of the C-terminal region of yeast Ctf4, selenomethionine protein.
Authors : Simon, A.C.; Pellegrini, L.
Deposited on : 2013-10-01
Resolution : 2.69 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

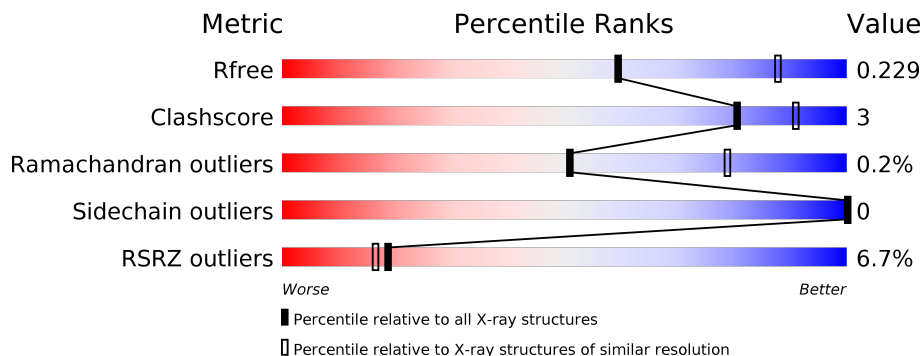
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	478	<div> <div>2%</div> <div>82% 8% 10%</div> </div>
1	B	478	<div> <div>9%</div> <div>81% 7% 12%</div> </div>
1	C	478	<div> <div>6%</div> <div>81% 8% 11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10421 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 CTF4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	Se	0	1	0
			3475	2233	577	649	5	11			
1	B	419	Total	C	N	O	S	Se	0	0	0
			3371	2170	557	629	5	10			
1	C	425	Total	C	N	O	S	Se	0	0	0
			3412	2192	565	640	5	10			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MSE	-	EXPRESSION TAG	UNP Q01454
A	451	GLY	-	EXPRESSION TAG	UNP Q01454
A	452	SER	-	EXPRESSION TAG	UNP Q01454
A	453	SER	-	EXPRESSION TAG	UNP Q01454
A	454	HIS	-	EXPRESSION TAG	UNP Q01454
A	455	HIS	-	EXPRESSION TAG	UNP Q01454
A	456	HIS	-	EXPRESSION TAG	UNP Q01454
A	457	HIS	-	EXPRESSION TAG	UNP Q01454
A	458	HIS	-	EXPRESSION TAG	UNP Q01454
A	459	HIS	-	EXPRESSION TAG	UNP Q01454
A	460	SER	-	EXPRESSION TAG	UNP Q01454
A	461	GLN	-	EXPRESSION TAG	UNP Q01454
A	462	ASP	-	EXPRESSION TAG	UNP Q01454
A	463	PRO	-	EXPRESSION TAG	UNP Q01454
A	464	GLU	-	EXPRESSION TAG	UNP Q01454
A	465	ASN	-	EXPRESSION TAG	UNP Q01454
A	466	LEU	-	EXPRESSION TAG	UNP Q01454
A	467	TYR	-	EXPRESSION TAG	UNP Q01454
A	468	PHE	-	EXPRESSION TAG	UNP Q01454
A	469	GLN	-	EXPRESSION TAG	UNP Q01454
A	470	GLY	-	EXPRESSION TAG	UNP Q01454
B	450	MSE	-	EXPRESSION TAG	UNP Q01454
B	451	GLY	-	EXPRESSION TAG	UNP Q01454

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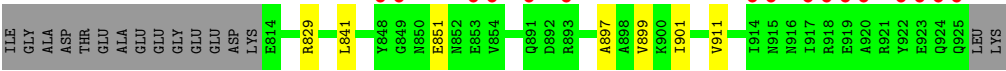
Chain	Residue	Modelled	Actual	Comment	Reference
B	452	SER	-	EXPRESSION TAG	UNP Q01454
B	453	SER	-	EXPRESSION TAG	UNP Q01454
B	454	HIS	-	EXPRESSION TAG	UNP Q01454
B	455	HIS	-	EXPRESSION TAG	UNP Q01454
B	456	HIS	-	EXPRESSION TAG	UNP Q01454
B	457	HIS	-	EXPRESSION TAG	UNP Q01454
B	458	HIS	-	EXPRESSION TAG	UNP Q01454
B	459	HIS	-	EXPRESSION TAG	UNP Q01454
B	460	SER	-	EXPRESSION TAG	UNP Q01454
B	461	GLN	-	EXPRESSION TAG	UNP Q01454
B	462	ASP	-	EXPRESSION TAG	UNP Q01454
B	463	PRO	-	EXPRESSION TAG	UNP Q01454
B	464	GLU	-	EXPRESSION TAG	UNP Q01454
B	465	ASN	-	EXPRESSION TAG	UNP Q01454
B	466	LEU	-	EXPRESSION TAG	UNP Q01454
B	467	TYR	-	EXPRESSION TAG	UNP Q01454
B	468	PHE	-	EXPRESSION TAG	UNP Q01454
B	469	GLN	-	EXPRESSION TAG	UNP Q01454
B	470	GLY	-	EXPRESSION TAG	UNP Q01454
C	450	MSE	-	EXPRESSION TAG	UNP Q01454
C	451	GLY	-	EXPRESSION TAG	UNP Q01454
C	452	SER	-	EXPRESSION TAG	UNP Q01454
C	453	SER	-	EXPRESSION TAG	UNP Q01454
C	454	HIS	-	EXPRESSION TAG	UNP Q01454
C	455	HIS	-	EXPRESSION TAG	UNP Q01454
C	456	HIS	-	EXPRESSION TAG	UNP Q01454
C	457	HIS	-	EXPRESSION TAG	UNP Q01454
C	458	HIS	-	EXPRESSION TAG	UNP Q01454
C	459	HIS	-	EXPRESSION TAG	UNP Q01454
C	460	SER	-	EXPRESSION TAG	UNP Q01454
C	461	GLN	-	EXPRESSION TAG	UNP Q01454
C	462	ASP	-	EXPRESSION TAG	UNP Q01454
C	463	PRO	-	EXPRESSION TAG	UNP Q01454
C	464	GLU	-	EXPRESSION TAG	UNP Q01454
C	465	ASN	-	EXPRESSION TAG	UNP Q01454
C	466	LEU	-	EXPRESSION TAG	UNP Q01454
C	467	TYR	-	EXPRESSION TAG	UNP Q01454
C	468	PHE	-	EXPRESSION TAG	UNP Q01454
C	469	GLN	-	EXPRESSION TAG	UNP Q01454
C	470	GLY	-	EXPRESSION TAG	UNP Q01454

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total 113	O 113	0	0
2	B	15	Total 15	O 15	0	0
2	C	35	Total 35	O 35	0	0

- Molecule 1: CTF4





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	107.29Å 118.43Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.69 49.19 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.19-2.69) 99.4 (49.19-2.69)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.225 0.194 , 0.229	Depositor DCC
R_{free} test set	2812 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10421	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.23	0/3552	0.39	0/4790
1	B	0.22	0/3445	0.39	0/4649
1	C	0.23	0/3487	0.40	0/4707
All	All	0.22	0/10484	0.39	0/14146

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3475	0	3433	26	0
1	B	3371	0	3319	20	0
1	C	3412	0	3356	23	0
2	A	113	0	0	0	0
2	B	15	0	0	0	0
2	C	35	0	0	0	0
All	All	10421	0	10108	63	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 3.

The worst 5 of 63 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:496:MSE:HE2	1:A:745:LEU:HD21	1.63	0.79
1:B:496:MSE:HE2	1:B:745:LEU:HD21	1.68	0.76
1:C:496:MSE:HE2	1:C:745:LEU:HD21	1.70	0.73
1:C:778:MSE:HE3	1:C:829:ARG:HA	1.77	0.66
1:B:533:GLY:O	1:B:548:GLN:NE2	2.28	0.66

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	426/478 (89%)	417 (98%)	8 (2%)	1 (0%)	51	79
1	B	411/478 (86%)	401 (98%)	9 (2%)	1 (0%)	51	79
1	C	419/478 (88%)	410 (98%)	8 (2%)	1 (0%)	51	79
All	All	1256/1434 (88%)	1228 (98%)	25 (2%)	3 (0%)	51	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	TYR
1	B	749	TYR
1	C	749	TYR

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	384/410 (94%)	384 (100%)	0	100	100
1	B	371/410 (90%)	371 (100%)	0	100	100
1	C	376/410 (92%)	376 (100%)	0	100	100
All	All	1131/1230 (92%)	1131 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 carbohydrates 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 [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	420/478 (87%)	0.30	8 (1%) 67 68	35, 57, 92, 134	0
1	B	409/478 (85%)	0.64	44 (10%) 6 5	50, 84, 124, 160	0
1	C	415/478 (86%)	0.48	31 (7%) 15 12	40, 71, 109, 151	0
All	All	1244/1434 (86%)	0.47	83 (6%) 19 16	35, 70, 116, 160	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PHE	7.4
1	B	917	ILE	7.0
1	C	922	TYR	6.8
1	C	646	SER	5.5
1	A	793	ILE	5.4

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 carbohydrates 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.