



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:06 PM GMT

PDB ID : 4NSC
Title : Crystal Structure of CBARA1 in the Apo-form
Authors : Wang, L.; Yang, X.; Li, S.; Shen, Y.
Deposited on : 2013-11-28
Resolution : 3.20 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

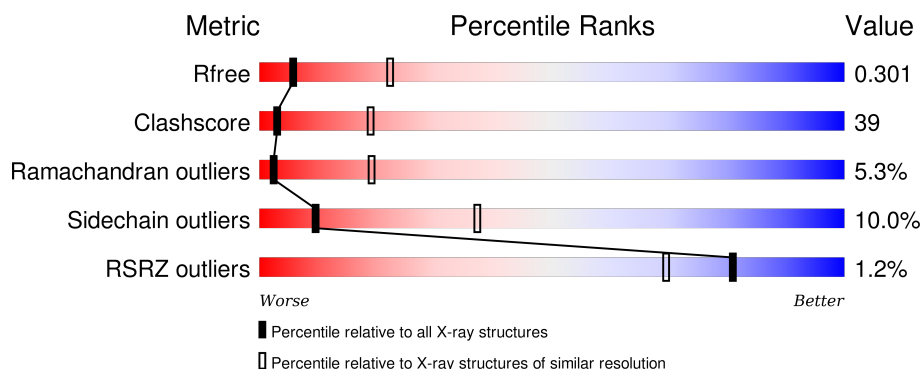
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	401	<div> <div>2%</div> <div> <div></div> <div>29%</div> <div>39%</div> <div>8%</div> <div>23%</div> </div> </div>
1	B	401	<div> <div>%</div> <div> <div></div> <div>35%</div> <div>36%</div> <div>7%</div> <div>21%</div> </div> </div>
1	C	401	<div> <div>%</div> <div> <div></div> <div>28%</div> <div>47%</div> <div>6%</div> <div>18%</div> </div> </div>
1	D	401	<div> <div>%</div> <div> <div></div> <div>37%</div> <div>36%</div> <div>7%</div> <div>19%</div> </div> </div>
1	E	401	<div> <div></div> <div> <div>35%</div> <div>40%</div> <div>6%</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	401	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (34%), yellow (35%), orange (7%), and grey (23%). A small red dot is located on the orange segment.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15349 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 Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2472	1583	419	454	16			
1	B	316	Total	C	N	O	S	0	0	0
			2539	1622	426	473	18			
1	C	330	Total	C	N	O	S	0	0	0
			2619	1673	442	486	18			
1	D	326	Total	C	N	O	S	0	0	0
			2604	1662	438	487	17			
1	E	330	Total	C	N	O	S	0	0	0
			2598	1657	439	487	15			
1	F	310	Total	C	N	O	S	0	0	0
			2504	1601	422	468	13			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
A	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
A	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
A	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
A	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
A	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
A	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
A	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
A	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
A	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
A	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
A	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
A	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
A	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
A	96	MET	-	EXPRESSION TAG	UNP Q9BPX6
B	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
B	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
B	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
B	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
B	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
B	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
B	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
B	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
B	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
B	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
B	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
B	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6
B	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
B	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
B	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
B	96	MET	-	EXPRESSION TAG	UNP Q9BPX6
C	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
C	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
C	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
C	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
C	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
C	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
C	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
C	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
C	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
C	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
C	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
C	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
C	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
C	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
C	96	MET	-	EXPRESSION TAG	UNP Q9BPX6
D	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
D	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
D	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
D	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
D	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
D	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
D	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
D	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
D	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
D	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
D	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
D	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6
D	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
D	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
D	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
D	96	MET	-	EXPRESSION TAG	UNP Q9BPX6
E	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
E	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
E	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
E	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
E	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
E	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
E	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
E	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
E	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
E	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
E	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
E	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
E	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
E	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
E	96	MET	-	EXPRESSION TAG	UNP Q9BPX6
F	76	MET	-	EXPRESSION TAG	UNP Q9BPX6
F	77	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	78	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	79	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	80	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	81	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	82	HIS	-	EXPRESSION TAG	UNP Q9BPX6
F	83	SER	-	EXPRESSION TAG	UNP Q9BPX6
F	84	SER	-	EXPRESSION TAG	UNP Q9BPX6
F	85	GLY	-	EXPRESSION TAG	UNP Q9BPX6
F	86	LEU	-	EXPRESSION TAG	UNP Q9BPX6
F	87	GLU	-	EXPRESSION TAG	UNP Q9BPX6
F	88	VAL	-	EXPRESSION TAG	UNP Q9BPX6
F	89	LEU	-	EXPRESSION TAG	UNP Q9BPX6
F	90	PHE	-	EXPRESSION TAG	UNP Q9BPX6
F	91	GLN	-	EXPRESSION TAG	UNP Q9BPX6
F	92	GLY	-	EXPRESSION TAG	UNP Q9BPX6
F	93	PRO	-	EXPRESSION TAG	UNP Q9BPX6
F	94	GLY	-	EXPRESSION TAG	UNP Q9BPX6
F	95	SER	-	EXPRESSION TAG	UNP Q9BPX6
F	96	MET	-	EXPRESSION TAG	UNP Q9BPX6

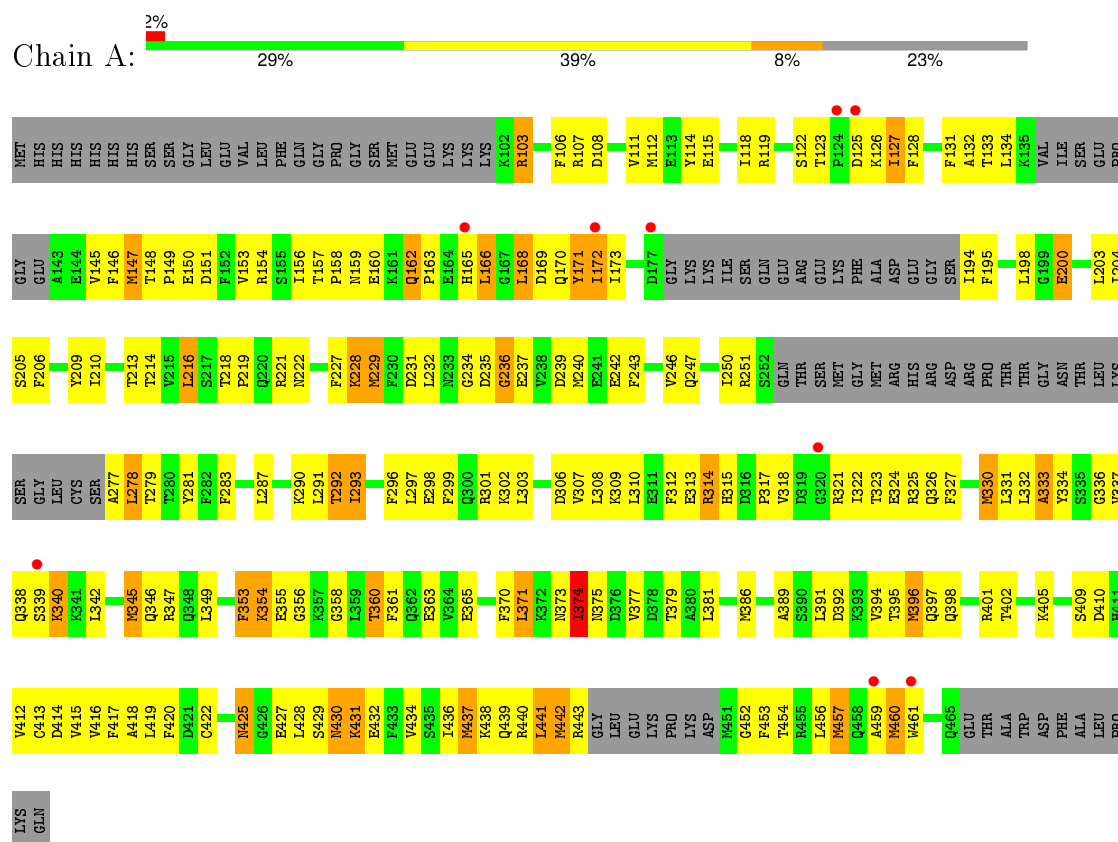
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	F	4	Total O 4 4	0	0

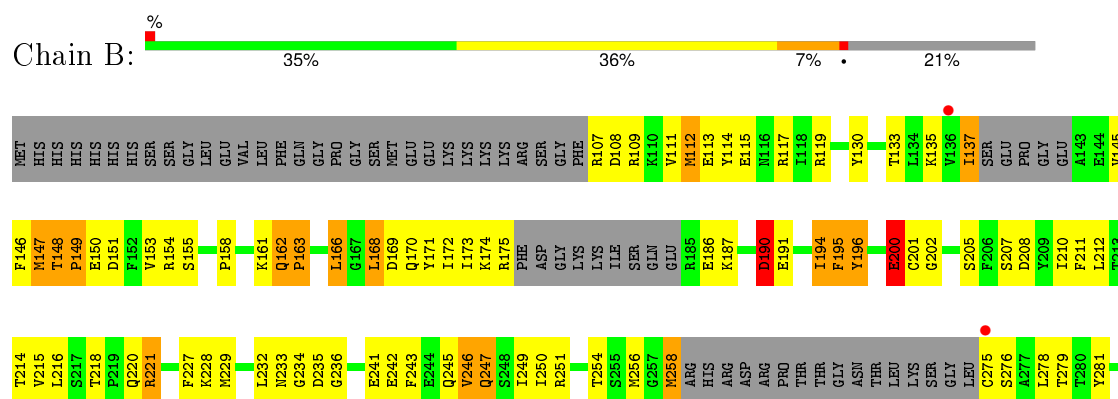
3 Residue-property plots

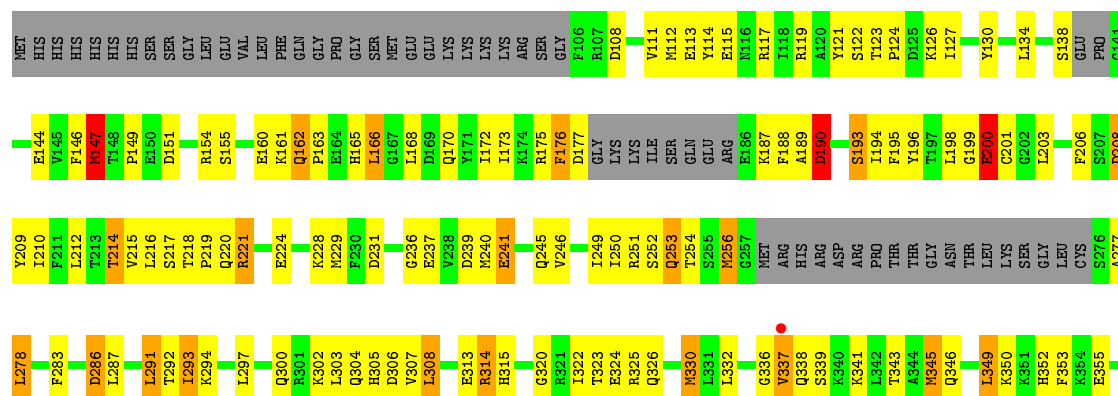
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

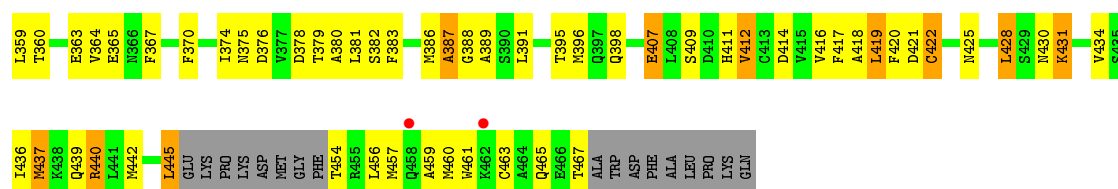
- Molecule 1: Calcium uptake protein 1, mitochondrial



- Molecule 1: Calcium uptake protein 1, mitochondrial

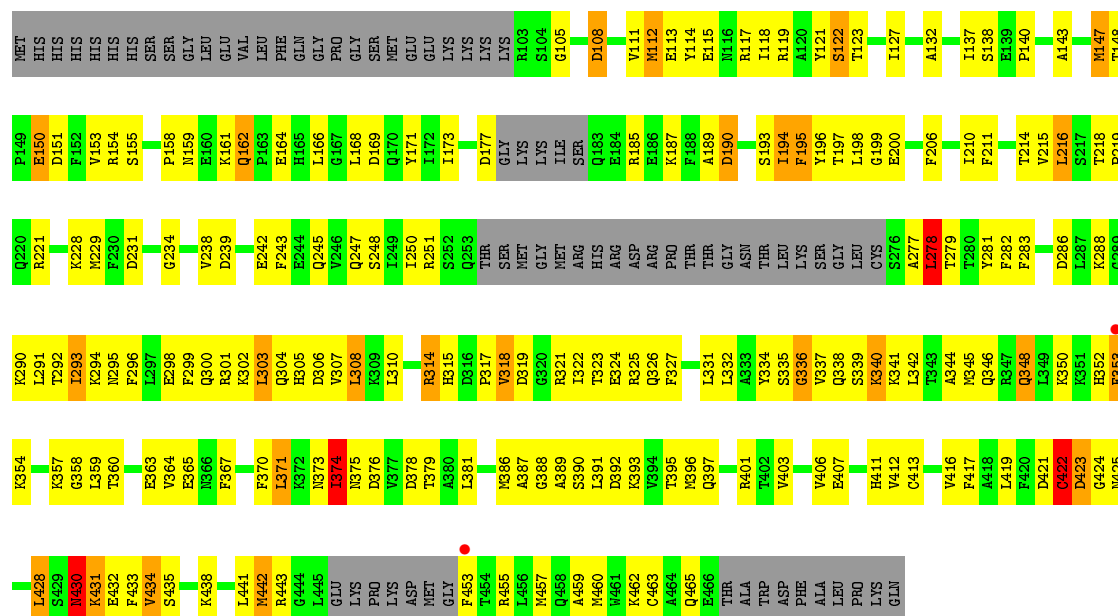






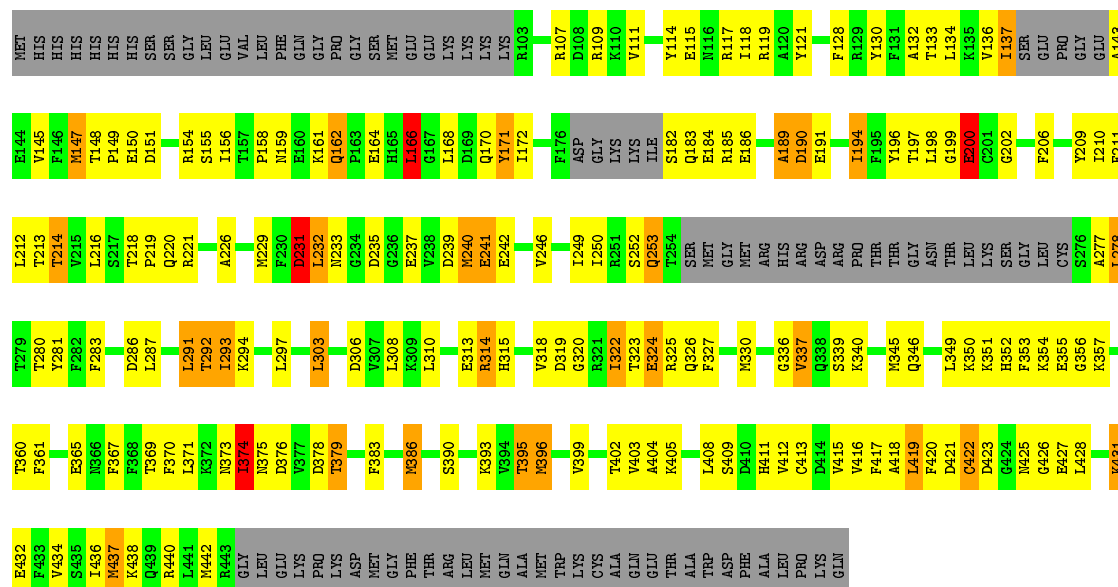
• Molecule 1: Calcium uptake protein 1, mitochondrial

Chain E: 35% 40% 6% 18%



• Molecule 1: Calcium uptake protein 1, mitochondrial

Chain F: 34% 35% 7% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 146.82Å 115.87Å 90.00° 111.08° 90.00°	Depositor
Resolution (Å)	36.72 – 3.20 36.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.72-3.20) 92.4 (36.71-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.254 , 0.307 0.254 , 0.301	Depositor DCC
R_{free} test set	1895 reflections (4.30%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.5	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 46620 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15349	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.61	10/2517 (0.4%)	0.66	1/3379 (0.0%)
1	B	0.67	10/2581 (0.4%)	0.68	0/3456
1	C	0.65	9/2665 (0.3%)	0.68	1/3577 (0.0%)
1	D	0.69	8/2649 (0.3%)	0.73	0/3551
1	E	0.62	4/2644 (0.2%)	0.73	1/3550 (0.0%)
1	F	0.64	5/2549 (0.2%)	0.74	2/3418 (0.1%)
All	All	0.65	46/15605 (0.3%)	0.71	5/20931 (0.0%)

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	B	0	1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	MET	CG-SD	9.03	2.04	1.81
1	D	147	MET	CG-SD	8.10	2.02	1.81
1	D	229	MET	CG-SD	7.68	2.01	1.81
1	F	442	MET	CG-SD	7.67	2.01	1.81
1	D	256	MET	CG-SD	7.62	2.00	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	PRO	N-CA-CB	6.02	110.52	103.30
1	F	356	GLY	N-CA-C	5.90	127.85	113.10
1	E	278	LEU	CA-CB-CG	5.53	128.02	115.30
1	F	166	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	441	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	TYR	Sidechain

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	2472	0	2397	221	0
1	B	2539	0	2496	197	0
1	C	2619	0	2542	230	0
1	D	2604	0	2547	208	0
1	E	2598	0	2494	184	1
1	F	2504	0	2458	197	1
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	4	0	0	0	0
All	All	15349	0	14934	1171	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 39.

The worst 5 of 1171 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:D:147:MET:SD	1:D:147:MET:CG	2.02	1.48
1:C:147:MET:CG	1:C:147:MET:SD	2.04	1.44
1:F:323:THR:HB	1:F:326:GLN:HG3	1.23	1.14
1:C:323:THR:HB	1:C:326:GLN:HG3	1.23	1.14
1:E:323:THR:HB	1:E:326:GLN:HG3	1.28	1.14

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)
1:E:171:TYR:O	1:F:357:LYS:NZ[2_756]	2.10	0.10

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	300/401 (75%)	227 (76%)	54 (18%)	19 (6%)	2	13
1	B	304/401 (76%)	235 (77%)	53 (17%)	16 (5%)	2	19
1	C	322/401 (80%)	248 (77%)	56 (17%)	18 (6%)	2	18
1	D	316/401 (79%)	262 (83%)	39 (12%)	15 (5%)	3	22
1	E	322/401 (80%)	261 (81%)	47 (15%)	14 (4%)	3	25
1	F	302/401 (75%)	237 (78%)	49 (16%)	16 (5%)	2	19
All	All	1866/2406 (78%)	1470 (79%)	298 (16%)	98 (5%)	2	19

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	172	ILE
1	A	354	LYS
1	A	453	PHE
1	B	374	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	259/354 (73%)	232 (90%)	27 (10%)	9	35
1	B	273/354 (77%)	243 (89%)	30 (11%)	8	33
1	C	274/354 (77%)	249 (91%)	25 (9%)	12	42
1	D	278/354 (78%)	256 (92%)	22 (8%)	15	53
1	E	269/354 (76%)	240 (89%)	29 (11%)	8	33
1	F	270/354 (76%)	241 (89%)	29 (11%)	8	34
All	All	1623/2124 (76%)	1461 (90%)	162 (10%)	9	37

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	379	THR
1	D	278	LEU
1	F	292	THR
1	C	396	MET
1	D	147	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	411	HIS
1	D	295	ASN
1	F	247	GLN
1	C	425	ASN
1	D	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	310/401 (77%)	0.12	9 (2%) 55 41	62, 86, 113, 127	0
1	B	316/401 (78%)	-0.09	3 (0%) 85 78	41, 73, 104, 122	0
1	C	330/401 (82%)	-0.13	6 (1%) 71 58	44, 70, 97, 114	0
1	D	326/401 (81%)	-0.15	3 (0%) 85 78	36, 60, 89, 111	0
1	E	330/401 (82%)	-0.28	2 (0%) 90 84	32, 59, 107, 122	0
1	F	310/401 (77%)	-0.31	0 100 100	36, 58, 95, 112	0
All	All	1922/2406 (79%)	-0.14	23 (1%) 81 69	32, 69, 104, 127	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	TRP	5.2
1	C	462	LYS	3.7
1	A	124	PRO	3.5
1	E	453	PHE	3.2
1	C	456	LEU	3.1

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 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.