wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 10:55 am BST

PDB ID	:	6C5R
Title	:	Crystal structure of the soluble domain of the mitochondrial calcium uniporter
Authors	:	Fan, C.; Fan, M.; Fastman, N.; Zhang, J.; Feng, L.
Deposited on	:	2018-01-16
Resolution	:	3.10 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 following versions of software and data (see references (1)) were used in the production of this report:

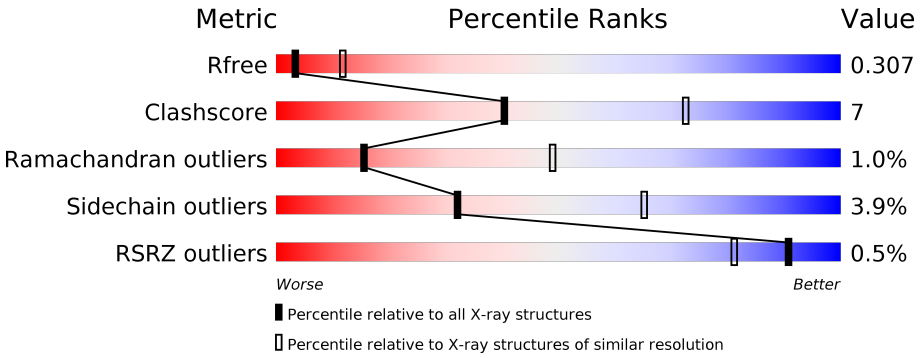
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	210	49% 18% • 32%
1	B	210	% 55% 10% 34%
1	C	210	% 52% 12% • 33%
1	D	210	67% 14% • 19%
1	E	210	57% 19% 24%
1	F	210	65% 15% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	210	
1	H	210	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9966 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 uniporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1178	750	215	209	4			
1	B	139	Total	C	N	O	S	0	0	0
			1065	681	192	190	2			
1	D	171	Total	C	N	O	S	0	0	0
			1405	896	250	254	5			
1	F	169	Total	C	N	O	S	0	0	0
			1380	883	246	246	5			
1	H	170	Total	C	N	O	S	0	0	0
			1377	886	243	243	5			
1	C	141	Total	C	N	O	S	0	0	0
			1104	704	199	197	4			
1	E	159	Total	C	N	O	S	0	0	0
			1257	808	224	220	5			
1	G	153	Total	C	N	O	S	0	0	0
			1200	770	213	213	4			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP E9DVV4
A	-2	PRO	-	expression tag	UNP E9DVV4
A	-1	MET	-	expression tag	UNP E9DVV4
A	0	MET	-	expression tag	UNP E9DVV4
A	?	-	LYS	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	ASP	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ARG	deletion	UNP E9DVV4
A	?	-	ARG	deletion	UNP E9DVV4
A	?	-	GLU	deletion	UNP E9DVV4
A	?	-	GLU	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	VAL	deletion	UNP E9DVV4
A	?	-	ALA	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	TYR	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	LEU	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ARG	deletion	UNP E9DVV4
A	?	-	GLU	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	PRO	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	LYS	deletion	UNP E9DVV4
A	167	ALA	CYS	engineered mutation	UNP E9DVV4
B	-3	GLY	-	expression tag	UNP E9DVV4
B	-2	PRO	-	expression tag	UNP E9DVV4
B	-1	MET	-	expression tag	UNP E9DVV4
B	0	MET	-	expression tag	UNP E9DVV4
B	?	-	LYS	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	ASP	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ARG	deletion	UNP E9DVV4
B	?	-	ARG	deletion	UNP E9DVV4
B	?	-	GLU	deletion	UNP E9DVV4
B	?	-	GLU	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP E9DVV4
B	?	-	ALA	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	TYR	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	LEU	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ARG	deletion	UNP E9DVV4
B	?	-	GLU	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	PRO	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	LYS	deletion	UNP E9DVV4
B	167	ALA	CYS	engineered mutation	UNP E9DVV4
D	-3	GLY	-	expression tag	UNP E9DVV4
D	-2	PRO	-	expression tag	UNP E9DVV4
D	-1	MET	-	expression tag	UNP E9DVV4
D	0	MET	-	expression tag	UNP E9DVV4
D	?	-	LYS	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	ASN	deletion	UNP E9DVV4
D	?	-	ASP	deletion	UNP E9DVV4
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	ARG	deletion	UNP E9DVV4
D	?	-	ARG	deletion	UNP E9DVV4
D	?	-	GLU	deletion	UNP E9DVV4
D	?	-	GLU	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	ASN	deletion	UNP E9DVV4
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	ASN	deletion	UNP E9DVV4
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	ASN	deletion	UNP E9DVV4
D	?	-	VAL	deletion	UNP E9DVV4
D	?	-	ALA	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	TYR	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	LEU	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	ARG	deletion	UNP E9DVV4
D	?	-	GLU	deletion	UNP E9DVV4
D	?	-	GLY	deletion	UNP E9DVV4
D	?	-	PRO	deletion	UNP E9DVV4
D	?	-	SER	deletion	UNP E9DVV4
D	?	-	LYS	deletion	UNP E9DVV4
D	167	ALA	CYS	engineered mutation	UNP E9DVV4
F	-3	GLY	-	expression tag	UNP E9DVV4
F	-2	PRO	-	expression tag	UNP E9DVV4
F	-1	MET	-	expression tag	UNP E9DVV4
F	0	MET	-	expression tag	UNP E9DVV4
F	?	-	LYS	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	ASN	deletion	UNP E9DVV4
F	?	-	ASP	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	ARG	deletion	UNP E9DVV4
F	?	-	ARG	deletion	UNP E9DVV4
F	?	-	GLU	deletion	UNP E9DVV4
F	?	-	GLU	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	ASN	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	ASN	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	ASN	deletion	UNP E9DVV4
F	?	-	VAL	deletion	UNP E9DVV4
F	?	-	ALA	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	TYR	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	LEU	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	ARG	deletion	UNP E9DVV4
F	?	-	GLU	deletion	UNP E9DVV4
F	?	-	GLY	deletion	UNP E9DVV4
F	?	-	PRO	deletion	UNP E9DVV4
F	?	-	SER	deletion	UNP E9DVV4
F	?	-	LYS	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	167	ALA	CYS	engineered mutation	UNP E9DVV4
H	-3	GLY	-	expression tag	UNP E9DVV4
H	-2	PRO	-	expression tag	UNP E9DVV4
H	-1	MET	-	expression tag	UNP E9DVV4
H	0	MET	-	expression tag	UNP E9DVV4
H	?	-	LYS	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	ASN	deletion	UNP E9DVV4
H	?	-	ASP	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	ARG	deletion	UNP E9DVV4
H	?	-	ARG	deletion	UNP E9DVV4
H	?	-	GLU	deletion	UNP E9DVV4
H	?	-	GLU	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	ASN	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	ASN	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	ASN	deletion	UNP E9DVV4
H	?	-	VAL	deletion	UNP E9DVV4
H	?	-	ALA	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	TYR	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	LEU	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	ARG	deletion	UNP E9DVV4
H	?	-	GLU	deletion	UNP E9DVV4
H	?	-	GLY	deletion	UNP E9DVV4
H	?	-	PRO	deletion	UNP E9DVV4
H	?	-	SER	deletion	UNP E9DVV4
H	?	-	LYS	deletion	UNP E9DVV4
H	167	ALA	CYS	engineered mutation	UNP E9DVV4
C	-3	GLY	-	expression tag	UNP E9DVV4
C	-2	PRO	-	expression tag	UNP E9DVV4
C	-1	MET	-	expression tag	UNP E9DVV4
C	0	MET	-	expression tag	UNP E9DVV4
C	?	-	LYS	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP E9DVV4
C	?	-	ASP	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	ARG	deletion	UNP E9DVV4
C	?	-	ARG	deletion	UNP E9DVV4
C	?	-	GLU	deletion	UNP E9DVV4
C	?	-	GLU	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4
C	?	-	ASN	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	ASN	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4
C	?	-	ASN	deletion	UNP E9DVV4
C	?	-	VAL	deletion	UNP E9DVV4
C	?	-	ALA	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4
C	?	-	TYR	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	LEU	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	ARG	deletion	UNP E9DVV4
C	?	-	GLU	deletion	UNP E9DVV4
C	?	-	GLY	deletion	UNP E9DVV4
C	?	-	PRO	deletion	UNP E9DVV4
C	?	-	SER	deletion	UNP E9DVV4
C	?	-	LYS	deletion	UNP E9DVV4
C	167	ALA	CYS	engineered mutation	UNP E9DVV4
E	-3	GLY	-	expression tag	UNP E9DVV4
E	-2	PRO	-	expression tag	UNP E9DVV4
E	-1	MET	-	expression tag	UNP E9DVV4
E	0	MET	-	expression tag	UNP E9DVV4
E	?	-	LYS	deletion	UNP E9DVV4
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	ASN	deletion	UNP E9DVV4
E	?	-	ASP	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	ARG	deletion	UNP E9DVV4
E	?	-	ARG	deletion	UNP E9DVV4
E	?	-	GLU	deletion	UNP E9DVV4
E	?	-	GLU	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	ASN	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	ASN	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	ASN	deletion	UNP E9DVV4
E	?	-	VAL	deletion	UNP E9DVV4
E	?	-	ALA	deletion	UNP E9DVV4
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	TYR	deletion	UNP E9DVV4
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	LEU	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	ARG	deletion	UNP E9DVV4
E	?	-	GLU	deletion	UNP E9DVV4
E	?	-	GLY	deletion	UNP E9DVV4
E	?	-	PRO	deletion	UNP E9DVV4
E	?	-	SER	deletion	UNP E9DVV4
E	?	-	LYS	deletion	UNP E9DVV4
E	167	ALA	CYS	engineered mutation	UNP E9DVV4
G	-3	GLY	-	expression tag	UNP E9DVV4
G	-2	PRO	-	expression tag	UNP E9DVV4
G	-1	MET	-	expression tag	UNP E9DVV4
G	0	MET	-	expression tag	UNP E9DVV4
G	?	-	LYS	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	ASN	deletion	UNP E9DVV4
G	?	-	ASP	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	ARG	deletion	UNP E9DVV4
G	?	-	ARG	deletion	UNP E9DVV4
G	?	-	GLU	deletion	UNP E9DVV4
G	?	-	GLU	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	ASN	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	ASN	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	ASN	deletion	UNP E9DVV4

Continued on next page...

Continued from previous page...

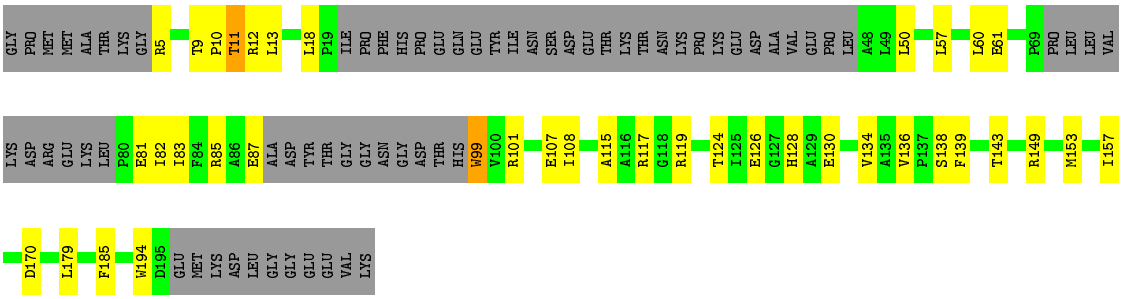
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	VAL	deletion	UNP E9DVV4
G	?	-	ALA	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	TYR	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	LEU	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	ARG	deletion	UNP E9DVV4
G	?	-	GLU	deletion	UNP E9DVV4
G	?	-	GLY	deletion	UNP E9DVV4
G	?	-	PRO	deletion	UNP E9DVV4
G	?	-	SER	deletion	UNP E9DVV4
G	?	-	LYS	deletion	UNP E9DVV4
G	167	ALA	CYS	engineered mutation	UNP E9DVV4

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

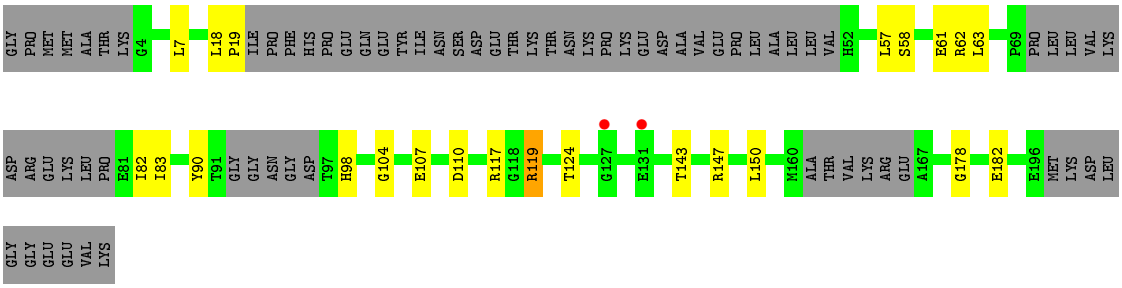
- Molecule 1: calcium uniporter

Chain A:



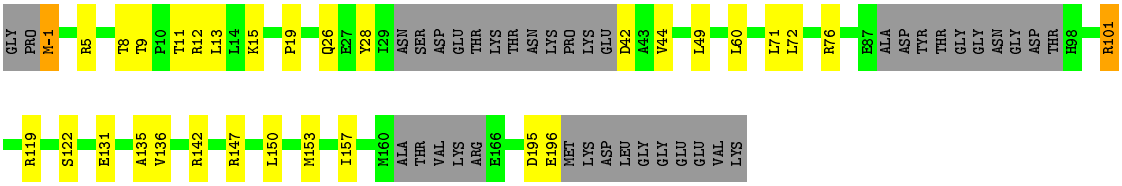
- Molecule 1: calcium uniporter

Chain B:



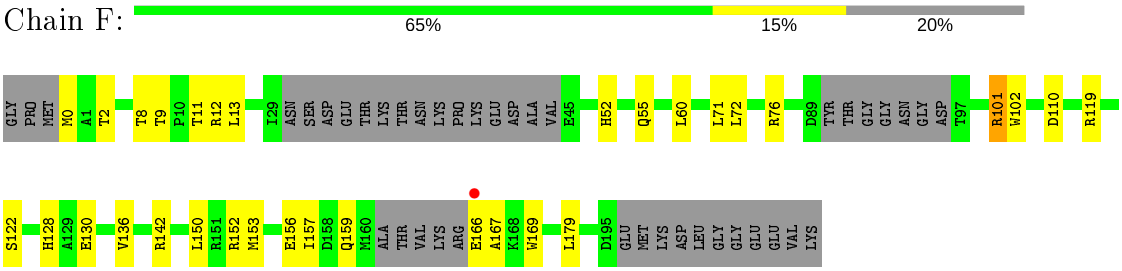
- Molecule 1: calcium uniporter

Chain D:



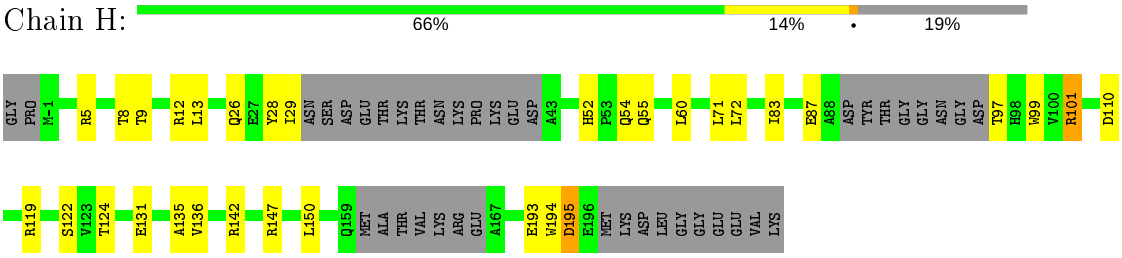
- Molecule 1: calcium uniporter

Chain F:



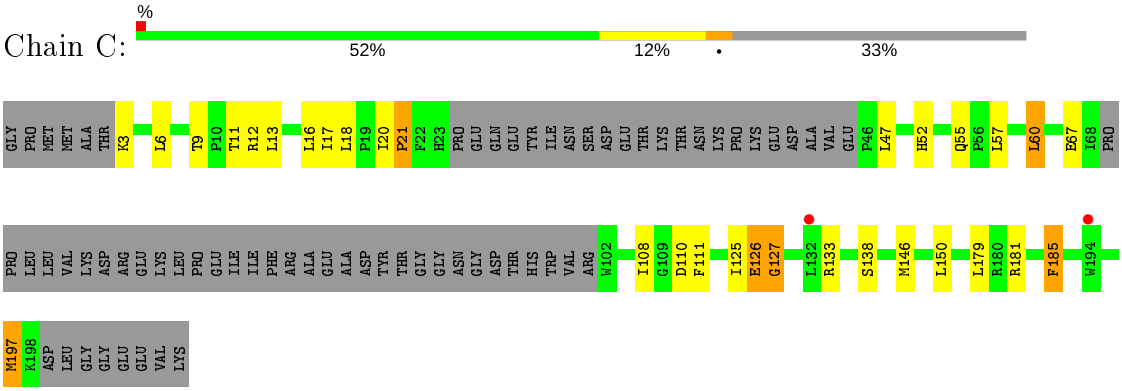
- Molecule 1: calcium uniporter

Chain H:



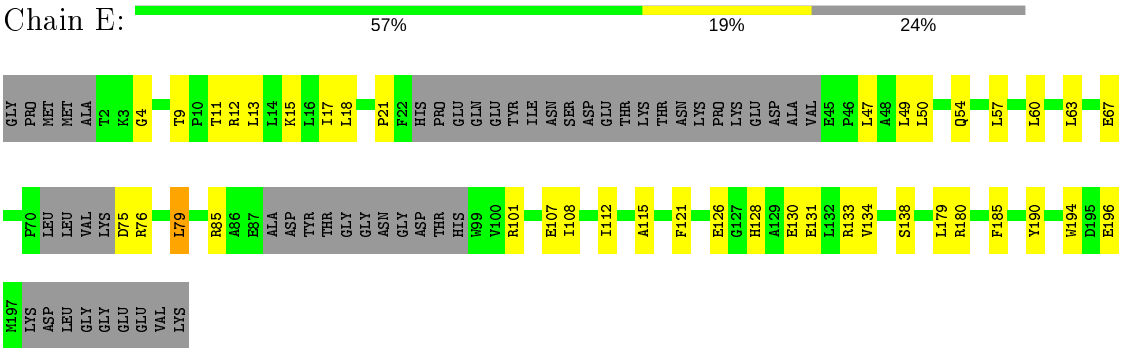
- Molecule 1: calcium uniporter

Chain C:



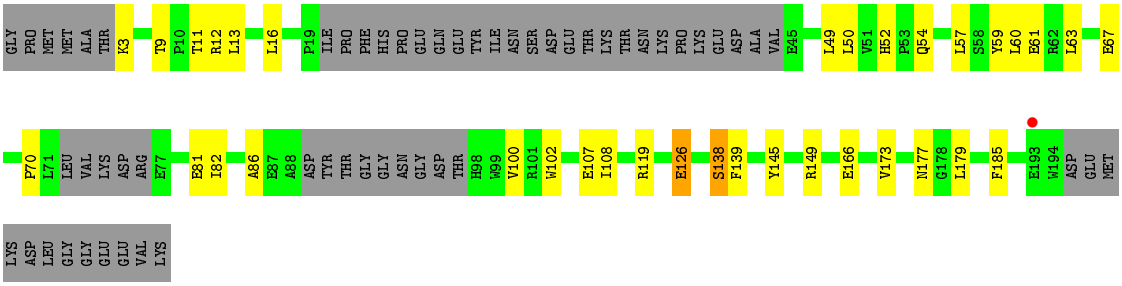
- Molecule 1: calcium uniporter

Chain E:



- Molecule 1: calcium uniporter

Chain G:


GLY PRO MET MET ALA THR K3 T9 P10 T11 R12 L13 L16 P19 ILE PRO PHE HIS PRO GLU GLN GLU TYR ILE ASN SER ASP GLU THR LYS THR ASN LYS PRO LYS GLU ASP ALA VAL E45 L49 L50 V51 H52 P53 Q54 L57 S58 Y59 L60 E61 R62 L63 E67
P70 L71 LEU VAL LYS ASP ARG E77 E81 I82 A86 E87 A88 ASP TYR THR GLY GLY ASN GLY ASP THR H98 W99 V100 R101 W102 E107 I108 R119 E126 S138 F139 Y145 R149 E166 V173 N177 G178 L179 F185 E193 W194 ASP GLU MET
LYS ASP LEU GLY GLY GLU GLU VAL LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.79Å 119.92Å 88.00Å 90.00° 106.89° 90.00°	Depositor
Resolution (Å)	42.11 – 3.10 48.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.11-3.10) 88.8 (48.35-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 3.12Å)	Xtriage
Refinement program	phenix.refine 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.262 , 0.306 0.262 , 0.307	Depositor DCC
R_{free} test set	2007 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9966	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

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	0.25	0/1201	0.43	0/1618
1	B	0.24	0/1087	0.44	0/1475
1	C	0.25	0/1124	0.46	0/1519
1	D	0.25	0/1434	0.44	0/1936
1	E	0.26	0/1283	0.46	1/1737 (0.1%)
1	F	0.26	0/1410	0.46	0/1906
1	G	0.25	0/1226	0.43	0/1662
1	H	0.26	0/1408	0.47	0/1906
All	All	0.25	0/10173	0.45	1/13759 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	79	LEU	CA-CB-CG	5.14	127.12	115.30

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	1178	0	1187	23	0
1	B	1065	0	989	14	0
1	C	1104	0	1098	18	0
1	D	1405	0	1407	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1257	0	1242	25	0
1	F	1380	0	1381	22	0
1	G	1200	0	1161	20	0
1	H	1377	0	1377	21	0
All	All	9966	0	9842	143	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 7.

The worst 5 of 143 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:H:142:ARG:NH1	1:H:142:ARG:O	2.16	0.77
1:A:83:ILE:HD11	1:A:101:ARG:HD3	1.70	0.72
1:D:150:LEU:HB2	1:E:179:LEU:HD11	1.70	0.72
1:H:119:ARG:HA	1:H:136:VAL:HB	1.71	0.72
1:F:12:ARG:NH1	1:G:107:GLU:OE2	2.24	0.70

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	134/210 (64%)	126 (94%)	7 (5%)	1 (1%)	22 57
1	B	129/210 (61%)	118 (92%)	10 (8%)	1 (1%)	19 54
1	C	135/210 (64%)	127 (94%)	5 (4%)	3 (2%)	6 29
1	D	163/210 (78%)	156 (96%)	7 (4%)	0	100 100
1	E	151/210 (72%)	143 (95%)	6 (4%)	2 (1%)	12 42
1	F	161/210 (77%)	151 (94%)	9 (6%)	1 (1%)	25 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	145/210 (69%)	135 (93%)	7 (5%)	3 (2%)	7 30
1	H	162/210 (77%)	154 (95%)	7 (4%)	1 (1%)	25 59
All	All	1180/1680 (70%)	1110 (94%)	58 (5%)	12 (1%)	15 49

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	167	ALA
1	C	126	GLU
1	H	195	ASP
1	E	126	GLU
1	G	126	GLU

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	124/182 (68%)	115 (93%)	9 (7%)	14 43
1	B	99/182 (54%)	96 (97%)	3 (3%)	41 71
1	C	111/182 (61%)	106 (96%)	5 (4%)	27 60
1	D	149/182 (82%)	143 (96%)	6 (4%)	31 65
1	E	126/182 (69%)	121 (96%)	5 (4%)	31 65
1	F	145/182 (80%)	141 (97%)	4 (3%)	43 73
1	G	118/182 (65%)	114 (97%)	4 (3%)	37 69
1	H	143/182 (79%)	139 (97%)	4 (3%)	43 73
All	All	1015/1456 (70%)	975 (96%)	40 (4%)	32 65

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	60	LEU
1	H	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	60	LEU
1	F	101	ARG
1	H	101	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	142/210 (67%)	-0.04	0 100 100	70, 101, 133, 155	0
1	B	139/210 (66%)	-0.15	2 (1%) 75 56	74, 120, 150, 176	0
1	C	141/210 (67%)	-0.17	2 (1%) 75 56	68, 99, 135, 157	0
1	D	171/210 (81%)	-0.20	0 100 100	61, 88, 129, 160	0
1	E	159/210 (75%)	-0.15	0 100 100	63, 93, 133, 167	0
1	F	169/210 (80%)	-0.17	1 (0%) 89 78	62, 87, 128, 166	0
1	G	153/210 (72%)	-0.18	1 (0%) 87 75	65, 94, 130, 142	0
1	H	170/210 (80%)	-0.21	0 100 100	61, 88, 127, 184	0
All	All	1244/1680 (74%)	-0.16	6 (0%) 91 81	61, 95, 138, 184	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	GLU	3.1
1	G	193	GLU	2.9
1	C	194	TRP	2.7
1	F	166	GLU	2.3
1	B	127	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.