wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 06:28 PM EST

PDB ID	:	3RFU
Title	:	Crystal structure of a copper-transporting PIB-type ATPase
Authors	:	Gourdon, P.; Liu, X.; Skjorringe, T.; Morth, J.P.; Birk Moller, L.; Panyella Pedersen, B.; Nissen, P.
Deposited on	:	2011-04-07
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
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:

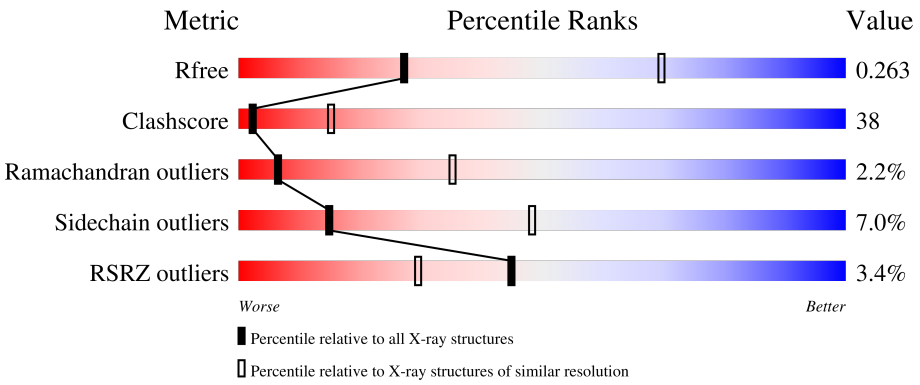
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	736	3% 38% 47% 5% 10%
1	B	736	3% 38% 47% 5% 10%
1	C	736	3% 38% 47% 5% 10%
1	D	736	3% 39% 46% 5% 10%

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
2	ALF	A	995	-	-	X	-
4	K	A	997	-	-	-	X

2 Entry composition (i)

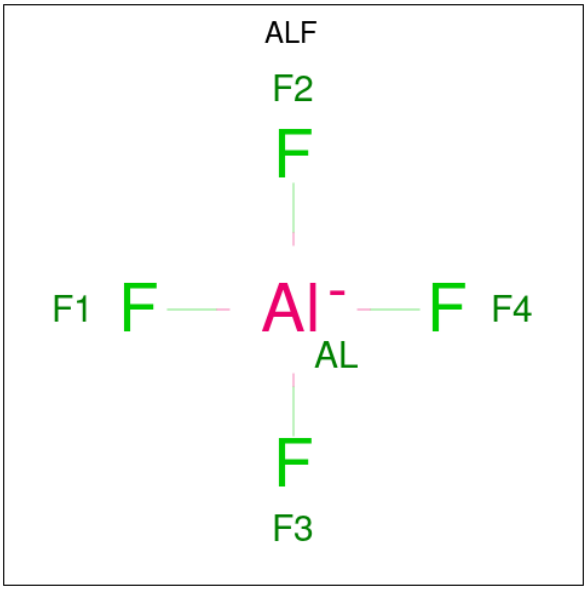
There are 4 unique types of molecules in this entry. The entry contains 19764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper efflux ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	663	4934	3156	844	909	25	0	0	0
1	B	663	4934	3156	844	909	25	0	0	0
1	C	663	4934	3156	844	909	25	0	0	0
1	D	663	4934	3156	844	909	25	0	0	0

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
2	A	1	5	1	4	0	0
2	B	1	5	1	4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Al F 5 1 4	0	0
2	D	1	Total Al F 5 1 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

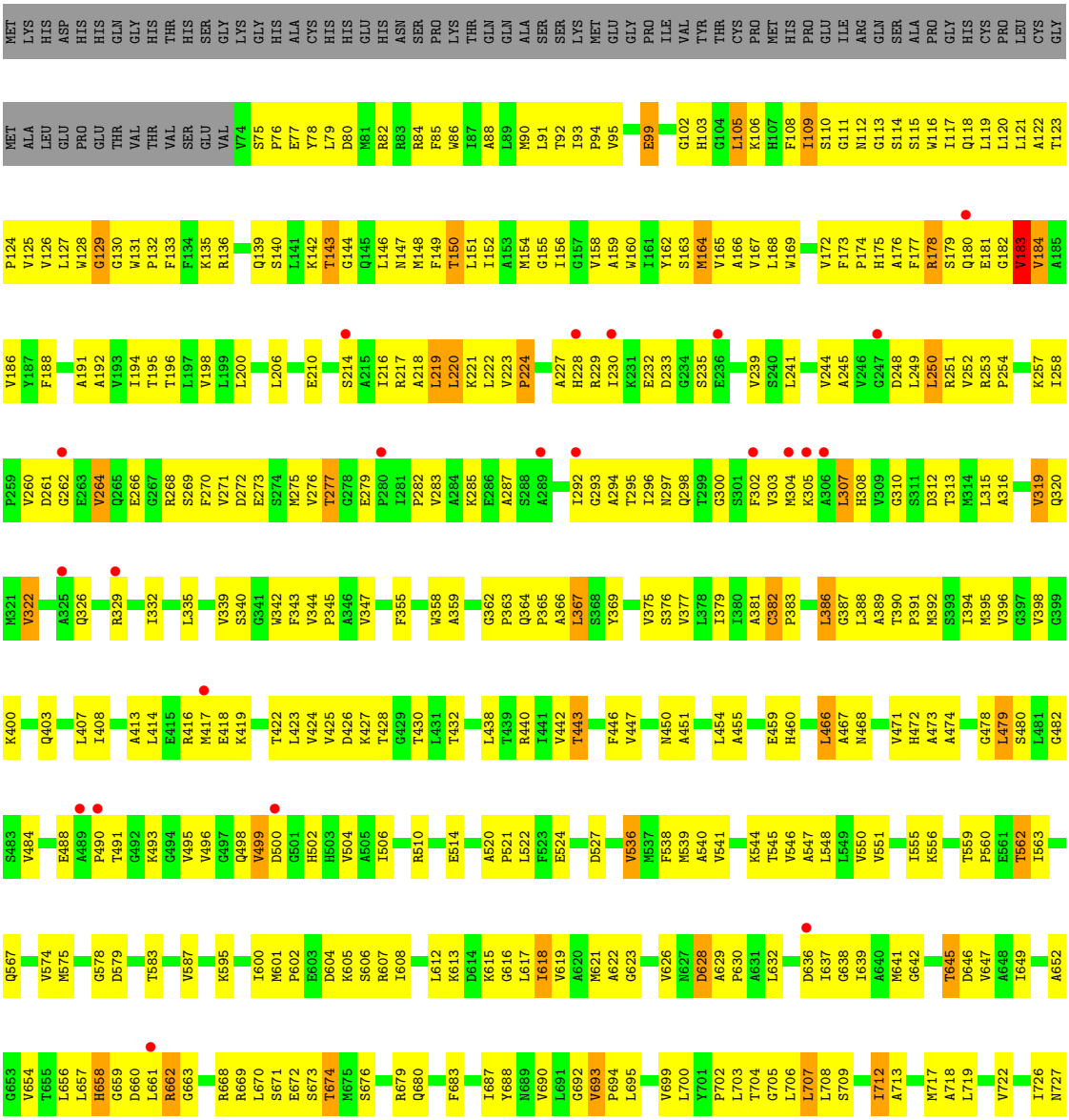
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

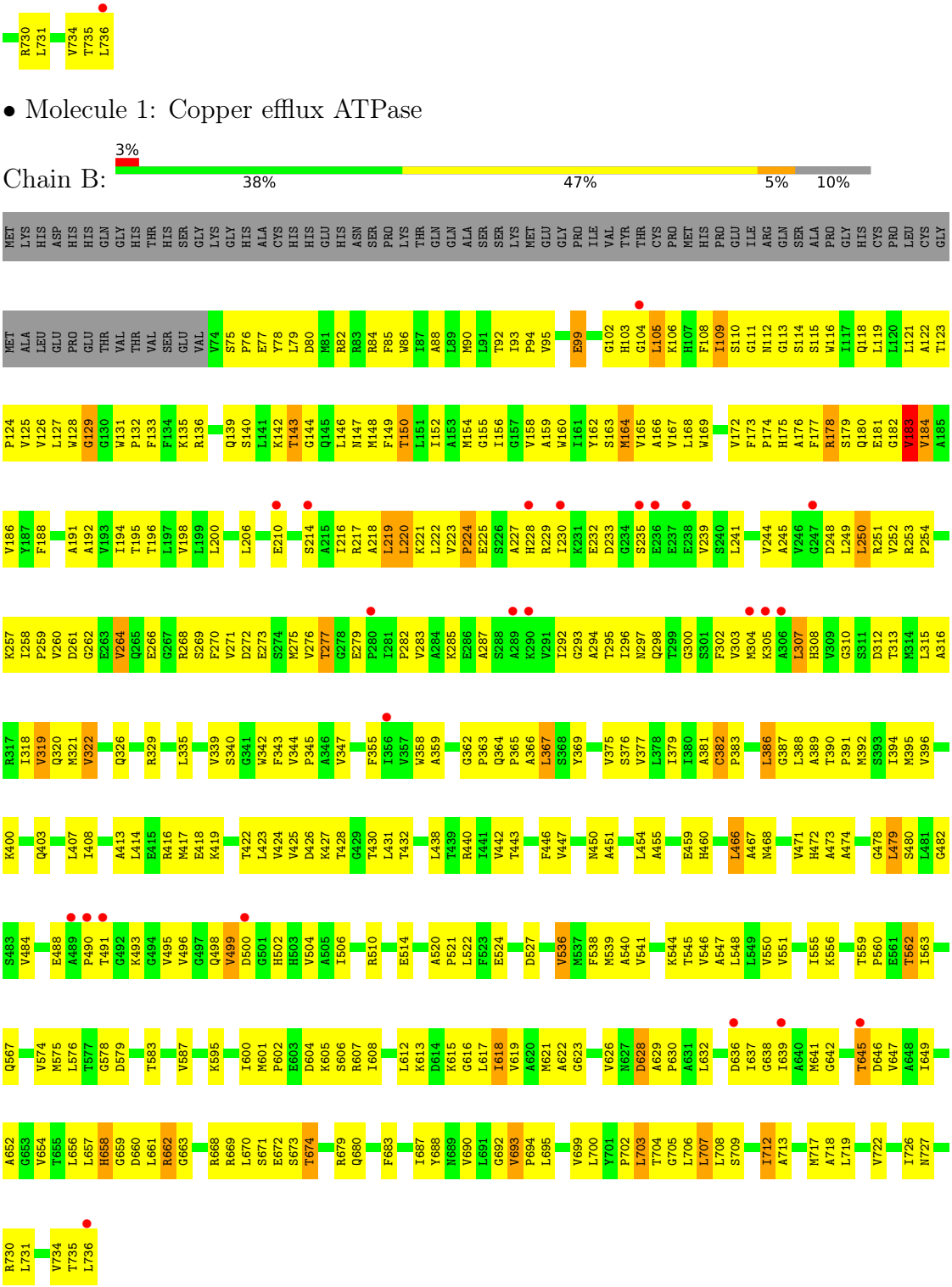
3 Residue-property plots (i)

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: Copper efflux ATPase

Chain A:



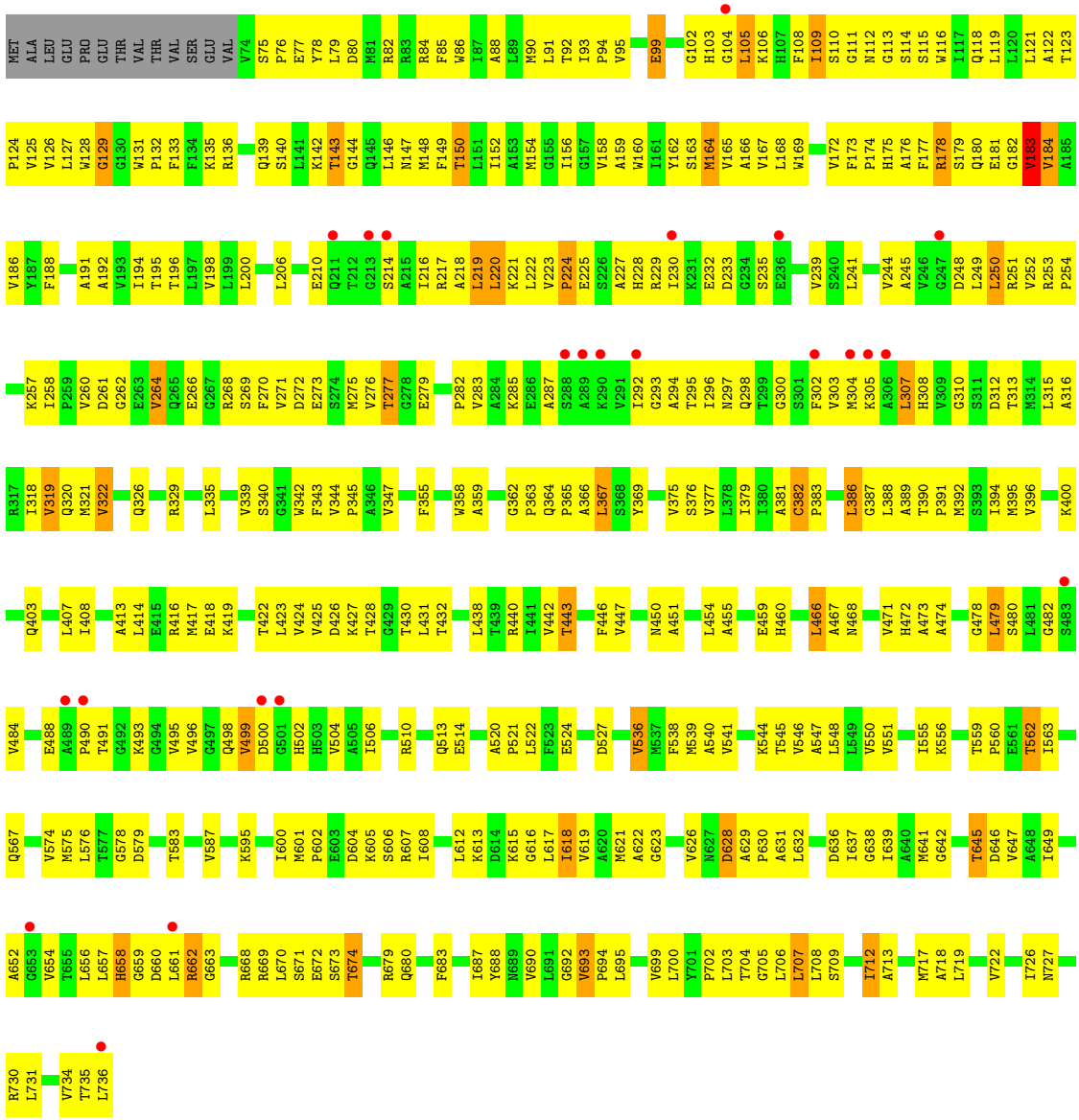


• Molecule 1: Copper efflux ATPase

Chain B: 3% 38% 47% 5% 10%

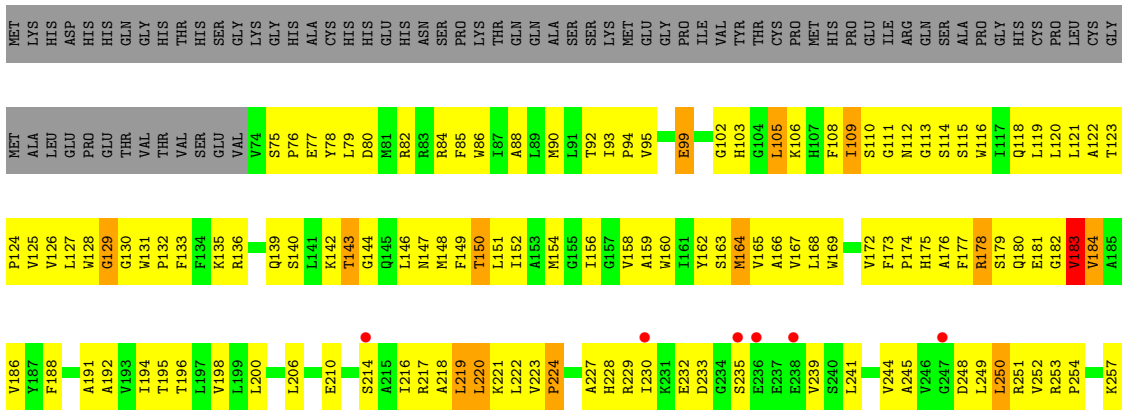
• Molecule 1: Copper efflux ATPase

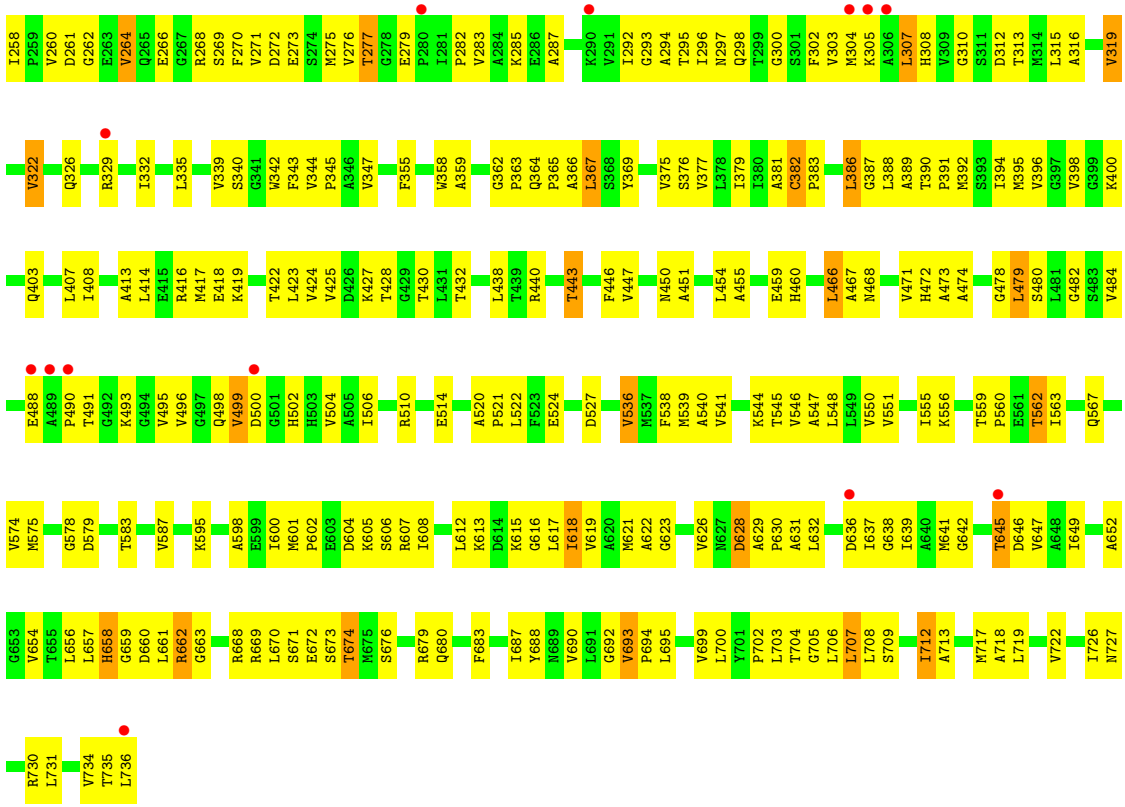
Chain C: 3% 38% 47% 5% 10%



- Molecule 1: Copper efflux ATPase

Chain D:




I258 P259 V260 D261 G262 E263 V264 Q265 E266 G267 R268 S269 F270 V271 D272 E273 S274 M275 V276 T277 G278 E279 P280 I281 P282 V283 A284 K285 E286 A287 K290 V291 I292 G293 A294 T295 I296 N297 Q298 T299 G300 S301 F302 V303 M304 K305 A306 L307 H308 V309 G310 S311 D312 T313 M314 L315 A316 V319
V322 Q326 R329 I332 L335 V339 S340 G341 W342 F343 V344 P345 A346 V347 F355 W358 A359 G362 P363 Q364 P365 A366 L367 S368 Y369 V375 S376 V377 L378 I379 I380 A381 C382 P383 L386 G387 L388 A389 T390 P391 M392 S393 I394 M395 V396 G397 V398 G399 K400
Q403 L407 I408 A413 L414 E415 R416 M417 E418 K419 T422 L423 V424 V425 D426 K427 T428 G429 T430 L431 T432 L438 T439 R440 T443 F446 V447 N450 A451 L454 A455 E459 H460 L466 A467 N468 V471 H472 A473 A474 G478 L479 S480 L481 G482 S483 V484
E488 A489 P490 T491 G492 K493 G494 V495 V496 G497 Q498 V499 D500 G501 H502 H503 V504 A505 I506 R510 E514 A520 P521 L522 F523 E524 D527 V536 M537 F538 M539 A540 V541 K544 T545 V546 A547 L548 L549 V550 V551 I555 K556 T559 P560 E561 T562 I563 Q567
V574 M575 G578 D579 T583 V587 K595 A598 E599 I600 M601 P602 E603 D604 K605 S606 R607 I608 L612 K613 D614 K615 G616 L617 I618 V619 A620 M621 A622 G623 V626 N627 D628 A629 P630 A631 L632 D636 I637 G638 I639 A640 M641 G642 T645 D646 V647 A648 I649 A652
G653 V654 T655 L656 L657 H658 G659 D660 L661 R662 G663 R668 R669 L670 S671 E672 S673 T674 M675 S676 R679 Q680 F683 I687 Y688 N689 V690 L691 G692 V693 P694 L695 V699 L700 Y701 P702 L703 T704 G705 L706 L707 L708 S709 I712 A713 M717 A718 L719 V722 I726 N727
R730 L731 V734 T735 L736

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.15Å 72.98Å 329.95Å 89.96° 90.04° 90.22°	Depositor
Resolution (Å)	20.00 – 3.20 71.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.20) 95.5 (71.27-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.261 0.243 , 0.263	Depositor DCC
R_{free} test set	1945 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 83.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l 0.428 for -h,k,-l 0.438 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19764	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: MG, ALF, K

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	0/5017	0.53	0/6812
1	B	0.25	0/5017	0.53	0/6812
1	C	0.25	0/5017	0.53	0/6812
1	D	0.25	0/5017	0.53	0/6812
All	All	0.25	0/20068	0.53	0/27248

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	4934	0	5125	387	0
1	B	4934	0	5125	393	0
1	C	4934	0	5125	394	0
1	D	4934	0	5125	385	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	19764	0	20500	1547	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 38.

The worst 5 of 1547 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:B:123:THR:HG23	1:B:124:PRO:HD3	1.31	1.12
1:C:123:THR:HG23	1:C:124:PRO:HD3	1.31	1.12
1:A:123:THR:HG23	1:A:124:PRO:HD3	1.31	1.12
1:D:123:THR:HG23	1:D:124:PRO:HD3	1.31	1.12
1:A:662:ARG:HB2	1:A:663:GLY:HA3	1.34	1.09

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	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	7 37
1	B	661/736 (90%)	578 (87%)	68 (10%)	15 (2%)	6 34
1	C	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	7 37
1	D	661/736 (90%)	579 (88%)	68 (10%)	14 (2%)	7 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2644/2944 (90%)	2313 (88%)	274 (10%)	57 (2%)	6 35

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO
1	A	662	ARG
1	B	224	PRO
1	C	224	PRO
1	C	662	ARG

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	523/586 (89%)	486 (93%)	37 (7%)	14 47
1	B	523/586 (89%)	486 (93%)	37 (7%)	14 47
1	C	523/586 (89%)	486 (93%)	37 (7%)	14 47
1	D	523/586 (89%)	487 (93%)	36 (7%)	15 49
All	All	2092/2344 (89%)	1945 (93%)	147 (7%)	15 48

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	164	MET
1	D	693	VAL
1	D	183	VAL
1	D	367	LEU
1	B	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	727	ASN
1	C	308	HIS
1	D	727	ASN
1	D	308	HIS
1	D	498	GLN

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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
2	ALF	A	995	-	0,4,4	-	-	-		
2	ALF	D	995	-	0,4,4	-	-	-		
2	ALF	C	995	-	0,4,4	-	-	-		
2	ALF	B	995	-	0,4,4	-	-	-		

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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	995	ALF	2	0
2	D	995	ALF	1	0
2	C	995	ALF	1	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	663/736 (90%)	0.02	23 (3%)	44	28	56, 106, 243, 371	0
1	B	663/736 (90%)	0.01	24 (3%)	42	27	55, 106, 244, 373	0
1	C	663/736 (90%)	0.03	23 (3%)	44	28	55, 106, 244, 371	0
1	D	663/736 (90%)	-0.05	19 (2%)	51	36	56, 106, 244, 369	0
All	All	2652/2944 (90%)	0.00	89 (3%)	45	29	55, 106, 244, 373	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	500	ASP	9.9
1	A	500	ASP	8.8
1	B	490	PRO	7.8
1	B	214	SER	7.5
1	D	489	ALA	7.5

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
4	K	A	997	1/1	0.59	0.40	141,141,141,141	0
4	K	C	997	1/1	0.72	0.38	144,144,144,144	0
4	K	D	997	1/1	0.84	0.27	160,160,160,160	0
4	K	B	997	1/1	0.90	0.34	154,154,154,154	0
2	ALF	D	995	5/5	0.95	0.21	57,62,80,127	0
2	ALF	B	995	5/5	0.96	0.20	48,60,80,130	0
3	MG	B	996	1/1	0.97	0.19	67,67,67,67	0
2	ALF	A	995	5/5	0.98	0.21	37,50,60,136	0
3	MG	A	996	1/1	0.98	0.17	68,68,68,68	0
2	ALF	C	995	5/5	0.98	0.19	45,57,62,117	0
3	MG	D	996	1/1	0.98	0.21	77,77,77,77	0
3	MG	C	996	1/1	0.99	0.22	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.