WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 07:12 pm GMT

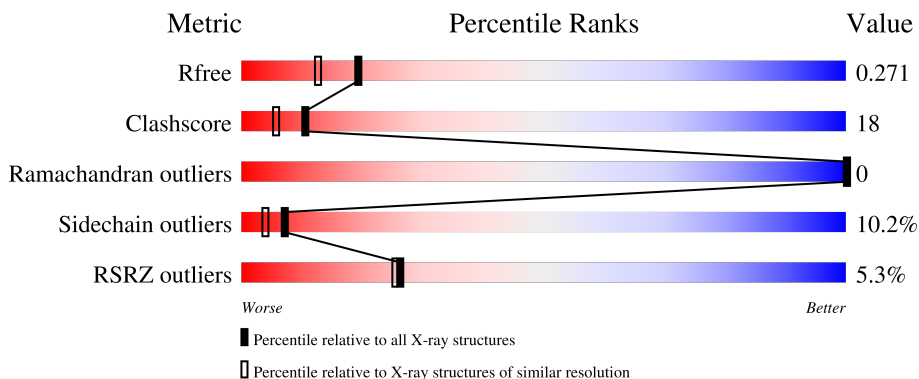|		
PDB ID	:	2X36
Title	:	Structure of the proteolytic domain of the Human Mitochondrial Lon protease
Authors	:	Garcia, J.; Ondrovicova, G.; Blagova, E.; Levdikov, V.M.; Bauer, J.A.; Kutejova, E.; Wilkinson, A.J.; Wilson, K.S.
Deposited on	:	2010-01-21
Resolution	:	2.00 Å(reported)

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 2.00 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.
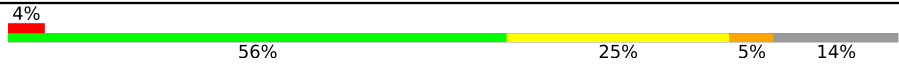
Metric	Percentile Ranks	Value
Rfree		0.271
Clashscore		18
Ramachandran outliers		0
Sidechain outliers		10.2%
RSRZ outliers		5.3%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	207	4% · 58% · 28% · 5% · 8%
1	B	207	6% · 56% · 25% · 6% · 13%
1	C	207	4% · 64% · 27% · · 7%
1	D	207	4% · 52% · 30% · · 14%
1	E	207	5% · 61% · 23% · · 13%

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	F	207	4% 56% 25% 5% 14%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8705 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 LON PROTEASE HOMOLOG, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total 1440	C 918	N 243	O 270	S 9	0	0	0
1	B	180	Total 1365	C 876	N 229	O 251	S 9	21	1	0
1	C	192	Total 1475	C 939	N 253	O 274	S 9	0	2	0
1	D	178	Total 1358	C 868	N 231	O 251	S 8	0	2	0
1	E	181	Total 1374	C 878	N 235	O 253	S 8	0	1	0
1	F	179	Total 1363	C 873	N 233	O 249	S 8	2	2	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total 74	O 74	0	0
2	B	42	Total 42	O 42	0	0
2	C	63	Total 65	O 65	1	2
2	D	42	Total 42	O 42	0	0
2	E	59	Total 59	O 59	0	0
2	F	48	Total 48	O 48	0	0

3 Residue-property plots ⓘ

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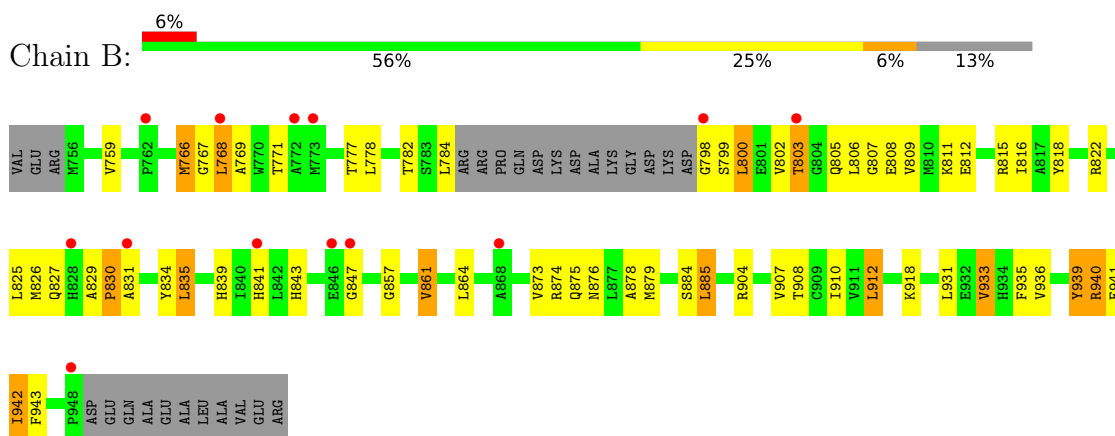 for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
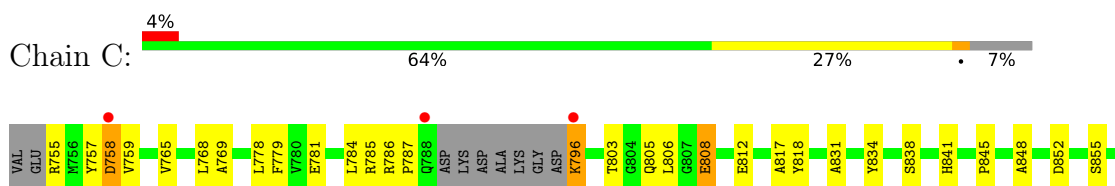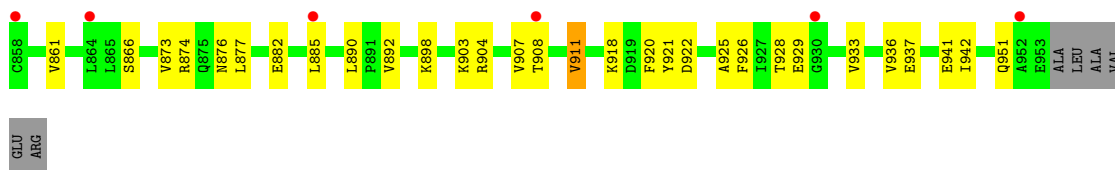
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain A:

• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain B:

• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain C:

C858 V861 L864 L865 S866 V873 R874 Q875 N876 L877 E882 L885 L890 P891 V892 K898 K903 R904 V907 T908 V911 K918 D919 F920 Y921 D922 A925 F926 I927 T928 E929 G930 V933 V936 E937 E941 I942 Q951 A952 E953 ALA LEU ALA VAL

GLU ARG

• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain D:

4%
52%   30%   •   14%

VAL GLU ARG MET TYR ASP VAL T760 G763 V764 V765 M766 G767 L768 T777 L778 E781 T782 S783 L784 R785 ARG PRO GLN LYS ASP ALA LYS GLY ASP LYS D797 L800 E801 V802 T803 G804 Q805 L806 M810 K811 E812 S813 A814 R815 I816 T819 F820 A823 F824 L825 M826

Q827 A831 Y834 L835 V836 T837 S838 H841 L842 K851 T859 T862 A863 L864 L865 A868 M869 G870 R871 P872 V873 R874 Q875 N876 L877 A878 M879 T880 G881 E882 V883 S884 L885 K888 I889 K896 K903 V907 T908 C909 I910 V911 L912 P913 N916 F920

L923 V933 H938 Y939 R940 E941 I942 F947 P948 ASP GLU GLN ALA GLU ALA LEU ALA VAL GLU ARG

• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain E:

5%
61%   23%   •   13%

VAL GLU ARG MET TYR D758 V759 T760 P761 P762 G763 V764 V765 M766 G767 L768 A772 M773 T777 L778 E781 L784 R785 R786 PRO GLN LYS ASP ALA LYS GLY ASP LYS D797 Q805 L806 M810 K811 E812 I816 A817 Y818 R822 A823 F824 L825 M826 Q827 H828 L835

V836 T837 S838 E846 A856 G857 C858 V861 L867 A868 R871 P872 V873 R874 Q875 N876 V883 L890 G894 K898 A902 V907 T908 C909 I910 V911 F920 L923 T928 L931 E932 V933 H934 F935 V936 R940 E941 I942 I945 P948 ASP GLU
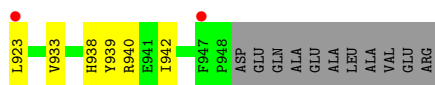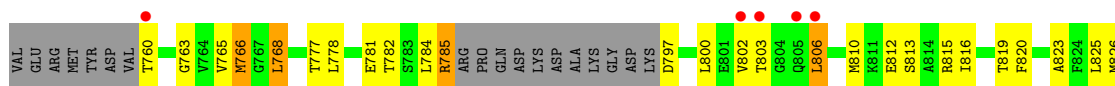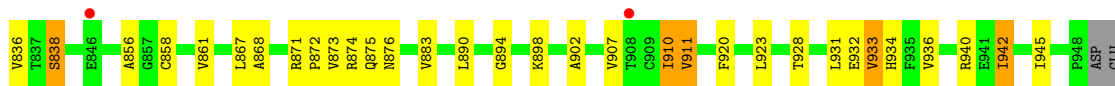
GLN ALA GLU ALA LEU ALA VAL GLU ARG

• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain F:

4%
56%   25%   5%   14%

VAL GLU ARG MET TYR ASP V759 T760 V764 V765 M766 G767 L768 A769 W770 T771 A772 M773 T777 E781 T782 S783 L784 R785 ARG PRO GLN LYS ASP ALA LYS GLY ASP LYS D797 G798 S799 T803 G804 Q805 L806 V809 M810 L825 M826 Q827 P830 Y834 L835 V836 T837

S838 H839 T840 H841 L842 H843 V844 G847 A848 T849 P854 S855 A856 G857 C858 T859 I860 V861 L865 A868 R871 P872 R874 Q875 N876 L877 A878 E882 L890 P891 V892 I895 K896 E897 K898 A902 K903 R904 V907 T908 C909 I910 N916 D919 L923

E929 V933 H938 Y939 R940 F943 P948 ASP GLU GLN ALA GLU ALA LEU ALA VAL GLU ARG

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.80Å 83.75Å 105.49Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	34.00 – 2.00 34.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.00-2.00) 96.8 (34.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.232 0.239 , 0.271	Depositor DCC
R_{free} test set	4328 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.6	EDS
L-test for twinning[2]	$<|L|> = 0.55, <L^2> = 0.39$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
Reported twinning fraction	0.321 for H, K, L 0.679 for -h,-k,l	Depositor
Outliers	0 of 80072 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8705	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	1.40	6/1470 (0.4%)	1.07	4/1995 (0.2%)
1	B	1.17	4/1394 (0.3%)	1.01	2/1892 (0.1%)
1	C	1.47	11/1506 (0.7%)	1.08	1/2041 (0.0%)
1	D	1.10	2/1386 (0.1%)	1.01	6/1880 (0.3%)
1	E	1.28	6/1403 (0.4%)	1.05	2/1904 (0.1%)
1	F	1.15	1/1395 (0.1%)	0.96	2/1893 (0.1%)
All	All	1.27	30/8554 (0.4%)	1.03	17/11605 (0.1%)

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 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	937	GLU	CD-OE1	5.90	1.32	1.25
1	D	820	PHE	CD1-CE1	5.79	1.50	1.39
1	C	834	TYR	CD2-CE2	-5.74	1.30	1.39
1	C	817	ALA	CA-CB	-5.74	1.40	1.52
1	A	873	VAL	CB-CG1	-5.68	1.41	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	786	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	D	871	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	E	835	LEU	CB-CG-CD1	5.90	121.03	111.00
1	C	904	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	904	ARG	NE-CZ-NH1	5.76	123.18	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	THR	Peptide

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	1440	0	1441	51	0
1	B	1365	0	1379	63	0
1	C	1475	0	1475	38	0
1	D	1358	0	1370	78	0
1	E	1374	0	1385	44	0
1	F	1363	0	1381	52	0
2	A	74	0	0	3	0
2	B	42	0	0	2	0
2	C	65	0	0	3	0
2	D	42	0	0	1	0
2	E	59	0	0	4	0
2	F	48	0	0	5	0
All	All	8705	0	8431	310	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 18.

The worst 5 of 310 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:766:MET:CE	1:D:878:ALA:HB2	1.73	1.18
1:D:825:LEU:HD23	1:D:835:LEU:HD13	1.24	1.17
1:D:766:MET:HE3	1:D:878:ALA:HB2	1.29	1.13
1:B:784:LEU:HD11	1:B:834:TYR:OH	1.55	1.07
1:F:877:LEU:HD12	1:F:878:ALA:N	1.70	1.06

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	186/207 (90%)	181 (97%)	5 (3%)	0	100	100
1	B	177/207 (86%)	174 (98%)	3 (2%)	0	100	100
1	C	190/207 (92%)	185 (97%)	5 (3%)	0	100	100
1	D	176/207 (85%)	169 (96%)	7 (4%)	0	100	100
1	E	178/207 (86%)	172 (97%)	6 (3%)	0	100	100
1	F	177/207 (86%)	170 (96%)	7 (4%)	0	100	100
All	All	1084/1242 (87%)	1051 (97%)	33 (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	152/165 (92%)	134 (88%)	18 (12%)	5	3
1	B	144/165 (87%)	128 (89%)	16 (11%)	6	3
1	C	155/165 (94%)	142 (92%)	13 (8%)	11	7
1	D	143/165 (87%)	130 (91%)	13 (9%)	9	5
1	E	145/165 (88%)	133 (92%)	12 (8%)	11	7
1	F	144/165 (87%)	126 (88%)	18 (12%)	4	2
All	All	883/990 (89%)	793 (90%)	90 (10%)	7	4

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	884	SER
1	E	933	VAL
1	D	888	LYS
1	E	867	LEU
1	F	803	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	827	GLN
1	F	805	GLN
1	F	938	HIS
1	F	827	GLN
1	E	875	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 monosaccharides 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 (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	190/207 (91%)	0.44	8 (4%)	36	35	25, 44, 66, 75	0
1	B	177/207 (85%)	0.63	13 (7%)	15	14	34, 53, 74, 86	0
1	C	192/207 (92%)	0.46	9 (4%)	31	30	26, 43, 62, 77	0
1	D	178/207 (85%)	0.49	9 (5%)	28	27	33, 52, 68, 93	0
1	E	181/207 (87%)	0.45	10 (5%)	25	24	27, 47, 70, 84	0
1	F	179/207 (86%)	0.59	9 (5%)	28	28	33, 55, 71, 87	1 (0%)
All	All	1097/1242 (88%)	0.51	58 (5%)	26	25	25, 49, 70, 93	1 (0%)

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	805	GLN	6.0
1	F	805	GLN	4.9
1	E	772	ALA	4.9
1	B	772	ALA	4.6
1	E	797	ASP	4.5

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)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.