



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:58 am BST

PDB ID : 2CBY
Title : Crystal structure of the ATP-dependent Clp Protease proteolytic subunit 1 (ClpP1) from Mycobacterium tuberculosis
Authors : Mate, M.J.; Portnoi, D.; Alzari, P.M.; Ortiz-Lombardia, M.
Deposited on : 2006-01-10
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
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

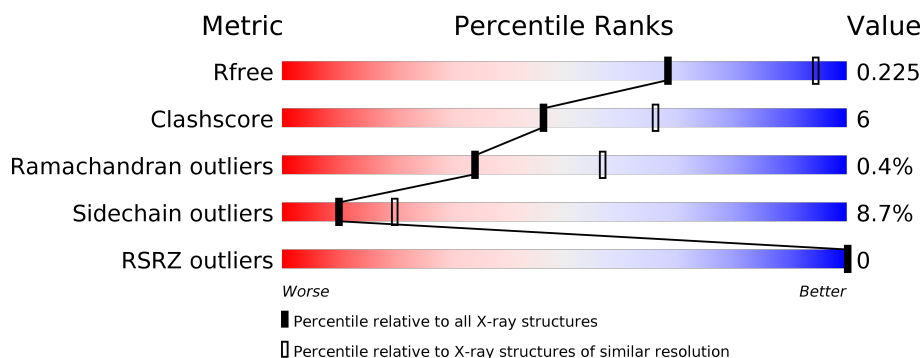
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	208	<div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
1	B	208	<div> <div>68%</div> <div>11%</div> <div>•</div> <div>18%</div> </div>
1	C	208	<div> <div>67%</div> <div>13%</div> <div>•</div> <div>19%</div> </div>
1	D	208	<div> <div>64%</div> <div>15%</div> <div>•</div> <div>18%</div> </div>
1	E	208	<div> <div>68%</div> <div>12%</div> <div>•</div> <div>19%</div> </div>
1	F	208	<div> <div>73%</div> <div>9%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	208	 A horizontal bar chart showing the quality of chain G. The bar is divided into three segments: a green segment representing 64%, a yellow segment representing 13%, and a grey segment representing 20%. A small black dot is located on the yellow segment.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9450 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 ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUB-UNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1304	827	220	248	9			
1	B	170	Total	C	N	O	S	0	0	0
			1314	833	223	249	9			
1	C	169	Total	C	N	O	S	0	0	0
			1304	827	220	248	9			
1	D	171	Total	C	N	O	S	0	0	0
			1321	838	224	250	9			
1	E	169	Total	C	N	O	S	0	0	0
			1304	827	220	248	9			
1	F	170	Total	C	N	O	S	0	0	0
			1314	833	223	249	9			
1	G	167	Total	C	N	O	S	0	0	0
			1288	818	215	246	9			

- Molecule 2 is water.

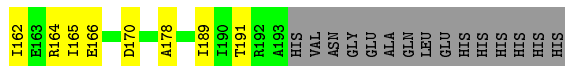
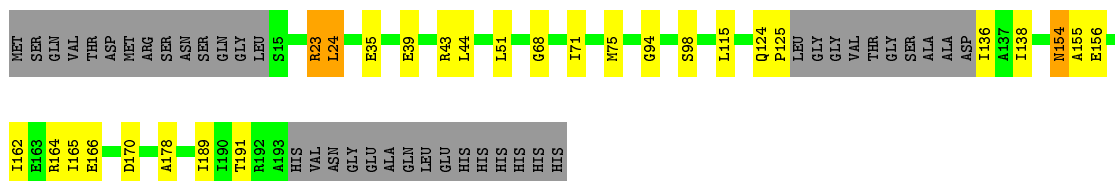
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	48	Total	O	0	0
			48	48		
2	C	55	Total	O	0	0
			55	55		
2	D	54	Total	O	0	0
			54	54		
2	E	46	Total	O	0	0
			46	46		
2	F	40	Total	O	0	0
			40	40		
2	G	23	Total	O	0	0
			23	23		

- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1

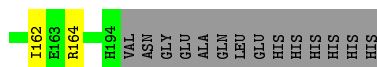
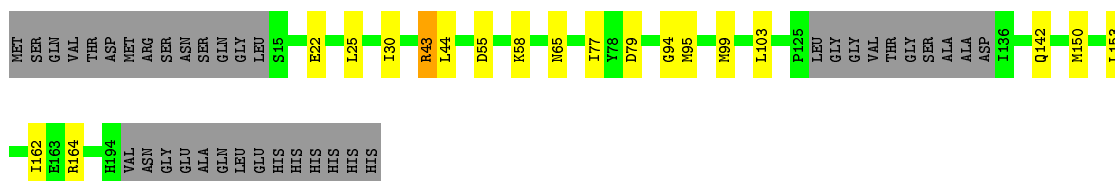




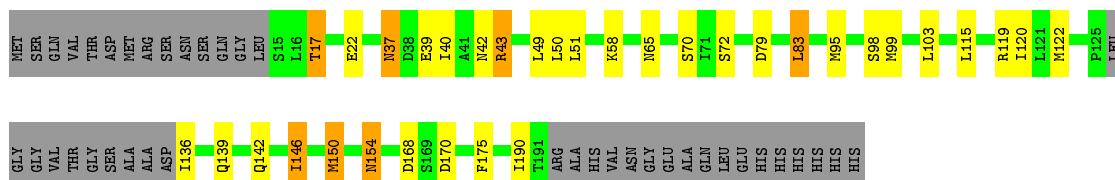
• Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



• Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



• Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	178.25Å 178.25Å 264.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	154.30 – 2.60 76.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.30-2.60) 100.0 (76.65-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.229 0.188 , 0.225	Depositor DCC
R_{free} test set	3895 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9450	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0.68	0/1325	0.70	0/1789
1	B	0.68	1/1336 (0.1%)	0.77	0/1804
1	C	0.71	0/1325	0.78	0/1789
1	D	0.74	0/1343	0.79	3/1814 (0.2%)
1	E	0.70	0/1325	0.74	1/1789 (0.1%)
1	F	0.67	0/1336	0.70	0/1804
1	G	0.62	0/1309	0.72	0/1768
All	All	0.69	1/9299 (0.0%)	0.75	4/12557 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	GLU	CG-CD	5.41	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	D	28	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	23	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	188	HIS	CB-CA-C	-5.33	99.73	110.40

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	1304	0	1298	12	0
1	B	1314	0	1305	22	0
1	C	1304	0	1298	16	0
1	D	1321	0	1314	27	0
1	E	1304	0	1298	14	0
1	F	1314	0	1305	15	0
1	G	1288	0	1280	24	0
2	A	35	0	0	0	0
2	B	48	0	0	1	0
2	C	55	0	0	1	0
2	D	54	0	0	1	0
2	E	46	0	0	0	0
2	F	40	0	0	0	0
2	G	23	0	0	0	0
All	All	9450	0	9098	114	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 6.

The worst 5 of 114 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:C:119:ARG:HB2	1:C:119:ARG:HH11	1.17	1.05
1:B:124:GLN:HE21	1:B:170:ASP:HB3	1.18	1.04
1:D:81:MET:CE	1:D:103:LEU:HD22	1.92	1.00
1:B:95:MET:HE1	1:B:121:LEU:HD13	1.45	0.98
1:B:95:MET:CE	1:B:121:LEU:HD13	1.96	0.96

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	165/208 (79%)	161 (98%)	3 (2%)	1 (1%)	25	47
1	B	166/208 (80%)	162 (98%)	3 (2%)	1 (1%)	25	47
1	C	165/208 (79%)	158 (96%)	6 (4%)	1 (1%)	25	47
1	D	167/208 (80%)	163 (98%)	4 (2%)	0	100	100
1	E	165/208 (79%)	160 (97%)	4 (2%)	1 (1%)	25	47
1	F	166/208 (80%)	162 (98%)	3 (2%)	1 (1%)	25	47
1	G	163/208 (78%)	160 (98%)	3 (2%)	0	100	100
All	All	1157/1456 (80%)	1126 (97%)	26 (2%)	5 (0%)	34	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	94	GLY
1	F	94	GLY
1	A	94	GLY
1	B	94	GLY
1	C	94	GLY

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	134/165 (81%)	125 (93%)	9 (7%)	16	33
1	B	135/165 (82%)	125 (93%)	10 (7%)	13	28
1	C	134/165 (81%)	122 (91%)	12 (9%)	9	18
1	D	136/165 (82%)	121 (89%)	15 (11%)	6	11
1	E	134/165 (81%)	122 (91%)	12 (9%)	9	18
1	F	135/165 (82%)	130 (96%)	5 (4%)	34	60
1	G	133/165 (81%)	114 (86%)	19 (14%)	3	5
All	All	941/1155 (82%)	859 (91%)	82 (9%)	10	20

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	95	MET
1	D	195	VAL
1	G	136	ILE
1	D	109	LYS
1	D	164	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	154	ASN
1	E	160	GLN
1	G	65	ASN
1	D	142	GLN
1	G	42	ASN

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	169/208 (81%)	-0.42	0 100 100	7, 19, 31, 43	0
1	B	170/208 (81%)	-0.49	0 100 100	8, 18, 29, 36	0
1	C	169/208 (81%)	-0.44	0 100 100	8, 18, 29, 40	0
1	D	171/208 (82%)	-0.48	0 100 100	11, 18, 29, 40	0
1	E	169/208 (81%)	-0.40	0 100 100	12, 19, 30, 40	0
1	F	170/208 (81%)	-0.47	0 100 100	8, 18, 28, 39	0
1	G	167/208 (80%)	-0.33	0 100 100	7, 19, 27, 38	0
All	All	1185/1456 (81%)	-0.43	0 100 100	7, 18, 30, 43	0

There are no RSRZ outliers to report.

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.