



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:47 PM UTC

PDB ID : 9DQK / pdb_00009dqk
Title : human ClpP - Apo - A192E / E196R
Authors : Forrester, T.J.B.; Kimber, M.S.
Deposited on : 2024-09-24
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

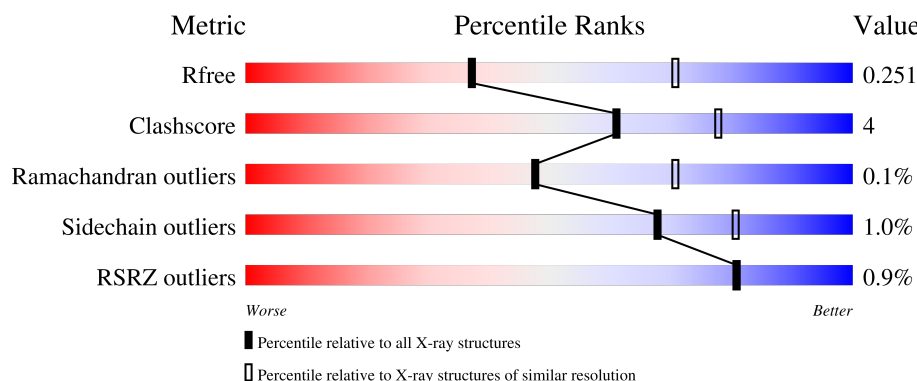
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



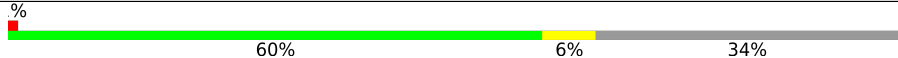
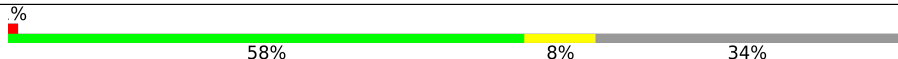
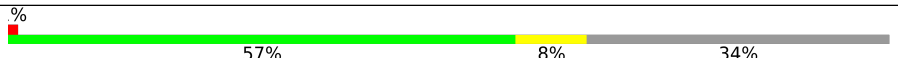
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	277	
1	B	277	
1	C	277	
1	D	277	
1	E	277	

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Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	
1	J	277	
1	K	277	
1	L	277	
1	M	277	
1	N	277	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19762 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 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1397	888	242	254	13			
1	B	185	Total	C	N	O	S	0	0	0
			1433	909	250	261	13			
1	C	180	Total	C	N	O	S	0	0	0
			1398	889	242	254	13			
1	D	180	Total	C	N	O	S	0	0	0
			1398	889	242	254	13			
1	E	180	Total	C	N	O	S	0	0	0
			1398	889	242	254	13			
1	F	181	Total	C	N	O	S	0	0	0
			1405	894	243	255	13			
1	G	182	Total	C	N	O	S	0	0	0
			1412	899	244	256	13			
1	H	183	Total	C	N	O	S	0	0	0
			1421	904	245	259	13			
1	I	184	Total	C	N	O	S	0	0	0
			1428	908	249	258	13			
1	J	182	Total	C	N	O	S	0	0	0
			1410	897	244	256	13			
1	K	178	Total	C	N	O	S	0	0	0
			1378	874	240	251	13			
1	L	183	Total	C	N	O	S	0	0	0
			1417	902	245	257	13			
1	M	178	Total	C	N	O	S	0	0	0
			1378	874	240	251	13			
1	N	182	Total	C	N	O	S	0	0	0
			1413	898	244	258	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLU	ALA	engineered mutation	UNP Q16740
A	196	ARG	GLU	engineered mutation	UNP Q16740
B	192	GLU	ALA	engineered mutation	UNP Q16740
B	196	ARG	GLU	engineered mutation	UNP Q16740
C	192	GLU	ALA	engineered mutation	UNP Q16740
C	196	ARG	GLU	engineered mutation	UNP Q16740
D	192	GLU	ALA	engineered mutation	UNP Q16740
D	196	ARG	GLU	engineered mutation	UNP Q16740
E	192	GLU	ALA	engineered mutation	UNP Q16740
E	196	ARG	GLU	engineered mutation	UNP Q16740
F	192	GLU	ALA	engineered mutation	UNP Q16740
F	196	ARG	GLU	engineered mutation	UNP Q16740
G	192	GLU	ALA	engineered mutation	UNP Q16740
G	196	ARG	GLU	engineered mutation	UNP Q16740
H	192	GLU	ALA	engineered mutation	UNP Q16740
H	196	ARG	GLU	engineered mutation	UNP Q16740
I	192	GLU	ALA	engineered mutation	UNP Q16740
I	196	ARG	GLU	engineered mutation	UNP Q16740
J	192	GLU	ALA	engineered mutation	UNP Q16740
J	196	ARG	GLU	engineered mutation	UNP Q16740
K	192	GLU	ALA	engineered mutation	UNP Q16740
K	196	ARG	GLU	engineered mutation	UNP Q16740
L	192	GLU	ALA	engineered mutation	UNP Q16740
L	196	ARG	GLU	engineered mutation	UNP Q16740
M	192	GLU	ALA	engineered mutation	UNP Q16740
M	196	ARG	GLU	engineered mutation	UNP Q16740
N	192	GLU	ALA	engineered mutation	UNP Q16740
N	196	ARG	GLU	engineered mutation	UNP Q16740

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	M	1	Total Cl 1 1	0	0
2	N	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	2	Total O 2 2	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0
3	E	4	Total O 4 4	0	0
3	F	1	Total O 1 1	0	0
3	G	7	Total O 7 7	0	0
3	H	5	Total O 5 5	0	0
3	I	9	Total O 9 9	0	0
3	J	3	Total O 3 3	0	0
3	K	4	Total O 4 4	0	0

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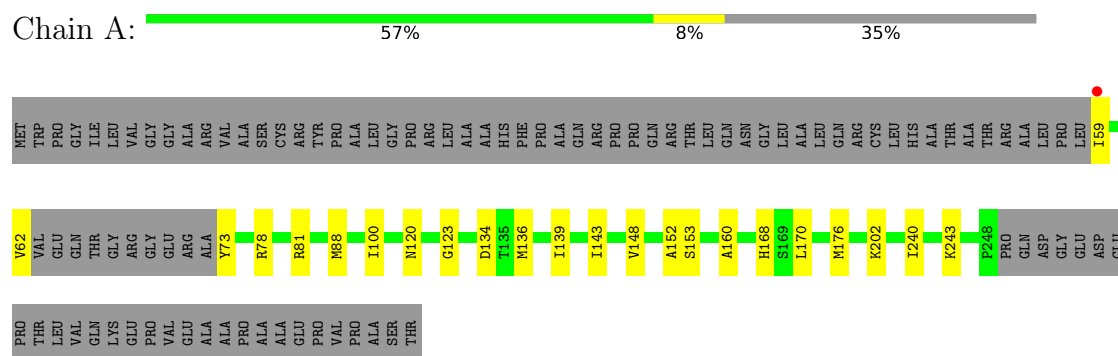
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	5	Total	O	0	0
			5	5		
3	M	3	Total	O	0	0
			3	3		
3	N	4	Total	O	0	0
			4	4		

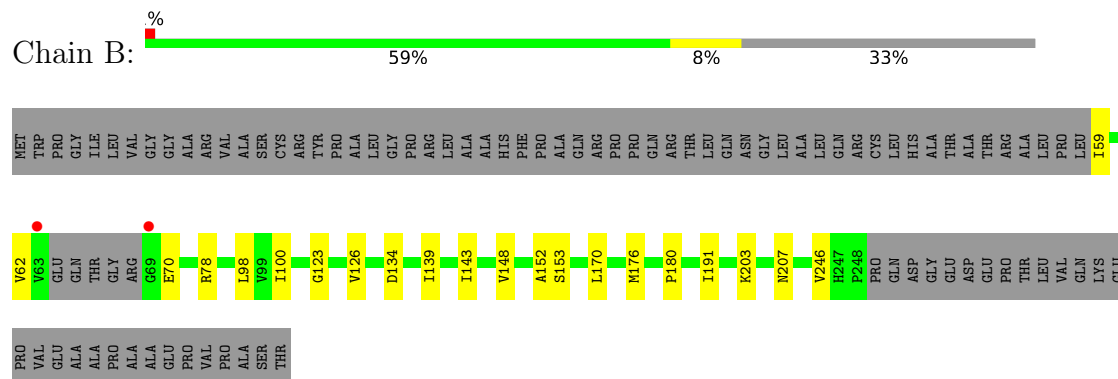
3 Residue-property plots [i](#)

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.

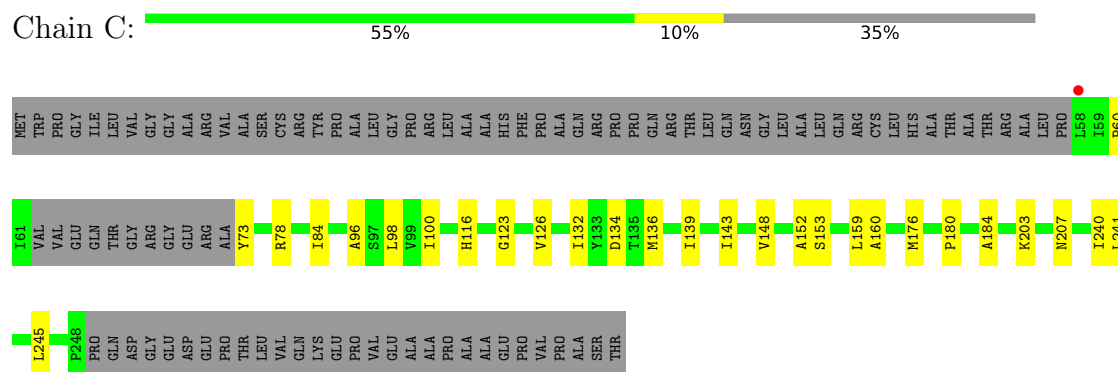
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



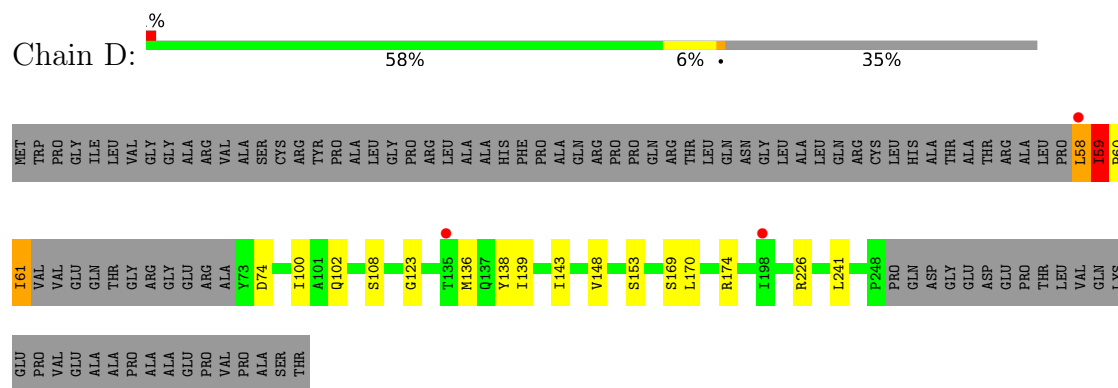
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



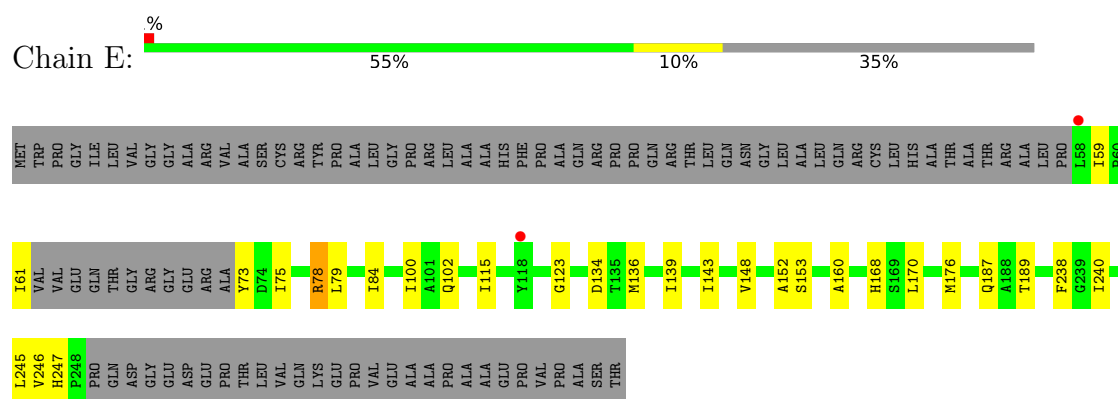
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



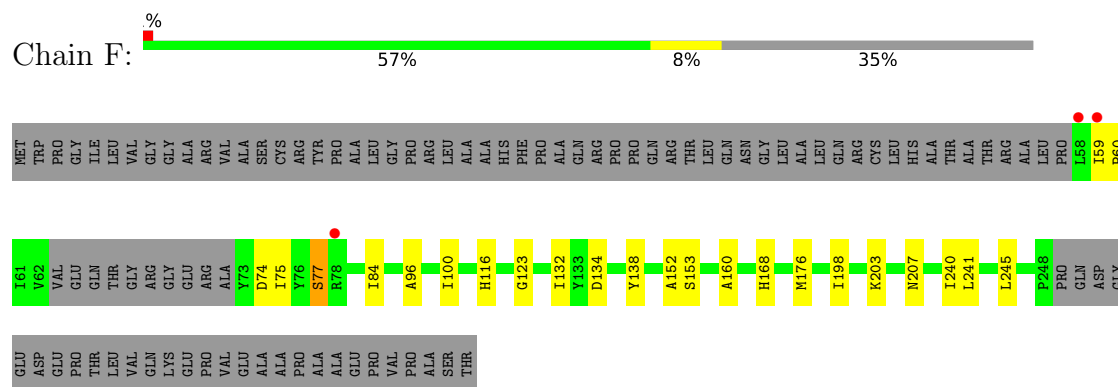
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



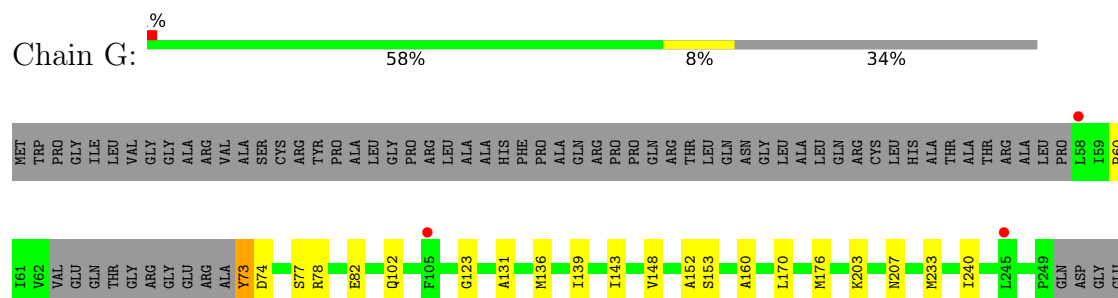
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



ASP
GLU
PRO
THR
LEU
VAL
GLN
LYS
GLU
PRO
VAL
GLU
ALA
ALA
PRO
THR
GLU
PRO
VAL
THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain H:  58% 8% 34%

MET TRP PRO GLY THR ILE LEU VAL GLN LYS GLY ARG VAL ALA SER CYS ARG TYR PRO PRO LEU LEU ALA ALA HIS PHE PRO PRO ALA ALA GLN ARG PRO GLN THR LEU LEU ASN GLY LEU LEU GLN CYS ARG HIS ALA THR PRO THR ARG ALA LEU PRO L58 I59

E64 GLN THR GLY ARG GLU VAL GLU ARG ALA Y73 D74 I75 I84 H116 G123 D134 I139 I143 V148 A152 S153 A160 L170 M176 A188 E197 K200 K203 N207 I240 V246 H247 P248 PRO GLN ASP THR PRO GLY LEU ASP PRO THR

LEU VAL GLN LYS GLU VAL GLU ALA ALA ALA GLU PRO VAL PRO ALA THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain I:  % 60% 6% 34%

MET TRP PRO GLY THR ILE LEU VAL GLN LYS GLY ARG VAL ALA SER CYS ARG TYR PRO PRO LEU LEU ALA ALA HIS PHE PRO PRO ALA ALA GLN ARG PRO GLN THR LEU LEU ASN GLY LEU LEU GLN CYS ARG HIS ALA THR PRO THR ARG ALA LEU PRO L58 V62

VAL GLU GLN THR GLY ARG GLU GLY R71 A72 Y73 S77 R81 G123 V126 D134 I139 I143 A152 S153 L170 M176 P180 K203 N207 L245 V246 P249 GLN ASP GLY GLU ASP GLU PRO THR LEU VAL VAL GLN LYS PRO PRO VAL GLU ALA

ALA PRO ALA ALA PRO VAL PRO ALA SER THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain J:  % 58% 8% 34%

MET TRP PRO GLY THR ILE LEU VAL GLN LYS GLY ARG VAL ALA SER CYS ARG TYR PRO PRO LEU LEU ALA ALA HIS PHE PRO PRO ALA ALA GLN ARG PRO GLN THR LEU LEU ASN GLY LEU LEU GLN CYS ARG HIS ALA THR PRO THR ARG ALA LEU PRO L58 V62

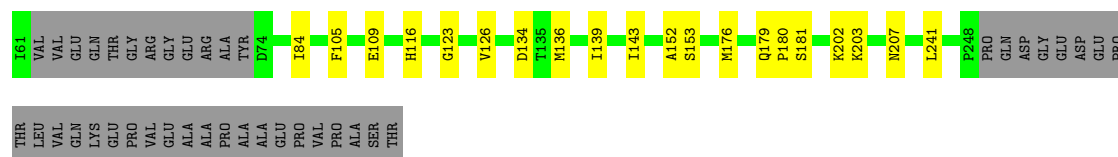
VAL GLU GLN THR GLY ARG GLU GLY A72 Y73 M111 Y113 G123 V126 D134 I139 L140 I143 A152 S153 A160 L170 R174 I175 M176 P180 I191 K203 N207 I240 V246 H247 P248 PRO GLN ASP THR PRO GLY LEU ASP PRO THR

LEU VAL GLN LYS GLU PRO VAL GLU ALA ALA ALA GLU PRO VAL PRO ALA THR

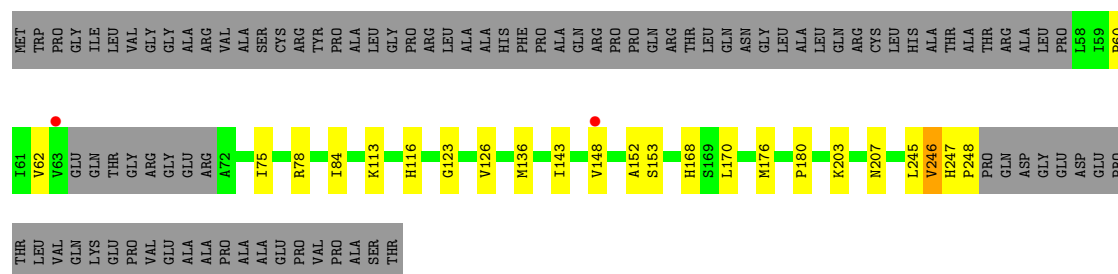
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain K:  57% 7% 36%

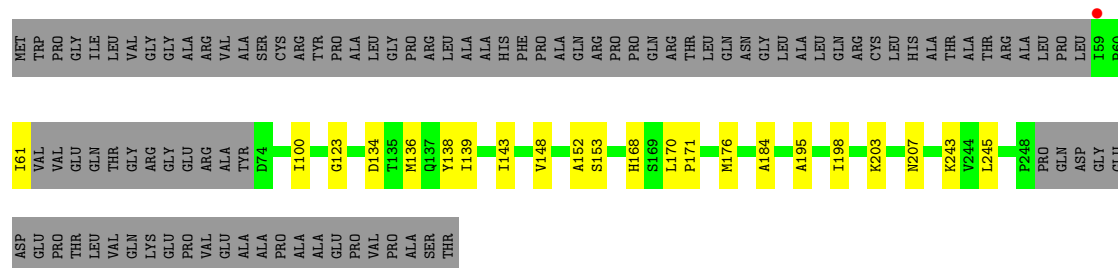
MET TRP PRO GLY THR ILE LEU VAL GLN LYS GLY ARG VAL ALA SER CYS ARG TYR PRO PRO LEU LEU ALA ALA HIS PHE PRO PRO ALA ALA GLN ARG PRO GLN THR LEU LEU ASN GLY LEU LEU GLN CYS ARG HIS ALA THR PRO THR ARG ALA LEU PRO L59 P60



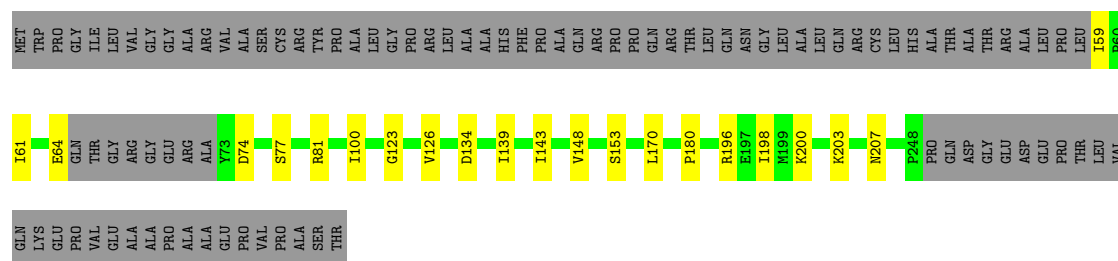
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.32Å 94.99Å 134.36Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	49.07 – 2.75 49.07 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-2.75) 91.0 (49.07-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.45 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.250 0.206 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19762	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.08	0/1422	0.23	0/1922
1	B	0.08	0/1458	0.23	0/1970
1	C	0.06	0/1423	0.20	0/1923
1	D	0.09	0/1423	0.24	0/1923
1	E	0.07	0/1423	0.23	0/1923
1	F	0.06	0/1430	0.20	0/1933
1	G	0.06	0/1438	0.20	0/1945
1	H	0.06	0/1446	0.20	0/1955
1	I	0.07	0/1454	0.24	1/1966 (0.1%)
1	J	0.07	0/1435	0.23	0/1940
1	K	0.07	0/1402	0.21	0/1894
1	L	0.08	0/1442	0.23	0/1950
1	M	0.08	0/1402	0.23	0/1894
1	N	0.08	0/1438	0.21	0/1944
All	All	0.07	0/20036	0.22	1/27082 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	246	VAL	N-CA-C	-5.33	107.63	112.96

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	1397	0	1436	16	0
1	B	1433	0	1472	14	0
1	C	1398	0	1438	18	0
1	D	1398	0	1438	16	0
1	E	1398	0	1438	21	0
1	F	1405	0	1447	14	0
1	G	1412	0	1454	15	0
1	H	1421	0	1462	12	0
1	I	1428	0	1472	10	0
1	J	1410	0	1452	13	0
1	K	1378	0	1418	11	0
1	L	1417	0	1461	15	0
1	M	1378	0	1418	15	0
1	N	1413	0	1451	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	8	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	1	0	0	0	0
3	G	7	0	0	1	0
3	H	5	0	0	0	0
3	I	9	0	0	0	0
3	J	3	0	0	0	0
3	K	4	0	0	0	0
3	L	5	0	0	0	0
3	M	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	4	0	0	0	0
All	All	19762	0	20257	168	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 4.

All (168) 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:152:ALA:HB1	1:C:176:MET:HE3	1.72	0.71
1:H:123:GLY:HA3	1:H:153:SER:HB3	1.72	0.70
1:A:152:ALA:HB1	1:A:176:MET:HE3	1.74	0.70
1:L:152:ALA:HB1	1:L:176:MET:HE3	1.73	0.69
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.75	0.69
1:G:152:ALA:HB1	1:G:176:MET:HE3	1.75	0.68
1:B:203:LYS:O	1:B:207:ASN:ND2	2.27	0.68
1:M:139:ILE:HD11	1:M:143:ILE:HD11	1.76	0.68
1:I:152:ALA:HB1	1:I:176:MET:HE3	1.76	0.67
1:F:203:LYS:O	1:F:207:ASN:ND2	2.29	0.66
1:I:203:LYS:O	1:I:207:ASN:ND2	2.28	0.66
1:K:203:LYS:O	1:K:207:ASN:ND2	2.30	0.65
1:F:152:ALA:HB1	1:F:176:MET:HE3	1.79	0.65
1:G:131:ALA:O	3:G:401:HOH:O	2.13	0.65
1:C:123:GLY:HA3	1:C:153:SER:HB3	1.77	0.65
1:N:139:ILE:HD11	1:N:143:ILE:HD11	1.78	0.64
1:J:123:GLY:HA3	1:J:153:SER:HB3	1.79	0.64
1:E:136:MET:HE3	1:E:143:ILE:HG21	1.79	0.64
1:L:203:LYS:O	1:L:207:ASN:ND2	2.29	0.64
1:B:170:LEU:HD13	1:C:134:ASP:HB3	1.79	0.64
1:C:203:LYS:O	1:C:207:ASN:ND2	2.30	0.64
1:J:203:LYS:O	1:J:207:ASN:ND2	2.30	0.64
1:K:152:ALA:HB1	1:K:176:MET:HE3	1.80	0.64
1:B:152:ALA:HB1	1:B:176:MET:HE3	1.81	0.63
1:H:203:LYS:O	1:H:207:ASN:ND2	2.30	0.63
1:I:123:GLY:HA3	1:I:153:SER:HB3	1.80	0.63
1:M:152:ALA:HB1	1:M:176:MET:HE3	1.80	0.63
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.81	0.63
1:H:134:ASP:HB3	1:N:170:LEU:HD13	1.80	0.62
1:J:152:ALA:HB1	1:J:176:MET:HE3	1.81	0.62
1:F:74:ASP:OD1	1:F:77:SER:OG	2.17	0.62
1:K:123:GLY:HA3	1:K:153:SER:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:203:LYS:O	1:N:207:ASN:ND2	2.32	0.62
1:M:203:LYS:O	1:M:207:ASN:ND2	2.34	0.61
1:L:123:GLY:HA3	1:L:153:SER:HB3	1.81	0.60
1:G:203:LYS:O	1:G:207:ASN:ND2	2.34	0.60
1:F:60:PRO:HG3	1:G:102:GLN:HE21	1.66	0.60
1:H:152:ALA:HB1	1:H:176:MET:HE3	1.83	0.60
1:N:123:GLY:HA3	1:N:153:SER:HB3	1.83	0.60
1:B:139:ILE:HD11	1:B:143:ILE:HD11	1.82	0.60
1:H:139:ILE:HD11	1:H:143:ILE:HD11	1.84	0.59
1:A:88:MET:HG2	1:A:120:ASN:HB3	1.83	0.59
1:A:123:GLY:HA3	1:A:153:SER:HB3	1.85	0.59
1:I:139:ILE:HD11	1:I:143:ILE:HD11	1.85	0.59
1:J:139:ILE:HD11	1:J:143:ILE:HD11	1.83	0.59
1:L:62:VAL:HG21	1:L:78:ARG:HG3	1.86	0.58
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.85	0.58
1:H:170:LEU:HD13	1:I:134:ASP:HB3	1.86	0.58
1:K:179:GLN:OE1	1:K:202:LYS:NZ	2.37	0.57
1:M:123:GLY:HA3	1:M:153:SER:HB3	1.85	0.57
1:A:160:ALA:HB2	1:A:240:ILE:HG23	1.86	0.57
1:C:126:VAL:HG21	1:C:180:PRO:HB3	1.87	0.57
1:C:60:PRO:HG3	1:D:102:GLN:HE21	1.69	0.57
1:L:84:ILE:HG12	1:L:116:HIS:HB2	1.87	0.56
1:K:84:ILE:HG12	1:K:116:HIS:HB2	1.88	0.56
1:E:61:ILE:O	1:E:78:ARG:NH1	2.39	0.55
1:L:136:MET:HE3	1:L:143:ILE:HG21	1.88	0.55
1:N:126:VAL:HG21	1:N:180:PRO:HB3	1.89	0.55
1:G:78:ARG:NH1	1:G:82:GLU:OE2	2.40	0.55
1:J:160:ALA:HB2	1:J:240:ILE:HG23	1.89	0.55
1:J:170:LEU:HD13	1:K:134:ASP:HB3	1.88	0.54
1:I:170:LEU:HD13	1:J:134:ASP:HB3	1.88	0.54
1:G:123:GLY:HA3	1:G:153:SER:HB3	1.88	0.54
1:M:170:LEU:HD13	1:N:134:ASP:HB3	1.90	0.53
1:C:136:MET:HE3	1:C:143:ILE:HG21	1.91	0.53
1:G:73:TYR:HB2	1:G:77:SER:HB2	1.90	0.53
1:N:59:ILE:HD11	1:N:74:ASP:HB2	1.90	0.52
1:F:60:PRO:HG2	1:F:75:ILE:HB	1.92	0.52
1:A:170:LEU:HD13	1:B:134:ASP:HB3	1.92	0.52
1:B:123:GLY:HA3	1:B:153:SER:HB3	1.91	0.51
1:E:61:ILE:HG13	1:E:78:ARG:HH12	1.74	0.51
1:B:191:ILE:HG21	1:N:198:ILE:HD12	1.92	0.51
1:N:64:GLU:OE1	1:N:81:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:HB3	1:G:170:LEU:HD13	1.93	0.51
1:N:196:ARG:HG2	1:N:200:LYS:HE3	1.93	0.51
1:L:168:HIS:HB3	1:L:245:LEU:HD13	1.93	0.50
1:D:61:ILE:HG22	1:D:74:ASP:HA	1.93	0.49
1:D:169:SER:HB2	1:D:241:LEU:HD22	1.94	0.49
1:F:168:HIS:HB3	1:F:245:LEU:HD13	1.94	0.49
1:L:246:VAL:C	1:L:247:HIS:HD1	2.20	0.49
1:A:73:TYR:OH	1:A:81:ARG:HD2	2.12	0.48
1:E:115:ILE:HB	1:E:143:ILE:HD13	1.94	0.48
1:G:74:ASP:OD1	1:G:77:SER:N	2.45	0.48
1:I:126:VAL:HG21	1:I:180:PRO:HB3	1.95	0.48
1:G:136:MET:HE3	1:G:143:ILE:HG21	1.94	0.48
1:M:61:ILE:N	1:N:77:SER:OG	2.42	0.48
1:D:59:ILE:HG13	1:D:60:PRO:HD2	1.94	0.48
1:D:148:VAL:HG11	1:E:100:ILE:HD13	1.96	0.48
1:E:152:ALA:HB1	1:E:176:MET:HE3	1.93	0.48
1:M:136:MET:HE3	1:M:143:ILE:HG21	1.95	0.48
1:A:62:VAL:HG21	1:A:78:ARG:HB2	1.94	0.48
1:F:198:ILE:HD12	1:J:191:ILE:HG21	1.96	0.48
1:H:148:VAL:HG13	1:H:170:LEU:HD12	1.96	0.48
1:J:111:ASN:HB2	1:J:140:LEU:HD21	1.95	0.48
1:L:247:HIS:N	1:L:248:PRO:HD3	2.29	0.47
1:A:136:MET:HE3	1:A:143:ILE:HG21	1.96	0.47
1:I:73:TYR:HB2	1:I:77:SER:HB2	1.97	0.47
1:H:197:GLU:HA	1:H:200:LYS:HE3	1.95	0.47
1:I:73:TYR:OH	1:I:81:ARG:NH2	2.48	0.47
1:L:170:LEU:HD13	1:M:134:ASP:HB3	1.97	0.46
1:K:139:ILE:HD11	1:K:143:ILE:HD11	1.96	0.46
1:C:148:VAL:HG11	1:D:100:ILE:HD13	1.97	0.46
1:K:136:MET:HE3	1:K:143:ILE:HG21	1.96	0.46
1:A:59:ILE:HD12	1:B:98:LEU:HD11	1.98	0.45
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.98	0.45
1:C:160:ALA:HB2	1:C:240:ILE:HG23	1.98	0.45
1:A:148:VAL:HG13	1:A:170:LEU:HD12	1.99	0.45
1:D:123:GLY:HA3	1:D:153:SER:HB3	1.97	0.45
1:E:59:ILE:HG22	1:E:75:ILE:HG22	1.98	0.45
1:B:126:VAL:HG21	1:B:180:PRO:HB3	1.99	0.45
1:E:246:VAL:HG22	1:E:247:HIS:H	1.81	0.45
1:M:168:HIS:CE1	1:M:243:LYS:HD2	2.52	0.45
1:M:195:ALA:O	1:M:198:ILE:HG22	2.16	0.45
1:L:60:PRO:HB2	1:L:75:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ALA:HA	1:C:132:ILE:HD11	2.00	0.44
1:E:170:LEU:HD13	1:F:134:ASP:HB3	1.99	0.44
1:F:123:GLY:HA3	1:F:153:SER:HB3	2.00	0.44
1:J:126:VAL:HG21	1:J:180:PRO:HB3	2.00	0.44
1:A:100:ILE:HD13	1:G:148:VAL:HG11	1.98	0.44
1:E:187:GLN:HA	1:K:181:SER:HA	1.99	0.44
1:I:245:LEU:HD13	1:I:249:PRO:HD3	1.99	0.44
1:H:59:ILE:HG23	1:H:75:ILE:HG22	2.00	0.43
1:L:245:LEU:HD23	1:M:138:TYR:CE1	2.53	0.43
1:N:148:VAL:HG13	1:N:170:LEU:HD12	1.99	0.43
1:K:105:PHE:O	1:K:109:GLU:HG2	2.18	0.43
1:K:126:VAL:HG21	1:K:180:PRO:HB3	2.01	0.43
1:C:184:ALA:HB3	1:M:184:ALA:HB3	2.00	0.43
1:D:60:PRO:HG3	1:E:102:GLN:HE21	1.84	0.43
1:J:140:LEU:HD22	1:J:140:LEU:H	1.84	0.43
1:C:159:LEU:HD21	1:C:241:LEU:HD21	2.01	0.42
1:E:238:PHE:HB3	1:E:240:ILE:HD12	2.01	0.42
1:M:148:VAL:HG11	1:N:100:ILE:HD13	2.00	0.42
1:A:168:HIS:CE1	1:A:243:LYS:HD2	2.54	0.42
1:G:160:ALA:HB2	1:G:240:ILE:HG23	2.00	0.42
1:F:160:ALA:HB2	1:F:240:ILE:HG23	2.00	0.42
1:F:96:ALA:HA	1:F:132:ILE:HD11	2.01	0.42
1:D:58:LEU:O	1:D:59:ILE:HB	2.19	0.42
1:E:245:LEU:HD13	1:F:138:TYR:CZ	2.54	0.42
1:E:59:ILE:H	1:E:59:ILE:HG12	1.59	0.42
1:G:233:MET:HA	1:G:233:MET:HE3	2.01	0.42
1:A:148:VAL:HG11	1:B:100:ILE:HD13	2.01	0.42
1:E:79:LEU:HB3	1:E:84:ILE:HB	2.01	0.42
1:B:59:ILE:HG12	1:C:98:LEU:HD21	2.02	0.41
1:B:78:ARG:O	1:B:78:ARG:NH1	2.54	0.41
1:E:123:GLY:HA3	1:E:153:SER:HB3	2.01	0.41
1:E:160:ALA:HB2	1:E:240:ILE:HG23	2.01	0.41
1:L:126:VAL:HG21	1:L:180:PRO:HB3	2.01	0.41
1:B:148:VAL:HG11	1:C:100:ILE:HD13	2.02	0.41
1:M:171:PRO:HG3	1:M:245:LEU:O	2.20	0.41
1:G:60:PRO:O	1:G:74:ASP:HA	2.21	0.41
1:H:84:ILE:HG12	1:H:116:HIS:HB2	2.03	0.41
1:C:245:LEU:HD23	1:D:138:TYR:CE1	2.55	0.41
1:F:84:ILE:HG12	1:F:116:HIS:HB2	2.02	0.41
1:A:202:LYS:HD2	1:H:188:ALA:HB3	2.02	0.41
1:C:84:ILE:HG12	1:C:116:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:HIS:N	1:J:248:PRO:HD3	2.36	0.41
1:D:59:ILE:HD12	1:D:59:ILE:HA	1.67	0.40
1:E:148:VAL:HG11	1:F:100:ILE:HD13	2.04	0.40
1:D:136:MET:HE3	1:D:143:ILE:HG21	2.01	0.40
1:J:246:VAL:C	1:J:248:PRO:HD3	2.47	0.40
1:L:113:LYS:HE3	1:L:113:LYS:HB2	1.95	0.40
1:B:62:VAL:HG21	1:B:78:ARG:HD3	2.03	0.40
1:D:170:LEU:HB3	1:E:134:ASP:HB3	2.02	0.40
1:L:148:VAL:HG11	1:M:100:ILE:HD13	2.02	0.40
1:E:139:ILE:HD11	1:E:143:ILE:HD11	2.03	0.40
1:H:160:ALA:HB2	1:H:240:ILE:HG23	2.02	0.40
1:C:78:ARG:HH22	1:D:108:SER:HB2	1.86	0.40
1:D:226:ARG:HH12	1:E:189:THR:HB	1.87	0.40

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	176/277 (64%)	171 (97%)	5 (3%)	0	100	100
1	B	181/277 (65%)	174 (96%)	6 (3%)	1 (1%)	21	38
1	C	176/277 (64%)	167 (95%)	9 (5%)	0	100	100
1	D	176/277 (64%)	168 (96%)	7 (4%)	1 (1%)	21	38
1	E	176/277 (64%)	166 (94%)	10 (6%)	0	100	100
1	F	177/277 (64%)	172 (97%)	5 (3%)	0	100	100
1	G	178/277 (64%)	172 (97%)	6 (3%)	0	100	100
1	H	179/277 (65%)	173 (97%)	6 (3%)	0	100	100
1	I	180/277 (65%)	175 (97%)	5 (3%)	0	100	100
1	J	178/277 (64%)	172 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	174/277 (63%)	169 (97%)	5 (3%)	0	100	100
1	L	179/277 (65%)	171 (96%)	8 (4%)	0	100	100
1	M	174/277 (63%)	167 (96%)	7 (4%)	0	100	100
1	N	178/277 (64%)	173 (97%)	5 (3%)	0	100	100
All	All	2482/3878 (64%)	2390 (96%)	90 (4%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	GLU
1	D	59	ILE

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	154/227 (68%)	154 (100%)	0	100	100
1	B	157/227 (69%)	156 (99%)	1 (1%)	78	88
1	C	154/227 (68%)	153 (99%)	1 (1%)	78	88
1	D	154/227 (68%)	150 (97%)	4 (3%)	40	63
1	E	154/227 (68%)	151 (98%)	3 (2%)	50	70
1	F	155/227 (68%)	152 (98%)	3 (2%)	50	70
1	G	156/227 (69%)	155 (99%)	1 (1%)	78	88
1	H	157/227 (69%)	156 (99%)	1 (1%)	78	88
1	I	157/227 (69%)	155 (99%)	2 (1%)	61	76
1	J	155/227 (68%)	152 (98%)	3 (2%)	50	70
1	K	152/227 (67%)	151 (99%)	1 (1%)	76	86
1	L	156/227 (69%)	155 (99%)	1 (1%)	78	88
1	M	152/227 (67%)	152 (100%)	0	100	100
1	N	156/227 (69%)	155 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2169/3178 (68%)	2147 (99%)	22 (1%)	68 81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	246	VAL
1	C	73	TYR
1	D	58	LEU
1	D	59	ILE
1	D	61	ILE
1	D	174	ARG
1	E	73	TYR
1	E	78	ARG
1	E	168	HIS
1	F	59	ILE
1	F	77	SER
1	F	241	LEU
1	G	73	TYR
1	H	73	TYR
1	I	58	LEU
1	I	73	TYR
1	J	73	TYR
1	J	140	LEU
1	J	174	ARG
1	K	241	LEU
1	L	246	VAL
1	N	61	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	120	ASN
1	A	137	GLN
1	A	236	GLN
1	B	137	GLN
1	D	102	GLN
1	D	137	GLN
1	F	247	HIS
1	G	102	GLN
1	G	120	ASN

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Mol	Chain	Res	Type
1	G	137	GLN
1	G	179	GLN
1	H	120	ASN
1	H	137	GLN
1	H	179	GLN
1	I	111	ASN
1	I	137	GLN
1	J	102	GLN
1	J	137	GLN
1	J	150	GLN
1	K	137	GLN
1	K	204	GLN
1	L	137	GLN
1	M	137	GLN
1	N	120	ASN
1	N	137	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

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, 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	180/277 (64%)	-0.20	1 (0%) 85 86	64, 80, 116, 154	0
1	B	185/277 (66%)	-0.13	2 (1%) 78 77	66, 83, 116, 154	0
1	C	180/277 (64%)	-0.03	1 (0%) 85 86	73, 94, 126, 156	0
1	D	180/277 (64%)	0.05	3 (1%) 69 67	87, 108, 153, 188	0
1	E	180/277 (64%)	0.09	2 (1%) 78 77	89, 112, 148, 201	0
1	F	181/277 (65%)	0.03	3 (1%) 69 67	77, 101, 139, 187	0
1	G	182/277 (65%)	-0.11	3 (1%) 70 69	69, 88, 138, 179	0
1	H	183/277 (66%)	-0.35	1 (0%) 87 87	60, 73, 101, 153	0
1	I	184/277 (66%)	-0.24	2 (1%) 78 77	62, 77, 106, 147	0
1	J	182/277 (65%)	-0.14	2 (1%) 78 77	66, 91, 118, 157	0
1	K	178/277 (64%)	-0.09	1 (0%) 85 86	75, 96, 120, 152	0
1	L	183/277 (66%)	-0.03	2 (1%) 78 77	81, 100, 129, 167	0
1	M	178/277 (64%)	-0.20	1 (0%) 85 86	67, 81, 114, 134	0
1	N	182/277 (65%)	-0.32	0 100 100	62, 76, 110, 133	0
All	All	2538/3878 (65%)	-0.12	24 (0%) 81 81	60, 91, 129, 201	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	72	ALA	4.9
1	B	69	GLY	4.1
1	D	58	LEU	2.9
1	I	62	VAL	2.8
1	B	63	VAL	2.8
1	E	58	LEU	2.7
1	G	105	PHE	2.7
1	L	63	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	118	TYR	2.6
1	A	59	ILE	2.5
1	C	58	LEU	2.4
1	J	58	LEU	2.4
1	D	135	THR	2.4
1	D	198	ILE	2.4
1	G	58	LEU	2.4
1	F	58	LEU	2.3
1	F	59	ILE	2.3
1	M	59	ILE	2.3
1	F	78	ARG	2.3
1	L	148	VAL	2.2
1	H	246	VAL	2.1
1	K	59	ILE	2.1
1	G	245	LEU	2.0
1	J	118	TYR	2.0

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 oligosaccharides 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
2	CL	L	301	1/1	0.82	0.10	108,108,108,108	0
2	CL	D	301	1/1	0.87	0.10	101,101,101,101	0
2	CL	G	301	1/1	0.88	0.08	93,93,93,93	0
2	CL	A	301	1/1	0.88	0.08	95,95,95,95	0
2	CL	C	301	1/1	0.89	0.08	92,92,92,92	0
2	CL	I	301	1/1	0.89	0.09	81,81,81,81	0
2	CL	K	301	1/1	0.89	0.09	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	E	301	1/1	0.89	0.07	109,109,109,109	0
2	CL	F	301	1/1	0.90	0.11	94,94,94,94	0
2	CL	J	301	1/1	0.90	0.08	80,80,80,80	0
2	CL	N	301	1/1	0.92	0.07	85,85,85,85	0
2	CL	B	301	1/1	0.93	0.06	88,88,88,88	0
2	CL	M	301	1/1	0.94	0.06	86,86,86,86	0
2	CL	H	301	1/1	0.97	0.06	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.