Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 01:26 PM EDT

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)

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

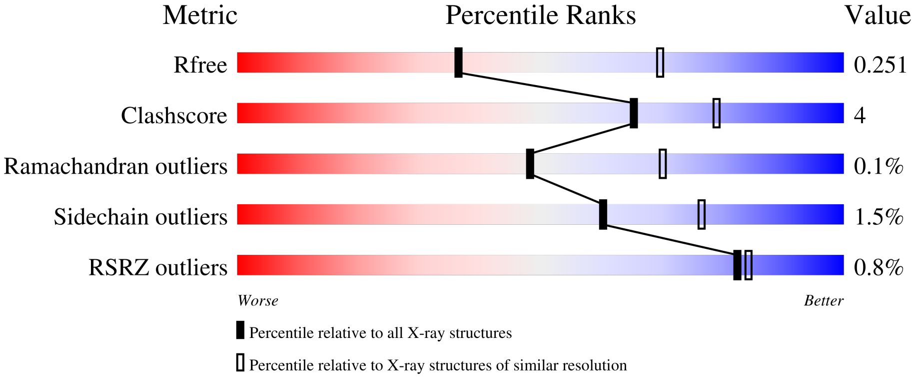
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

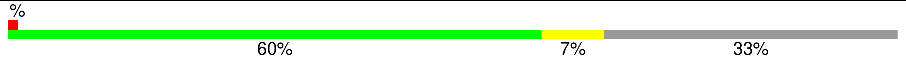
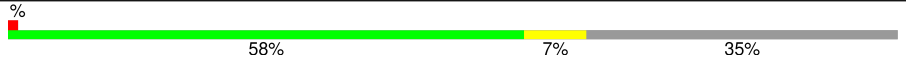
The reported resolution of this entry is 2.75 Å.

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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	277	
1	B	277	
1	C	277	
1	D	277	
1	E	277	

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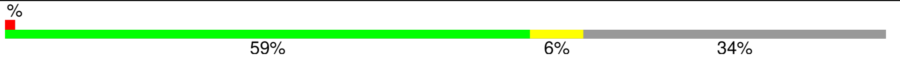
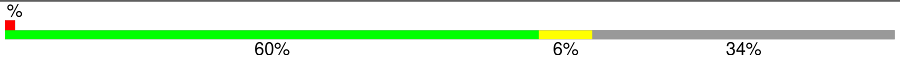
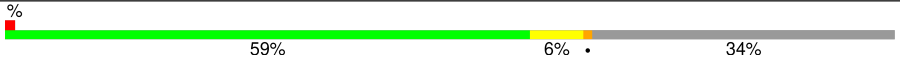
Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	
1	J	277	
1	K	277	
1	L	277	
1	M	277	
1	N	277	

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

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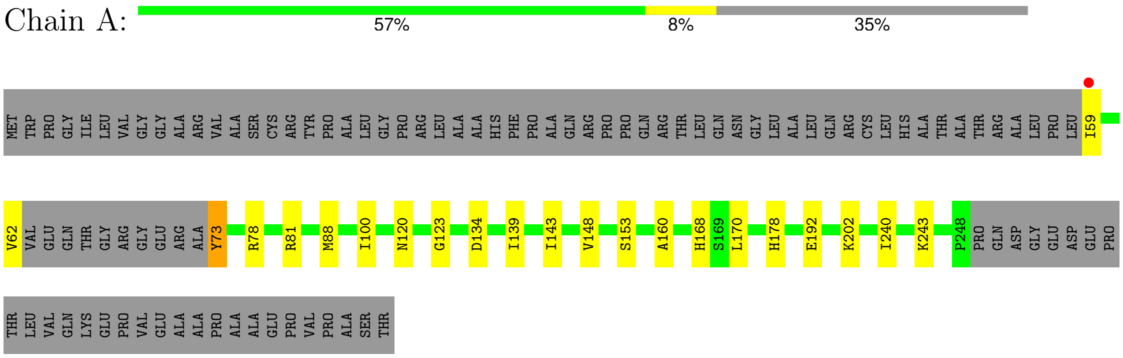
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	5	Total O 5 5	0	0
3	M	3	Total O 3 3	0	0
3	N	4	Total O 4 4	0	0

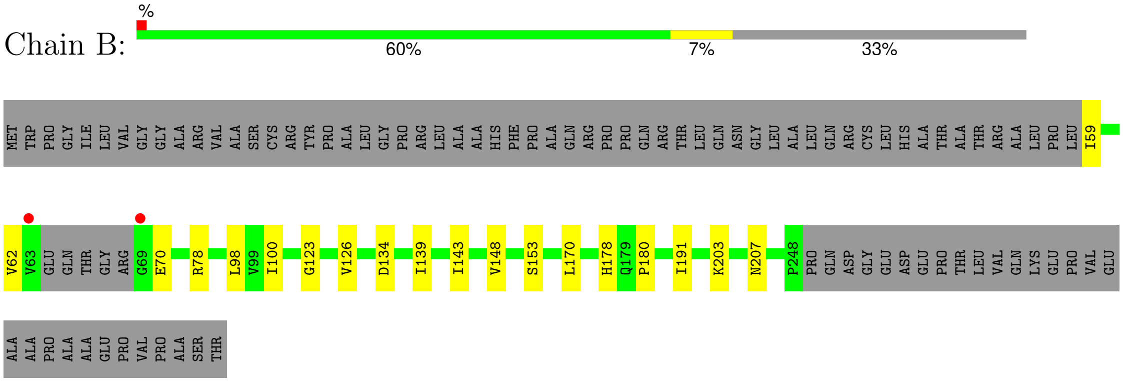
3 Residue-property plots

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.

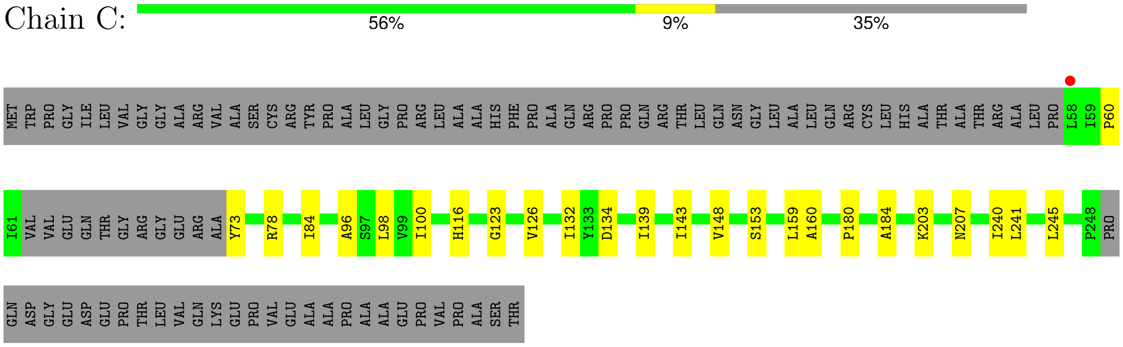
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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

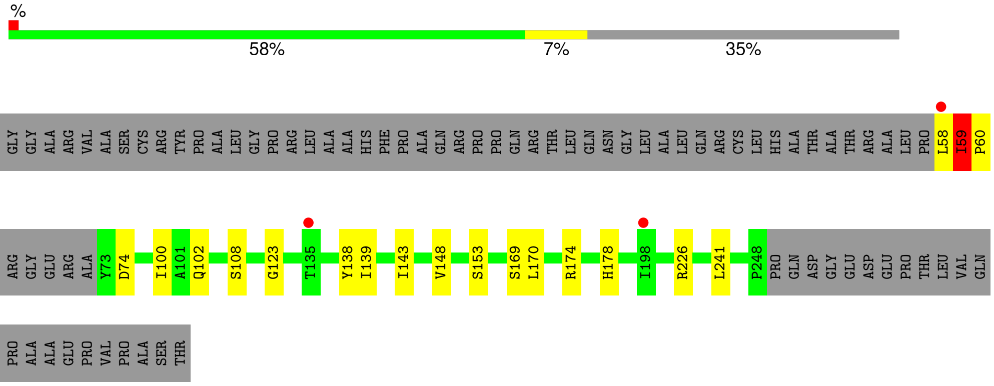


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



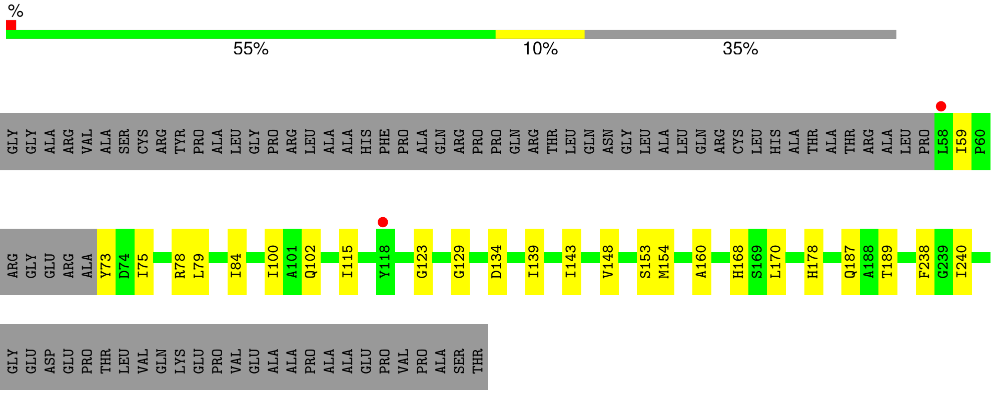
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain D:



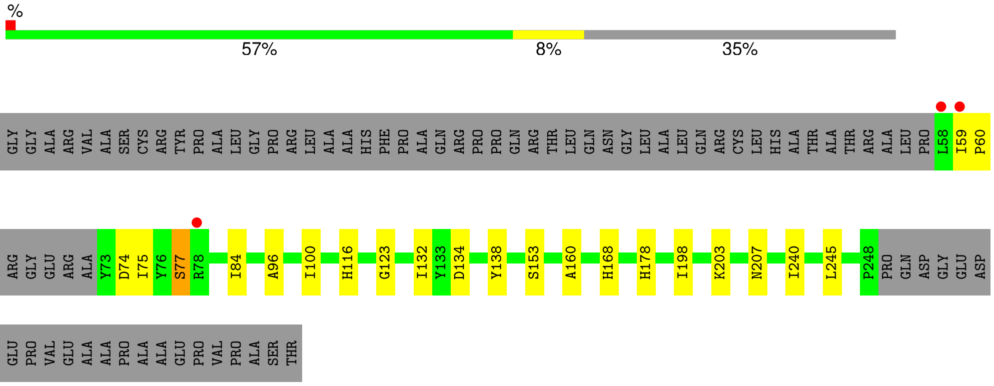
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



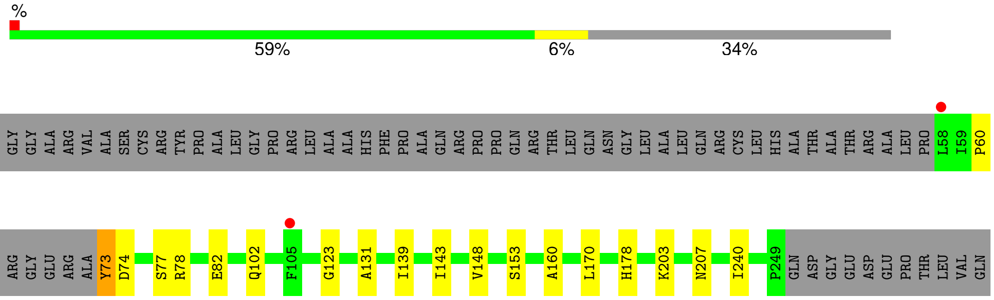
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:

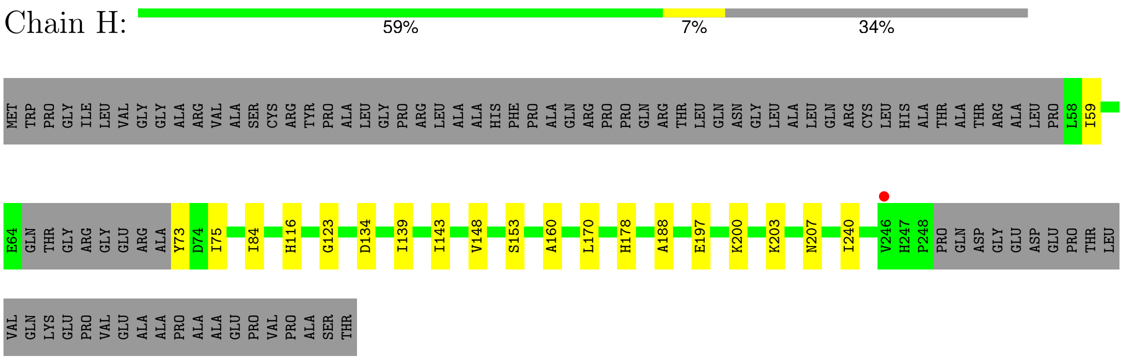


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

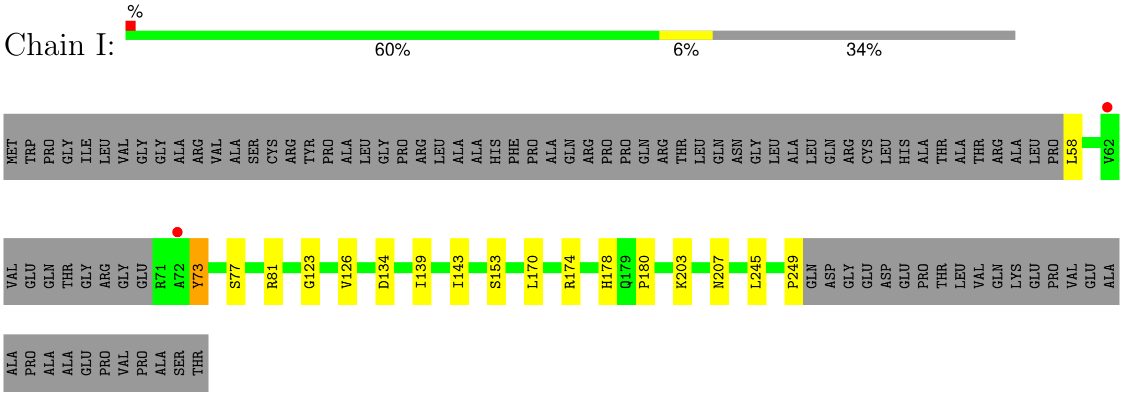
Chain G:



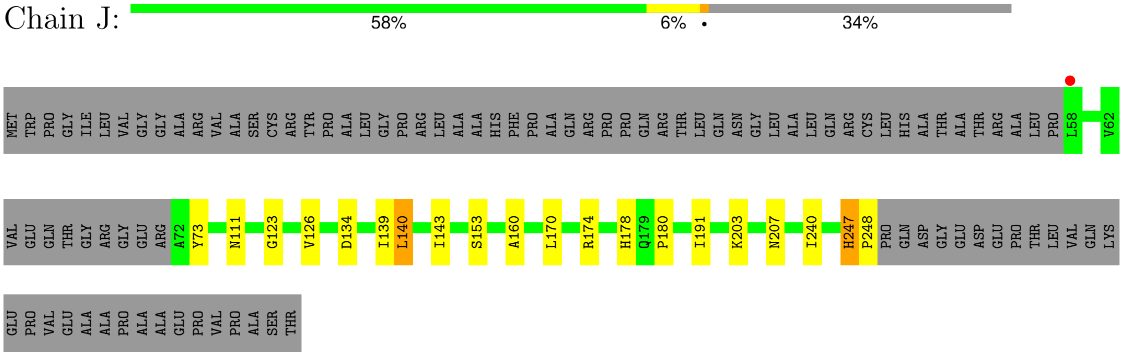
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



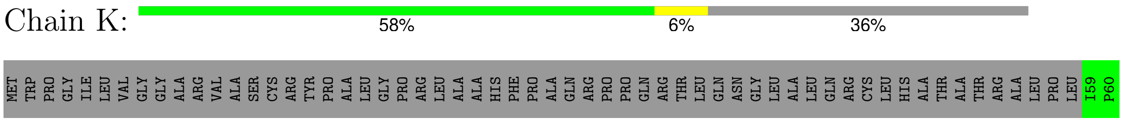
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

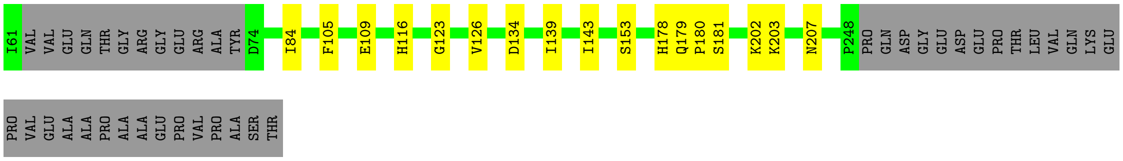


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



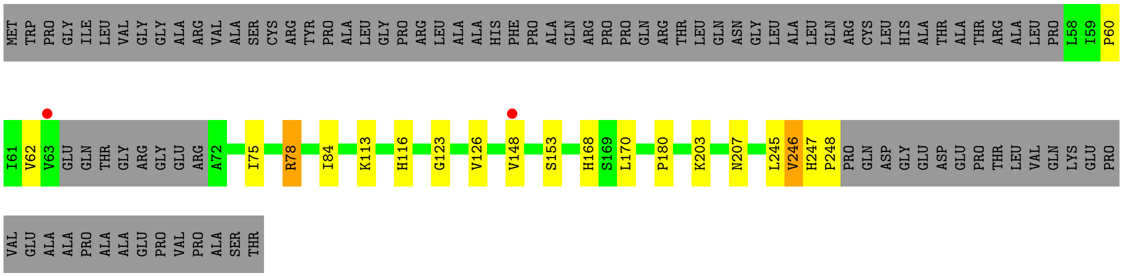
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial





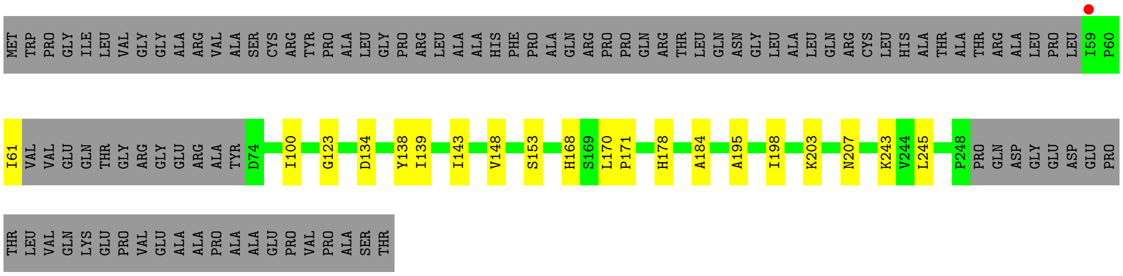
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain L:



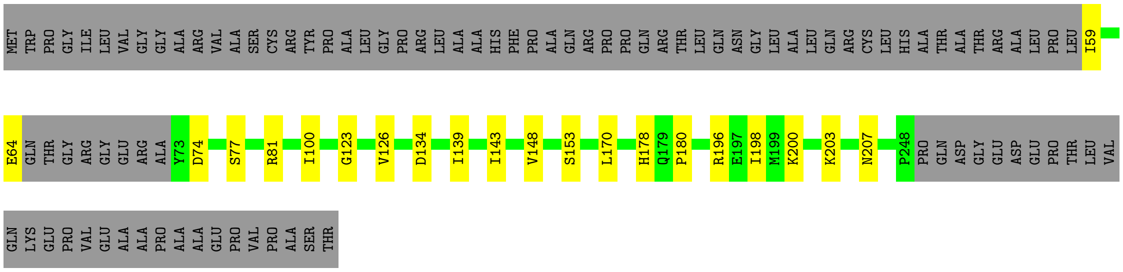
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain M:



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

Chain N:



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
$< I/\sigma(I) >$ [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	77415 reflections (2.17%)	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]	$< \lvert L\rvert > = 0.49$, $< L^2 > = 0.32$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L\rvert >$, $< L^2 >$ 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 ⓘ

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	0.23	0/1422	0.45	0/1922
1	B	0.24	0/1458	0.46	0/1970
1	C	0.23	0/1423	0.45	0/1923
1	D	0.23	0/1423	0.45	0/1923
1	E	0.23	0/1423	0.45	0/1923
1	F	0.23	0/1430	0.45	0/1933
1	G	0.23	0/1438	0.45	0/1945
1	H	0.23	0/1446	0.45	0/1955
1	I	0.23	0/1454	0.46	0/1966
1	J	0.24	0/1435	0.47	0/1940
1	K	0.23	0/1402	0.45	0/1894
1	L	0.23	0/1442	0.46	0/1950
1	M	0.23	0/1402	0.45	0/1894
1	N	0.23	0/1438	0.44	0/1944
All	All	0.23	0/20036	0.45	0/27082

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 ⓘ

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	14	0
1	B	1433	0	1472	13	0
1	C	1398	0	1438	16	0
1	D	1398	0	1438	15	0
1	E	1398	0	1438	20	0
1	F	1405	0	1447	13	0
1	G	1412	0	1454	12	0
1	H	1421	0	1462	11	0
1	I	1428	0	1472	9	0
1	J	1410	0	1452	11	0
1	K	1378	0	1418	9	0
1	L	1417	0	1461	13	0
1	M	1378	0	1418	13	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
3	N	4	0	0	0	0
All	All	19762	0	20257	147	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 (147) 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:123:GLY:HA3	1:H:153:SER:HB3	1.72	0.70
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.75	0.69
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: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: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: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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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:I:73:TYR:HB2	1:I:77:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:L:246:VAL:C	1:L:247:HIS:HD1	2.20	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:D:58:LEU:O	1:D:59:ILE:HB	2.19	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:E:245:LEU:HD13	1:F:138:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ILE:H	1:E:59:ILE:HG12	1.59	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:129:GLY:HA3	1:E:154:MET:HE2	2.02	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
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: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%)	22	36
1	C	176/277 (64%)	167 (95%)	9 (5%)	0	100	100
1	D	176/277 (64%)	168 (96%)	7 (4%)	1 (1%)	22	36
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
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	70

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%)	151 (98%)	3 (2%)	52	71
1	B	157/227 (69%)	156 (99%)	1 (1%)	84	90
1	C	154/227 (68%)	153 (99%)	1 (1%)	84	90
1	D	154/227 (68%)	151 (98%)	3 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	154/227 (68%)	151 (98%)	3 (2%)	52	71
1	F	155/227 (68%)	152 (98%)	3 (2%)	52	71
1	G	156/227 (69%)	154 (99%)	2 (1%)	65	80
1	H	157/227 (69%)	155 (99%)	2 (1%)	65	80
1	I	157/227 (69%)	153 (98%)	4 (2%)	42	64
1	J	155/227 (68%)	150 (97%)	5 (3%)	34	55
1	K	152/227 (67%)	151 (99%)	1 (1%)	81	89
1	L	156/227 (69%)	154 (99%)	2 (1%)	65	80
1	M	152/227 (67%)	151 (99%)	1 (1%)	81	89
1	N	156/227 (69%)	155 (99%)	1 (1%)	84	90
All	All	2169/3178 (68%)	2137 (98%)	32 (2%)	60	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	TYR
1	A	178	HIS
1	A	192	GLU
1	B	178	HIS
1	C	73	TYR
1	D	59	ILE
1	D	174	ARG
1	D	178	HIS
1	E	73	TYR
1	E	168	HIS
1	E	178	HIS
1	F	59	ILE
1	F	77	SER
1	F	178	HIS
1	G	73	TYR
1	G	178	HIS
1	H	73	TYR
1	H	178	HIS
1	I	58	LEU
1	I	73	TYR
1	I	174	ARG
1	I	178	HIS
1	J	73	TYR

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Mol	Chain	Res	Type
1	J	140	LEU
1	J	174	ARG
1	J	178	HIS
1	J	247	HIS
1	K	178	HIS
1	L	78	ARG
1	L	246	VAL
1	M	178	HIS
1	N	178	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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, 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%)	-0.34	1 (0%)	85	87	64, 80, 116, 154	0
1	B	185/277 (66%)	-0.26	2 (1%)	77	80	66, 83, 116, 154	0
1	C	180/277 (64%)	-0.16	1 (0%)	85	87	73, 94, 126, 156	0
1	D	180/277 (64%)	-0.08	3 (1%)	69	70	87, 108, 153, 188	0
1	E	180/277 (64%)	-0.04	2 (1%)	77	80	89, 112, 148, 201	0
1	F	181/277 (65%)	-0.10	3 (1%)	69	70	77, 101, 139, 187	0
1	G	182/277 (65%)	-0.24	2 (1%)	77	80	69, 88, 138, 179	0
1	H	183/277 (66%)	-0.48	1 (0%)	87	89	60, 73, 101, 153	0
1	I	184/277 (66%)	-0.37	2 (1%)	77	80	62, 77, 106, 147	0
1	J	182/277 (65%)	-0.27	1 (0%)	87	89	66, 91, 118, 157	0
1	K	178/277 (64%)	-0.22	0	100	100	75, 96, 120, 152	0
1	L	183/277 (66%)	-0.17	2 (1%)	77	80	81, 100, 129, 167	0
1	M	178/277 (64%)	-0.34	1 (0%)	85	87	67, 81, 114, 134	0
1	N	182/277 (65%)	-0.46	0	100	100	62, 76, 110, 133	0
All	All	2538/3878 (65%)	-0.25	21 (0%)	82	84	60, 91, 129, 201	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	72	ALA	4.8
1	B	69	GLY	3.9
1	D	58	LEU	2.7
1	I	62	VAL	2.7
1	B	63	VAL	2.7
1	E	58	LEU	2.6
1	L	63	VAL	2.6
1	G	105	PHE	2.5

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

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
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

There are no such residues in this entry.