



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2016 – 07:27 PM EDT

PDB ID : 5DZK
Title : Crystal structure of the active form of the proteolytic complex clpP1 and clpP2
Authors : LI, M.; Wlodawer, A.; Maurizi, M.
Deposited on : 2015-09-25
Resolution : 3.07 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

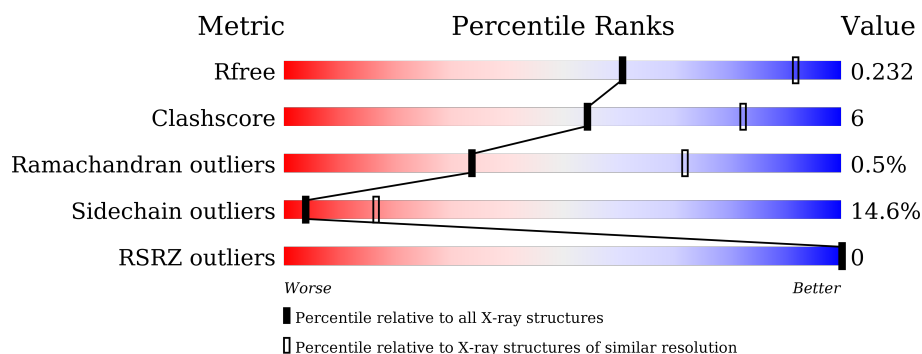
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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.















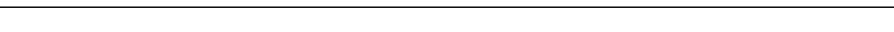

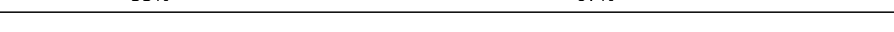

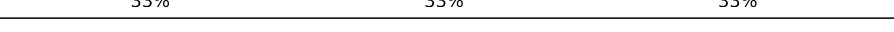
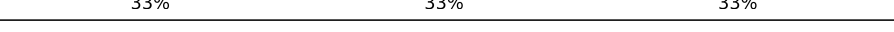
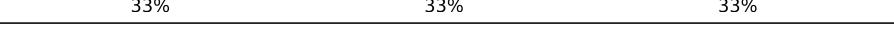






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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. 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	214	
1	B	214	
1	C	214	
1	D	214	
1	E	214	
1	F	214	

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Mol	Chain	Length	Quality of chain
1	G	214	
1	a	214	
1	b	214	
1	c	214	
1	d	214	
1	e	214	
1	f	214	
1	g	214	
2	1	3	
2	2	3	
2	3	3	
2	4	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	
2	T	3	
2	U	3	
2	V	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	
2	o	3	

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Mol	Chain	Length	Quality of chain
2	p	3	
2	q	3	
2	r	3	
2	s	3	
2	t	3	
2	u	3	
2	v	3	
2	w	3	
2	x	3	
2	y	3	
2	z	3	
3	H	200	
3	I	200	
3	J	200	
3	K	200	
3	L	200	
3	M	200	
3	N	200	
3	h	200	
3	i	200	
3	j	200	
3	k	200	
3	l	200	
3	m	200	
3	n	200	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40976 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	B	200	Total	C	N	O	S	0	0	0
			1534	963	262	301	8			
1	C	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	D	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	E	200	Total	C	N	O	S	0	0	0
			1534	963	262	301	8			
1	F	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	G	195	Total	C	N	O	S	0	0	0
			1502	945	256	293	8			
1	a	197	Total	C	N	O	S	0	0	0
			1513	951	258	296	8			
1	b	200	Total	C	N	O	S	0	0	0
			1534	963	262	301	8			
1	c	197	Total	C	N	O	S	0	0	0
			1513	951	258	296	8			
1	d	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	e	200	Total	C	N	O	S	0	0	0
			1534	963	262	301	8			
1	f	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			
1	g	196	Total	C	N	O	S	0	0	0
			1508	948	257	295	8			

- Molecule 2 is a protein called BEZ-LEU-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	P	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	Q	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	R	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	S	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	T	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	U	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	V	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	W	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	X	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	Y	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	Z	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	1	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	2	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	o	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	p	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	q	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	r	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	s	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	t	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	u	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	v	3	Total	C	N	O	0	0	0
			25	19	2	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	w	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	x	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	y	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	z	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	3	3	Total	C	N	O	0	0	0
			25	19	2	4			
2	4	3	Total	C	N	O	0	0	0
			25	19	2	4			

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	I	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	J	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	K	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	L	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	M	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	N	179	Total	C	N	O	S	0	0	0
			1362	861	230	262	9			
3	h	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	i	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	j	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	k	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	l	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
3	m	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	n	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	G	2	Total	O	0	0
			2	2		
4	H	2	Total	O	0	0
			2	2		
4	I	4	Total	O	0	0
			4	4		
4	J	1	Total	O	0	0
			1	1		
4	K	2	Total	O	0	0
			2	2		
4	L	2	Total	O	0	0
			2	2		
4	M	3	Total	O	0	0
			3	3		
4	N	2	Total	O	0	0
			2	2		
4	a	1	Total	O	0	0
			1	1		
4	b	1	Total	O	0	0
			1	1		
4	c	1	Total	O	0	0
			1	1		
4	d	2	Total	O	0	0
			2	2		
4	e	1	Total	O	0	0
			1	1		
4	h	4	Total	O	0	0
			4	4		

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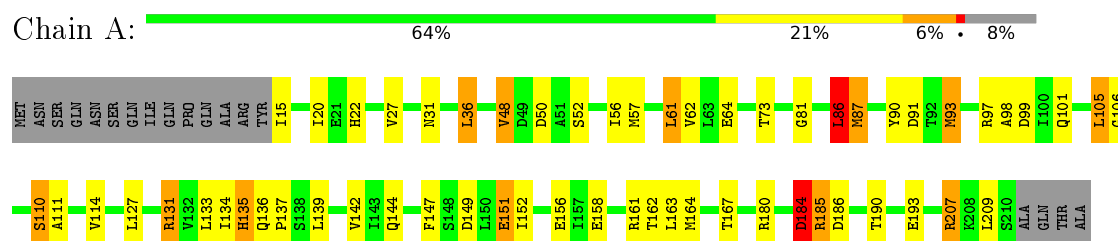
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	i	3	Total 3	O 3	0	0
4	j	3	Total 3	O 3	0	0
4	k	6	Total 6	O 6	0	0
4	l	2	Total 2	O 2	0	0
4	m	4	Total 4	O 4	0	0
4	n	3	Total 3	O 3	0	0

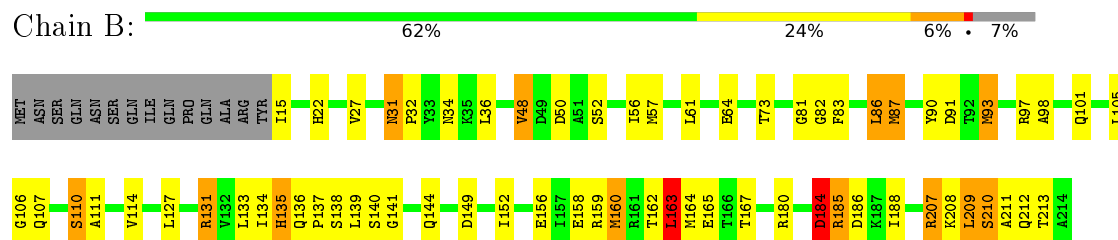
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

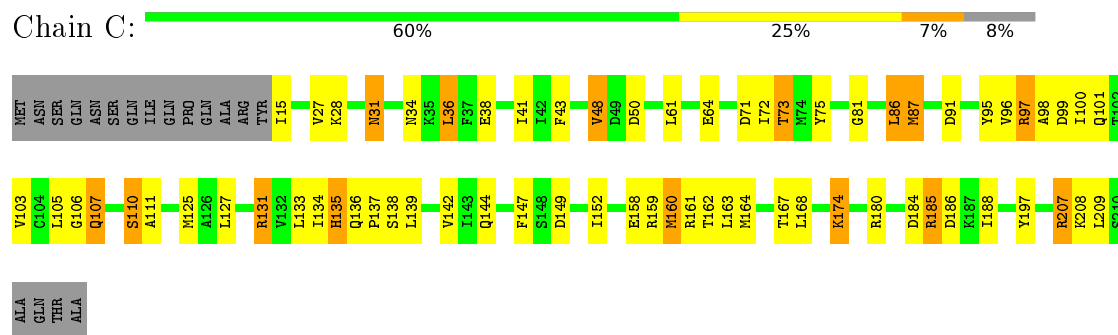
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



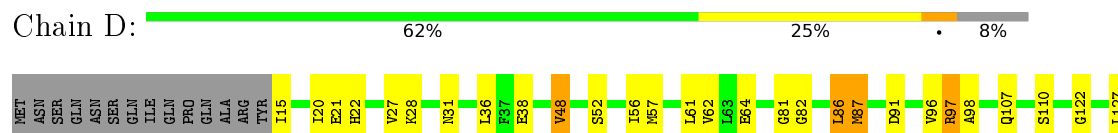
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

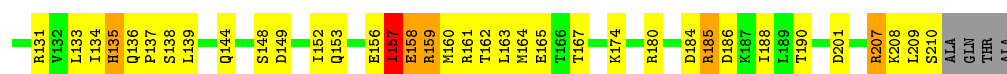


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



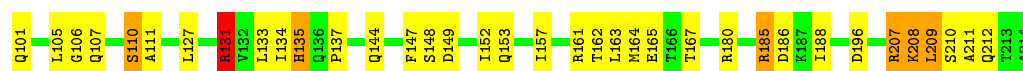
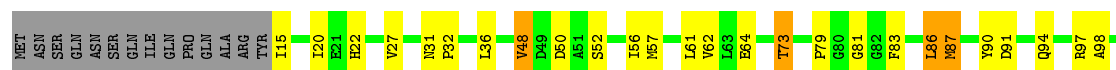
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2





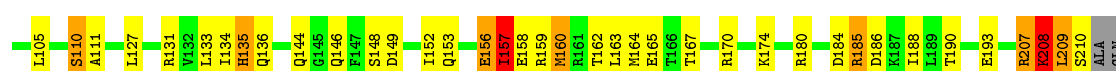
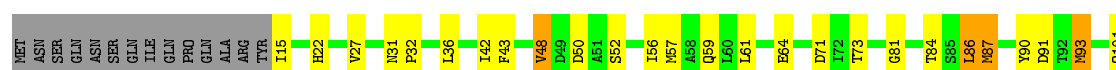
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E: 64% 24% 5% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F: 62% 24% 5% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain G: 66% 20% 5% 9%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain a: 82% 9% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

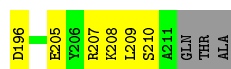
Chain b: 79% 14% 7%





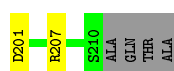
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain c: 78% 14% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain d: 79% 11% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain e: 80% 12% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f: 80% 12% 8%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain g: 78% 14% 8%





- Molecule 2: BEZ-LEU-LEU



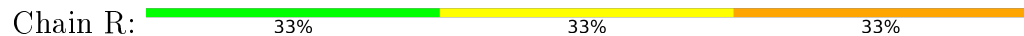
- Molecule 2: BEZ-LEU-LEU



- Molecule 2: BEZ-LEU-LEU



- Molecule 2: BEZ-LEU-LEU



- Molecule 2: BEZ-LEU-LEU



- Molecule 2: BEZ-LEU-LEU



- Molecule 2: BEZ-LEU-LEU



• Molecule 2: BEZ-LEU-LEU

Chain V:  67% 33%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain W:  67% 33%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain X:  33% 67%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain Y:  67% 33%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain Z:  67% 33%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain 1:  33% 67%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain 2:  67% 33%
7801
L802
L803

• Molecule 2: BEZ-LEU-LEU

Chain o:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain p:  33% 67%



- Molecule 2: BEZ-LEU-LEU

Chain q:  33% 33% 33%




- Molecule 2: BEZ-LEU-LEU

Chain r:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain s:  33% 67%



- Molecule 2: BEZ-LEU-LEU

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: BEZ-LEU-LEU

Chain u:  33% 67%



- Molecule 2: BEZ-LEU-LEU

Chain v:  67% 33%




- Molecule 2: BEZ-LEU-LEU

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: BEZ-LEU-LEU

Chain x:  33% 67%



- Molecule 2: BEZ-LEU-LEU

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: BEZ-LEU-LEU

Chain z:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain 3:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain 4:  67% 33%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

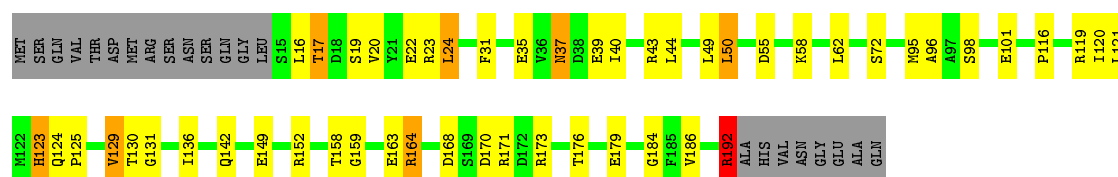
Chain H:  66% 18% 5% • 11%





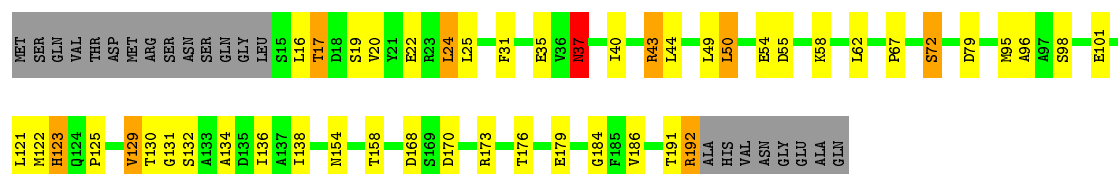
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain I:  64% 22% • • 11%



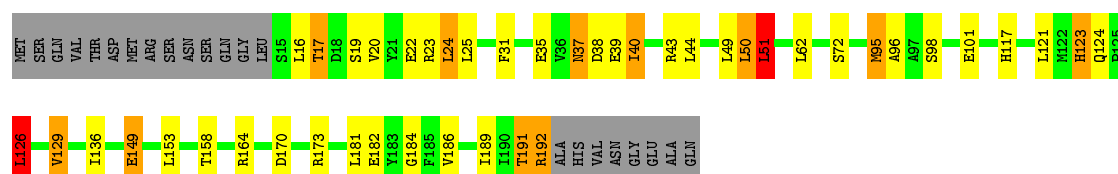
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain J: 65% 20% 11%



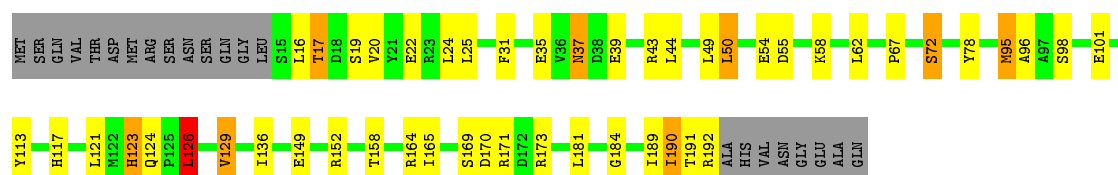
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain K: 67% 16% 6% 11%



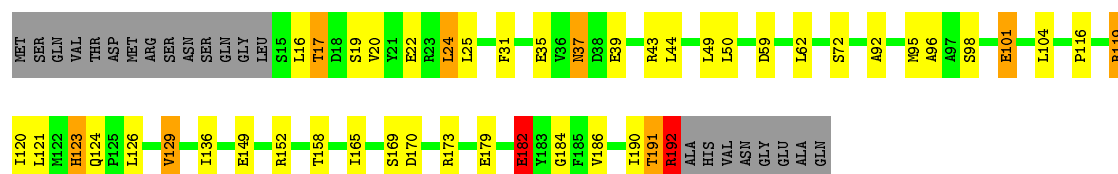
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain L: 65% 20% 11%



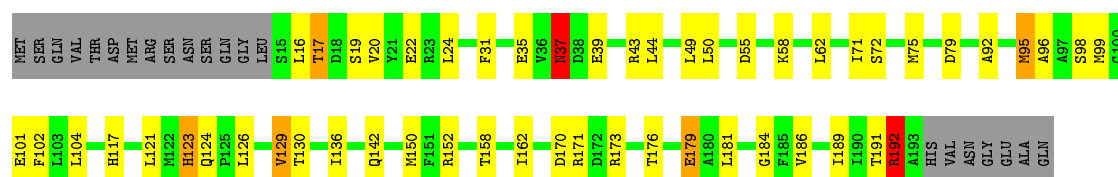
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain M: 66% 19% 11%



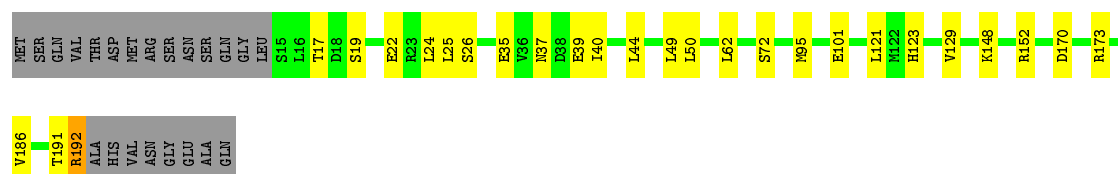
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain N: 63% 23% 11%



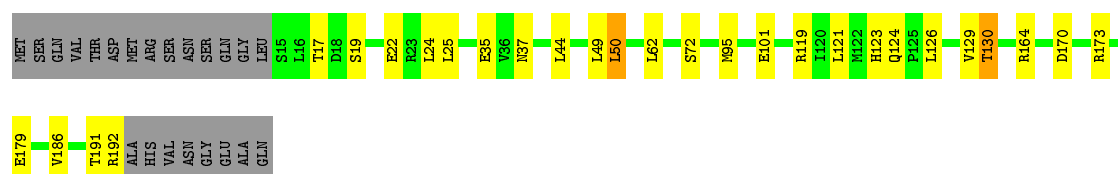
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain h: 76% 13% 11%



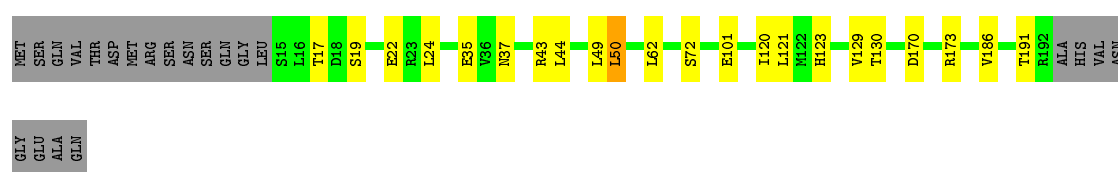
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain i: 75% 13% 11%



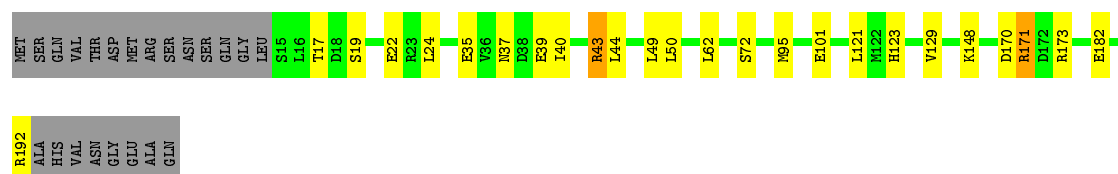
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain j: 78% 11% 11%



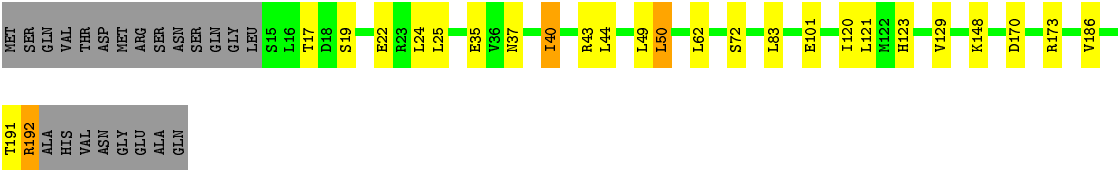
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain k: 77% 12% 11%

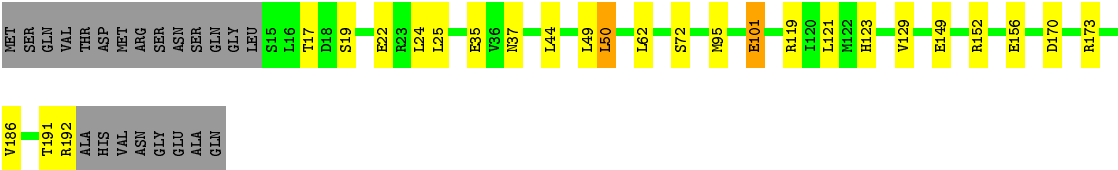


- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

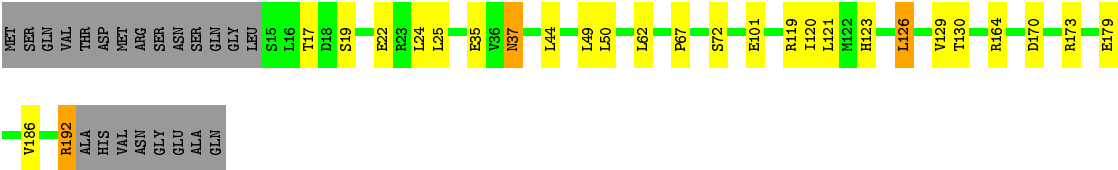
Chain l: 76% 12% 11%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.94Å 183.35Å 188.45Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	72.24 – 3.07 72.14 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.2 (72.24-3.07) 93.2 (72.14-3.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.232 0.201 , 0.232	Depositor DCC
R_{free} test set	6092 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	7 of 121114 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40976	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2426e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BEZ

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	0.82	0/1529	1.03	8/2068 (0.4%)
1	B	0.83	0/1555	1.04	7/2104 (0.3%)
1	C	0.86	0/1529	1.06	6/2068 (0.3%)
1	D	0.91	1/1529 (0.1%)	1.08	5/2068 (0.2%)
1	E	0.87	0/1555	0.99	3/2104 (0.1%)
1	F	0.83	0/1529	1.07	8/2068 (0.4%)
1	G	0.83	0/1523	1.01	5/2060 (0.2%)
1	a	0.84	0/1534	1.01	3/2075 (0.1%)
1	b	0.86	0/1555	1.07	5/2104 (0.2%)
1	c	0.91	2/1534 (0.1%)	1.22	11/2075 (0.5%)
1	d	0.84	1/1529 (0.1%)	1.07	9/2068 (0.4%)
1	e	0.87	2/1555 (0.1%)	1.14	9/2104 (0.4%)
1	f	0.86	1/1529 (0.1%)	1.04	4/2068 (0.2%)
1	g	0.86	1/1529 (0.1%)	1.13	9/2068 (0.4%)
2	1	0.85	0/16	1.53	0/19
2	2	1.06	0/16	1.61	0/19
2	3	0.61	0/16	1.52	0/19
2	4	0.80	0/16	1.91	1/19 (5.3%)
2	O	0.83	0/16	1.13	0/19
2	P	0.66	0/16	1.88	0/19
2	Q	0.69	0/16	1.35	0/19
2	R	0.78	0/16	1.46	0/19
2	S	0.45	0/16	1.94	1/19 (5.3%)
2	T	0.89	0/16	1.32	0/19
2	U	0.71	0/16	1.13	0/19
2	V	0.58	0/16	1.86	1/19 (5.3%)
2	W	0.95	0/16	1.50	0/19
2	X	0.76	0/16	1.15	0/19
2	Y	0.93	0/16	1.19	0/19
2	Z	1.21	0/16	1.99	1/19 (5.3%)
2	o	0.61	0/16	1.67	0/19
2	p	0.52	0/16	1.54	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q	0.44	0/16	2.09	1/19 (5.3%)
2	r	0.92	0/16	1.35	0/19
2	s	0.66	0/16	1.84	0/19
2	t	0.61	0/16	1.47	0/19
2	u	0.57	0/16	1.76	0/19
2	v	0.64	0/16	1.29	0/19
2	w	0.75	0/16	1.47	0/19
2	x	0.69	0/16	1.81	1/19 (5.3%)
2	y	0.92	0/16	1.60	0/19
2	z	0.82	0/16	2.09	1/19 (5.3%)
3	H	0.86	0/1379	1.03	8/1864 (0.4%)
3	I	0.92	1/1379 (0.1%)	1.14	9/1864 (0.5%)
3	J	0.90	0/1379	1.11	8/1864 (0.4%)
3	K	0.83	0/1379	1.03	6/1864 (0.3%)
3	L	0.82	0/1379	1.02	4/1864 (0.2%)
3	M	0.84	1/1379 (0.1%)	1.03	10/1864 (0.5%)
3	N	0.82	1/1384 (0.1%)	1.04	6/1871 (0.3%)
3	h	0.84	2/1379 (0.1%)	1.03	5/1864 (0.3%)
3	i	0.84	1/1379 (0.1%)	1.10	10/1864 (0.5%)
3	j	0.80	0/1379	1.05	6/1864 (0.3%)
3	k	0.82	0/1379	1.05	7/1864 (0.4%)
3	l	0.81	0/1379	1.01	6/1864 (0.3%)
3	m	0.85	1/1379 (0.1%)	1.03	4/1864 (0.2%)
3	n	0.87	0/1379	1.10	12/1864 (0.6%)
All	All	0.85	15/41273 (0.0%)	1.07	200/55737 (0.4%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	26	SER	CB-OG	-9.46	1.29	1.42
3	N	179	GLU	CD-OE2	-7.57	1.17	1.25
1	e	94	GLN	CG-CD	-7.03	1.34	1.51
1	c	205	GLU	CD-OE2	-6.52	1.18	1.25
1	e	151	GLU	CD-OE1	-6.52	1.18	1.25

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	99	ASP	CB-CG-OD1	-19.46	100.79	118.30
1	c	99	ASP	CB-CG-OD2	18.03	134.53	118.30
1	g	99	ASP	CB-CG-OD1	-15.39	104.45	118.30
1	g	99	ASP	CB-CG-OD2	15.32	132.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	94	GLN	CA-CB-CG	-14.42	81.67	113.40

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	1508	0	1520	52	0
1	B	1534	0	1545	72	0
1	C	1508	0	1520	60	0
1	D	1508	0	1520	58	0
1	E	1534	0	1545	63	1
1	F	1508	0	1517	54	0
1	G	1502	0	1515	48	0
1	a	1513	0	1525	0	0
1	b	1534	0	1545	0	0
1	c	1513	0	1525	0	0
1	d	1508	0	1520	0	0
1	e	1534	0	1545	0	0
1	f	1508	0	1520	0	0
1	g	1508	0	1520	0	0
2	1	25	0	27	4	0
2	2	25	0	27	2	0
2	3	25	0	27	4	0
2	4	25	0	27	2	0
2	O	25	0	27	4	0
2	P	25	0	27	11	0
2	Q	25	0	27	4	0
2	R	25	0	27	5	0
2	S	25	0	27	8	0
2	T	25	0	27	1	0
2	U	25	0	27	5	0
2	V	25	0	27	4	0
2	W	25	0	27	2	0
2	X	25	0	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	25	0	27	3	0
2	Z	25	0	27	3	0
2	o	25	0	27	0	0
2	p	25	0	27	0	0
2	q	25	0	27	0	0
2	r	25	0	27	0	0
2	s	25	0	27	0	0
2	t	25	0	27	0	0
2	u	25	0	27	0	0
2	v	25	0	27	0	0
2	w	25	0	27	0	0
2	x	25	0	27	0	0
2	y	25	0	27	0	0
2	z	25	0	27	0	0
3	H	1357	0	1349	37	1
3	I	1357	0	1349	39	0
3	J	1357	0	1349	35	0
3	K	1357	0	1349	37	0
3	L	1357	0	1349	39	0
3	M	1357	0	1349	29	0
3	N	1362	0	1354	49	0
3	h	1357	0	1349	0	0
3	i	1357	0	1349	0	0
3	j	1357	0	1349	0	0
3	k	1357	0	1349	0	0
3	l	1357	0	1349	0	0
3	m	1357	0	1349	0	0
3	n	1357	0	1349	0	0
4	A	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	G	2	0	0	1	0
4	H	2	0	0	1	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
4	K	2	0	0	2	0
4	L	2	0	0	0	0
4	M	3	0	0	3	0
4	N	2	0	0	0	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c	1	0	0	0	0
4	d	2	0	0	0	0
4	e	1	0	0	0	0
4	h	4	0	0	0	0
4	i	3	0	0	0	0
4	j	3	0	0	0	0
4	k	6	0	0	0	0
4	l	2	0	0	0	0
4	m	4	0	0	0	0
4	n	3	0	0	0	0
All	All	40976	0	41029	528	1

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 528 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)
3:I:159:GLY:O	3:L:191:THR:HG21	93.36	1.34
1:E:98:ALA:O	1:F:208:LYS:HE2	1.40	1.17
3:I:159:GLY:O	3:L:191:THR:CG2	92.56	1.10
1:C:142:VAL:HG22	3:J:130:THR:CG2	3.52	1.07
1:E:97:ARG:C	1:F:208:LYS:CE	2.24	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ASP:OD1	3:H:152:ARG:NH1[4_546]	2.07	0.13

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	194/214 (91%)	187 (96%)	6 (3%)	1 (0%)	34	72
1	B	198/214 (92%)	191 (96%)	5 (2%)	2 (1%)	19	58
1	C	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
1	D	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	34	72
1	E	198/214 (92%)	190 (96%)	6 (3%)	2 (1%)	19	58
1	F	194/214 (91%)	187 (96%)	5 (3%)	2 (1%)	19	58
1	G	193/214 (90%)	186 (96%)	6 (3%)	1 (0%)	34	72
1	a	195/214 (91%)	189 (97%)	5 (3%)	1 (0%)	34	72
1	b	198/214 (92%)	189 (96%)	6 (3%)	3 (2%)	13	47
1	c	195/214 (91%)	189 (97%)	4 (2%)	2 (1%)	19	58
1	d	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
1	e	198/214 (92%)	188 (95%)	8 (4%)	2 (1%)	19	58
1	f	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	34	72
1	g	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
2	1	1/3 (33%)	1 (100%)	0	0	100	100
2	2	1/3 (33%)	1 (100%)	0	0	100	100
2	3	1/3 (33%)	1 (100%)	0	0	100	100
2	4	1/3 (33%)	1 (100%)	0	0	100	100
2	O	1/3 (33%)	1 (100%)	0	0	100	100
2	P	1/3 (33%)	1 (100%)	0	0	100	100
2	Q	1/3 (33%)	1 (100%)	0	0	100	100
2	R	1/3 (33%)	1 (100%)	0	0	100	100
2	S	1/3 (33%)	1 (100%)	0	0	100	100
2	T	1/3 (33%)	1 (100%)	0	0	100	100
2	U	1/3 (33%)	1 (100%)	0	0	100	100
2	V	1/3 (33%)	1 (100%)	0	0	100	100
2	W	1/3 (33%)	1 (100%)	0	0	100	100
2	X	1/3 (33%)	1 (100%)	0	0	100	100
2	Y	1/3 (33%)	1 (100%)	0	0	100	100
2	Z	1/3 (33%)	1 (100%)	0	0	100	100
2	o	1/3 (33%)	1 (100%)	0	0	100	100
2	p	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	1/3 (33%)	0	1 (100%)	0	100	100
2	r	1/3 (33%)	1 (100%)	0	0	100	100
2	s	1/3 (33%)	1 (100%)	0	0	100	100
2	t	1/3 (33%)	1 (100%)	0	0	100	100
2	u	1/3 (33%)	1 (100%)	0	0	100	100
2	v	1/3 (33%)	1 (100%)	0	0	100	100
2	w	1/3 (33%)	1 (100%)	0	0	100	100
2	x	1/3 (33%)	1 (100%)	0	0	100	100
2	y	1/3 (33%)	1 (100%)	0	0	100	100
2	z	1/3 (33%)	1 (100%)	0	0	100	100
3	H	176/200 (88%)	169 (96%)	7 (4%)	0	100	100
3	I	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	J	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	K	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	L	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	M	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	N	177/200 (88%)	170 (96%)	7 (4%)	0	100	100
3	h	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	i	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	j	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	k	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	l	176/200 (88%)	169 (96%)	7 (4%)	0	100	100
3	m	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	n	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
All	All	5226/5880 (89%)	5047 (97%)	155 (3%)	24 (0%)	34	72

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	209	LEU
1	B	48	VAL
1	E	48	VAL
1	G	48	VAL
1	b	48	VAL

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	163/178 (92%)	142 (87%)	21 (13%)	5	21
1	B	165/178 (93%)	142 (86%)	23 (14%)	4	19
1	C	163/178 (92%)	140 (86%)	23 (14%)	4	18
1	D	163/178 (92%)	141 (86%)	22 (14%)	5	20
1	E	165/178 (93%)	145 (88%)	20 (12%)	6	24
1	F	163/178 (92%)	137 (84%)	26 (16%)	3	13
1	G	162/178 (91%)	143 (88%)	19 (12%)	7	26
1	a	163/178 (92%)	143 (88%)	20 (12%)	6	23
1	b	165/178 (93%)	140 (85%)	25 (15%)	3	15
1	c	163/178 (92%)	142 (87%)	21 (13%)	5	21
1	d	163/178 (92%)	142 (87%)	21 (13%)	5	21
1	e	165/178 (93%)	145 (88%)	20 (12%)	6	24
1	f	163/178 (92%)	143 (88%)	20 (12%)	6	23
1	g	163/178 (92%)	142 (87%)	21 (13%)	5	21
2	1	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	2	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	3	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	4	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	O	2/2 (100%)	2 (100%)	0	100	100
2	P	2/2 (100%)	0	2 (100%)	0	0
2	Q	2/2 (100%)	2 (100%)	0	100	100
2	R	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	S	2/2 (100%)	0	2 (100%)	0	0
2	T	2/2 (100%)	0	2 (100%)	0	0
2	U	2/2 (100%)	2 (100%)	0	100	100
2	V	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	2/2 (100%)	2 (100%)	0	100	100
2	X	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	Y	2/2 (100%)	2 (100%)	0	100	100
2	Z	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	o	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	p	2/2 (100%)	0	2 (100%)	0	0
2	q	2/2 (100%)	0	2 (100%)	0	0
2	r	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	s	2/2 (100%)	0	2 (100%)	0	0
2	t	2/2 (100%)	2 (100%)	0	100	100
2	u	2/2 (100%)	0	2 (100%)	0	0
2	v	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	w	2/2 (100%)	2 (100%)	0	100	100
2	x	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	y	2/2 (100%)	2 (100%)	0	100	100
2	z	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	H	139/157 (88%)	117 (84%)	22 (16%)	3	13
3	I	139/157 (88%)	121 (87%)	18 (13%)	5	21
3	J	139/157 (88%)	119 (86%)	20 (14%)	4	17
3	K	139/157 (88%)	114 (82%)	25 (18%)	2	9
3	L	139/157 (88%)	120 (86%)	19 (14%)	4	19
3	M	139/157 (88%)	117 (84%)	22 (16%)	3	13
3	N	139/157 (88%)	121 (87%)	18 (13%)	5	21
3	h	139/157 (88%)	115 (83%)	24 (17%)	2	11
3	i	139/157 (88%)	116 (84%)	23 (16%)	3	12
3	j	139/157 (88%)	121 (87%)	18 (13%)	5	21
3	k	139/157 (88%)	117 (84%)	22 (16%)	3	13
3	l	139/157 (88%)	116 (84%)	23 (16%)	3	12
3	m	139/157 (88%)	115 (83%)	24 (17%)	2	11
3	n	139/157 (88%)	118 (85%)	21 (15%)	3	15
All	All	4291/4746 (90%)	3663 (85%)	628 (15%)	4	16

5 of 628 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	129	VAL
1	b	188	ILE
2	z	803	LEU
3	N	19	SER
1	a	110	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	124	GLN
3	N	124	GLN
3	m	37	ASN
3	M	37	ASN
3	N	37	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 ⓘ

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	196/214 (91%)	-0.16	0 100 100	51, 66, 90, 117	0
1	B	200/214 (93%)	-0.20	0 100 100	48, 64, 93, 118	0
1	C	196/214 (91%)	-0.16	0 100 100	46, 60, 88, 101	0
1	D	196/214 (91%)	-0.25	0 100 100	48, 60, 82, 102	0
1	E	200/214 (93%)	-0.12	0 100 100	48, 65, 92, 141	0
1	F	196/214 (91%)	0.00	0 100 100	57, 75, 92, 115	0
1	G	195/214 (91%)	-0.03	0 100 100	55, 72, 93, 107	0
1	a	197/214 (92%)	-0.14	0 100 100	52, 63, 91, 112	0
1	b	200/214 (93%)	-0.20	0 100 100	50, 63, 93, 124	0
1	c	197/214 (92%)	-0.21	0 100 100	50, 67, 92, 110	0
1	d	196/214 (91%)	-0.21	0 100 100	48, 64, 91, 113	0
1	e	200/214 (93%)	-0.13	0 100 100	47, 65, 93, 125	0
1	f	196/214 (91%)	-0.08	0 100 100	48, 67, 91, 111	0
1	g	196/214 (91%)	-0.08	0 100 100	49, 66, 89, 109	0
2	1	2/3 (66%)	0.38	0 100 100	91, 91, 91, 97	0
2	2	2/3 (66%)	1.14	0 100 100	86, 86, 86, 112	0
2	3	2/3 (66%)	0.82	0 100 100	94, 94, 94, 100	0
2	4	2/3 (66%)	0.25	0 100 100	87, 87, 87, 88	0
2	O	2/3 (66%)	0.34	0 100 100	99, 99, 99, 99	0
2	P	2/3 (66%)	0.00	0 100 100	96, 96, 96, 101	0
2	Q	2/3 (66%)	-0.04	0 100 100	92, 92, 92, 95	0
2	R	2/3 (66%)	0.58	0 100 100	89, 89, 89, 95	0
2	S	2/3 (66%)	0.30	0 100 100	90, 90, 90, 112	0
2	T	2/3 (66%)	1.41	0 100 100	102, 102, 102, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	U	2/3 (66%)	0.43	0 100 100	93, 93, 93, 105	0
2	V	2/3 (66%)	-0.02	0 100 100	83, 83, 83, 89	0
2	W	2/3 (66%)	-0.12	0 100 100	76, 76, 76, 84	0
2	X	2/3 (66%)	0.38	0 100 100	82, 82, 82, 91	0
2	Y	2/3 (66%)	-0.24	0 100 100	85, 85, 85, 88	0
2	Z	2/3 (66%)	0.70	0 100 100	89, 89, 89, 103	0
2	o	2/3 (66%)	-0.13	0 100 100	98, 98, 98, 100	0
2	p	2/3 (66%)	0.09	0 100 100	95, 95, 95, 102	0
2	q	2/3 (66%)	0.40	0 100 100	97, 97, 97, 109	0
2	r	2/3 (66%)	0.49	0 100 100	91, 91, 91, 100	0
2	s	2/3 (66%)	0.32	0 100 100	89, 89, 89, 98	0
2	t	2/3 (66%)	0.97	0 100 100	98, 98, 98, 105	0
2	u	2/3 (66%)	0.41	0 100 100	98, 98, 98, 108	0
2	v	2/3 (66%)	-0.22	0 100 100	82, 82, 82, 88	0
2	w	2/3 (66%)	-0.23	0 100 100	88, 88, 88, 89	0
2	x	2/3 (66%)	0.28	0 100 100	77, 77, 77, 97	0
2	y	2/3 (66%)	-0.13	0 100 100	88, 88, 88, 90	0
2	z	2/3 (66%)	1.03	0 100 100	80, 80, 80, 95	0
3	H	178/200 (89%)	-0.15	0 100 100	46, 61, 82, 117	0
3	I	178/200 (89%)	-0.16	0 100 100	44, 54, 81, 121	0
3	J	178/200 (89%)	-0.18	0 100 100	48, 53, 82, 96	0
3	K	178/200 (89%)	0.00	0 100 100	45, 60, 87, 116	0
3	L	178/200 (89%)	-0.01	0 100 100	51, 71, 95, 104	0
3	M	178/200 (89%)	0.08	0 100 100	53, 73, 91, 114	0
3	N	179/200 (89%)	-0.10	0 100 100	48, 67, 88, 110	0
3	h	178/200 (89%)	-0.15	0 100 100	46, 64, 86, 113	0
3	i	178/200 (89%)	-0.11	0 100 100	48, 67, 92, 118	0
3	j	178/200 (89%)	-0.10	0 100 100	49, 65, 94, 116	0
3	k	178/200 (89%)	-0.09	0 100 100	48, 61, 84, 101	0
3	l	178/200 (89%)	-0.09	0 100 100	46, 59, 80, 100	0
3	m	178/200 (89%)	-0.18	0 100 100	44, 58, 82, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	n	178/200 (89%)	-0.06	0 100 100	45, 59, 85, 126	0
All	All	5310/5880 (90%)	-0.11	0 100 100	44, 64, 91, 141	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.