



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:12 AM UTC

PDB ID : 5DZK / pdb_00005dzk
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

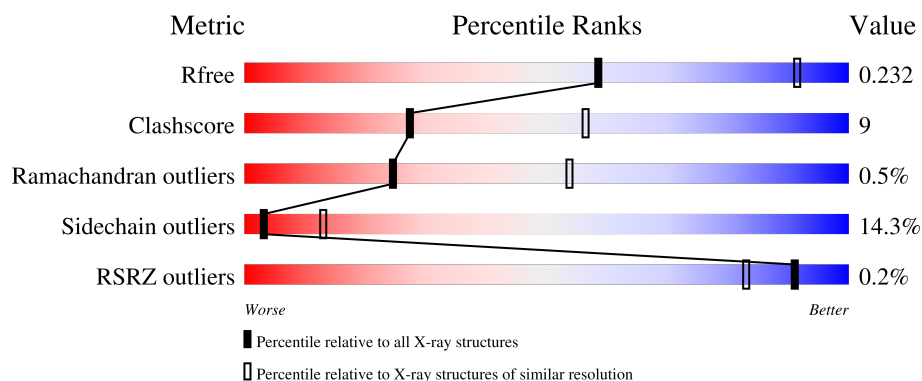
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



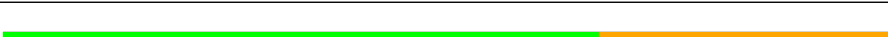
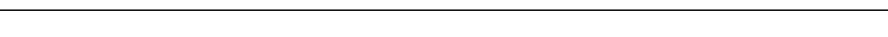
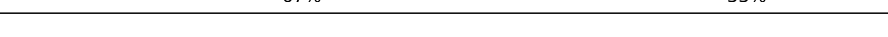
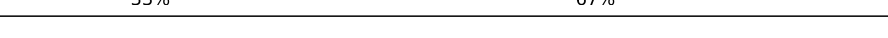
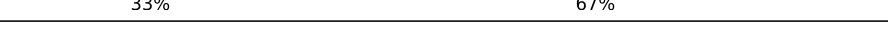
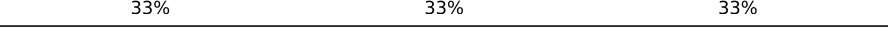
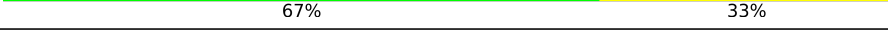
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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 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	214	 66% 20% 6% 8%
1	B	214	 66% 19% 8% 7%
1	C	214	 64% 20% 8% 8%
1	D	214	 65% 21% 8% 8%
1	E	214	 68% 19% 7% 7%

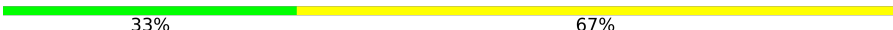
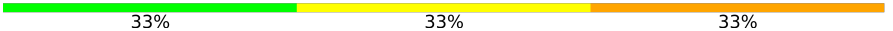
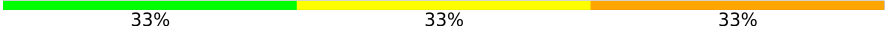
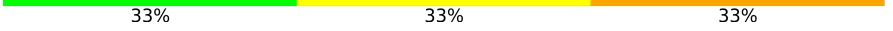
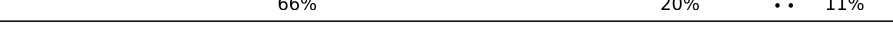
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Mol	Chain	Length	Quality of chain
1	F	214	
1	G	214	
1	a	214	
1	b	214	
1	c	214	
1	d	214	
1	e	214	
1	f	214	
1	g	214	
2	1	3	
2	2	3	
2	3	3	
2	4	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	
2	T	3	
2	U	3	
2	V	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	

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Mol	Chain	Length	Quality of chain
2	o	3	 33% 67%
2	p	3	 33% 67%
2	q	3	 33% 33% 33%
2	r	3	 33% 33% 33%
2	s	3	 33% 67%
2	t	3	 67% 33%
2	u	3	 33% 33% 33%
2	v	3	 33% 67%
2	w	3	 67% 33%
2	x	3	 67% 33%
2	y	3	 67% 33%
2	z	3	 67% 33%
3	H	200	 68% 16% . . 11%
3	I	200	 66% 20% . . 11%
3	J	200	 66% 20% . 11%
3	K	200	 66% 18% . . 11%
3	L	200	 65% 20% . . 11%
3	M	200	 68% 17% . 11%
3	N	200	 66% 20% . 10%
3	h	200	 70% 14% . 11%
3	i	200	 67% 18% . . 11%
3	j	200	 68% 16% . 11%
3	k	200	 70% 14% . . 11%
3	l	200	 65% 20% . 11%
3	m	200	 70% 15% . 11%

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Mol	Chain	Length	Quality of chain
3	n	200	66% 18% • • 11%

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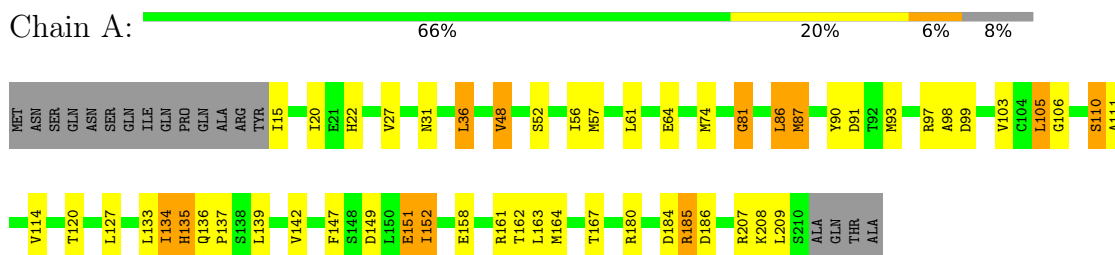
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	i	3	Total 3	O 3	0	0
4	j	3	Total 3	O 3	0	0
4	k	6	Total 6	O 6	0	0
4	l	2	Total 2	O 2	0	0
4	m	4	Total 4	O 4	0	0
4	n	3	Total 3	O 3	0	0

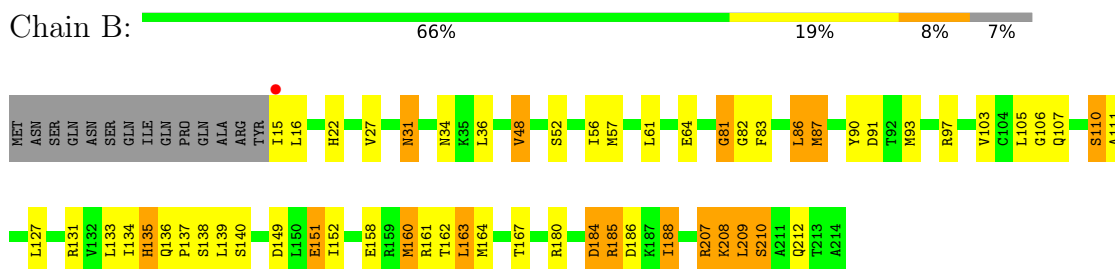
3 Residue-property plots [i](#)

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.

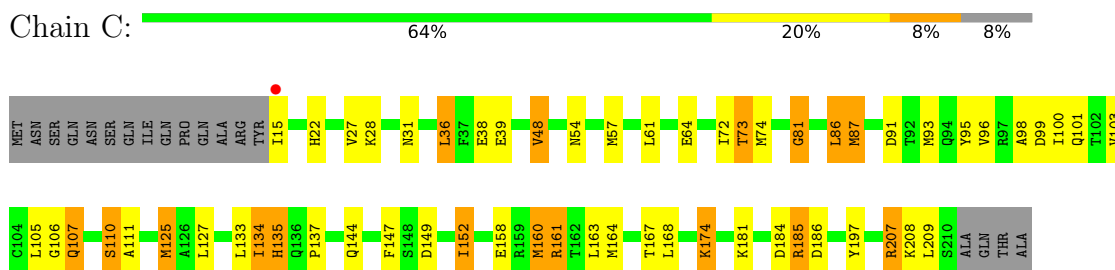
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



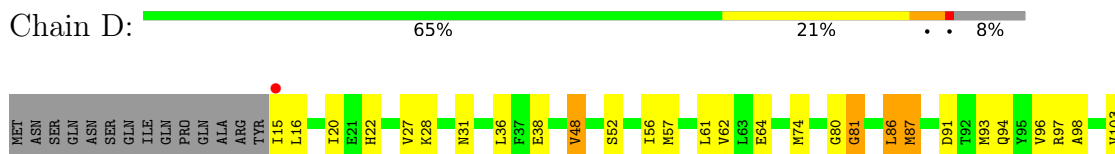
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



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



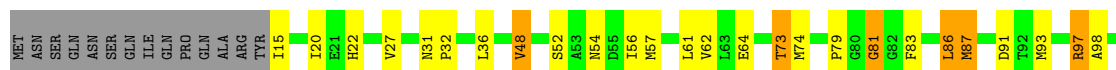
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2





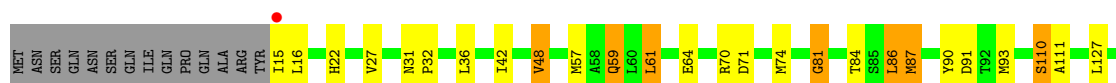
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E: 68% 19% 7% 7%



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

Chain F: 67% 17% 6% 8%



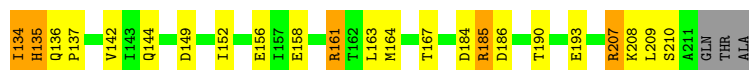
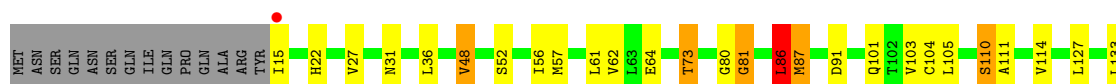
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain G: 67% 18% 6% 9%



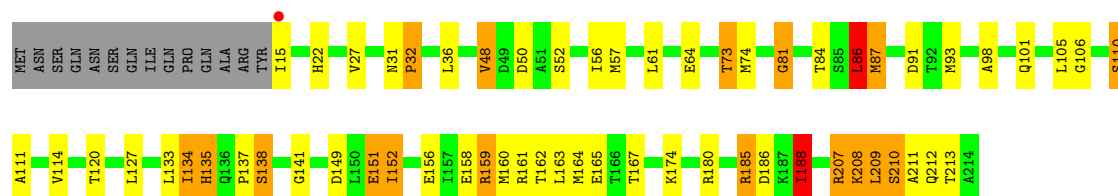
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain a: 69% 18% 5% 8%



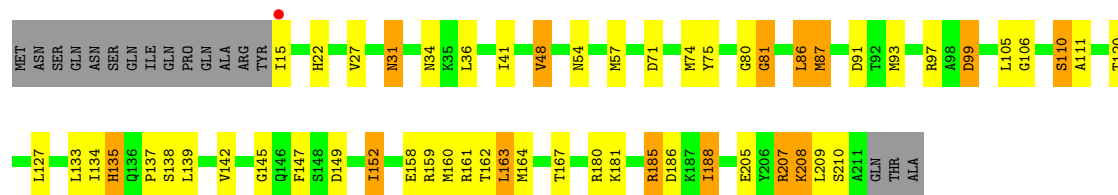
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain b: 65% 20% 8% 7%



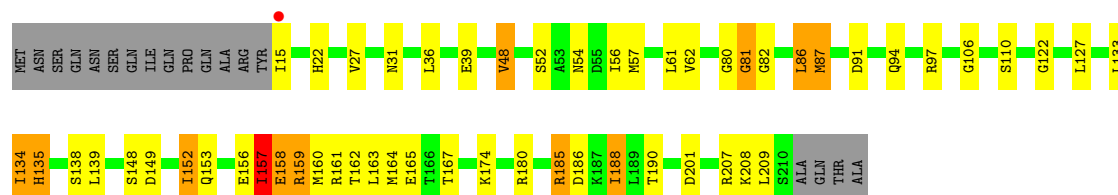
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain c: 66% 20% 7% 8%



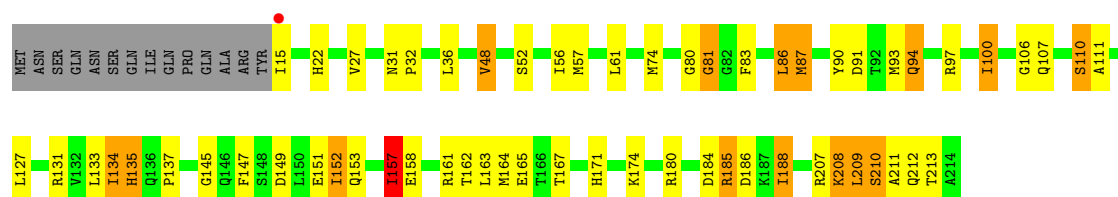
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain d: 66% 20% 5% 8%



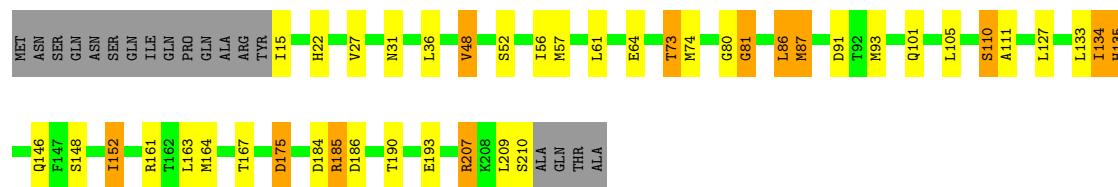
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain e: 65% 21% 7% 7%

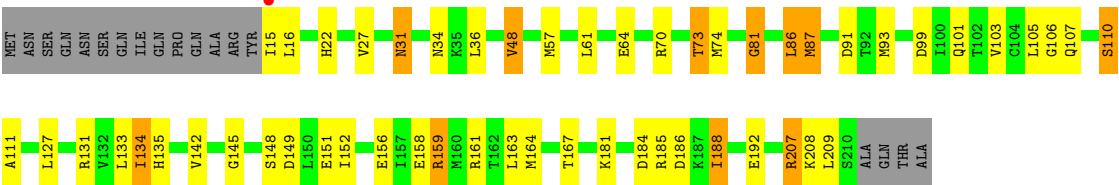
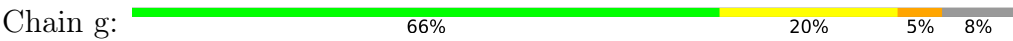


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f: 71% 14% 6% 8%



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



● Molecule 2: BEZ-LEU-LEU



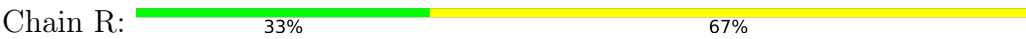
● Molecule 2: BEZ-LEU-LEU



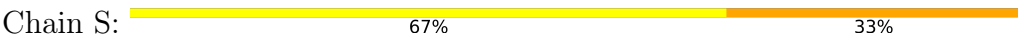
● Molecule 2: BEZ-LEU-LEU



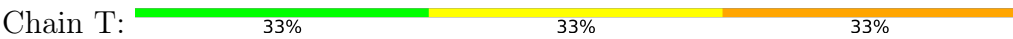
● Molecule 2: BEZ-LEU-LEU



● Molecule 2: BEZ-LEU-LEU



● Molecule 2: BEZ-LEU-LEU



• Molecule 2: BEZ-LEU-LEU

Chain U:  67% 33%

• Molecule 2: BEZ-LEU-LEU

Chain V:  67% 33%

• Molecule 2: BEZ-LEU-LEU

Chain W:  67% 33%

• Molecule 2: BEZ-LEU-LEU

Chain X:  33% 67%

• Molecule 2: BEZ-LEU-LEU

Chain Y:  67% 33%

• Molecule 2: BEZ-LEU-LEU

Chain Z:  67% 33%

• Molecule 2: BEZ-LEU-LEU

Chain 1:  33% 67%

• Molecule 2: BEZ-LEU-LEU

Chain 2:  67% 33%



• Molecule 2: BEZ-LEU-LEU

Chain o:  33% 67%



• 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:  33% 33% 33%



• Molecule 2: BEZ-LEU-LEU

Chain s:  33% 67%



• Molecule 2: BEZ-LEU-LEU

Chain t:  67% 33%

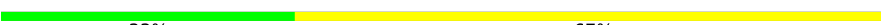


• Molecule 2: BEZ-LEU-LEU

Chain u:  33% 33% 33%



- Molecule 2: BEZ-LEU-LEU

Chain v:  33% 67%



- Molecule 2: BEZ-LEU-LEU

Chain w:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain x:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain y:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain z:  67% 33%



- Molecule 2: BEZ-LEU-LEU

Chain 3:  67% 33%



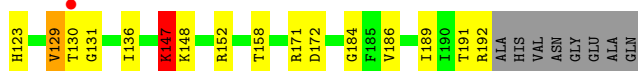
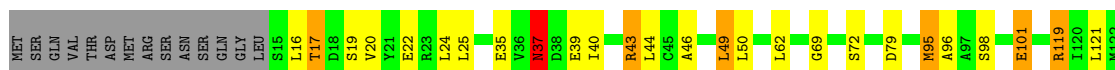
- Molecule 2: BEZ-LEU-LEU

Chain 4:  67% 33%



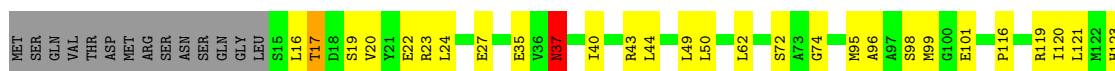
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain H: 68% 16% 11%



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

Chain I: 66% 20% 11%



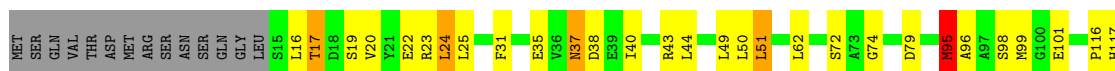
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain J: 66% 20% 11%



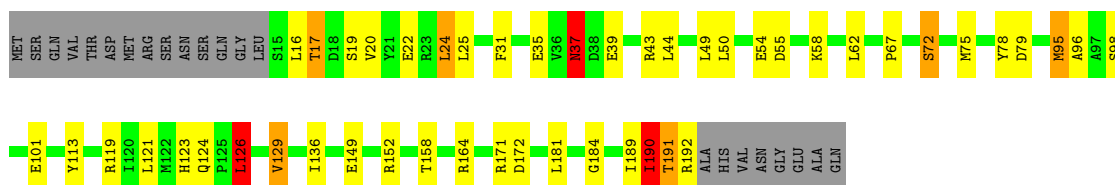
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain K: 66% 18% 11%

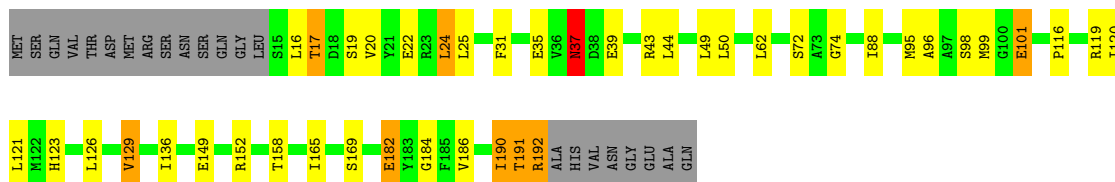


- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

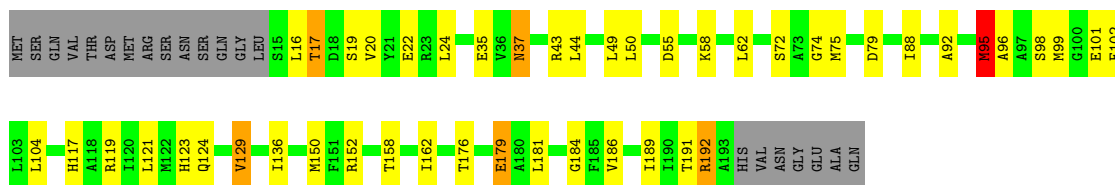
Chain L: 65% 20% 11%



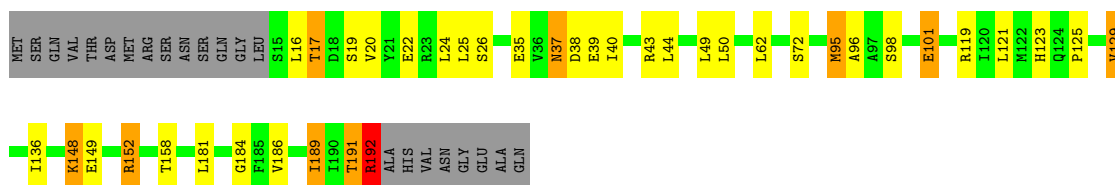
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



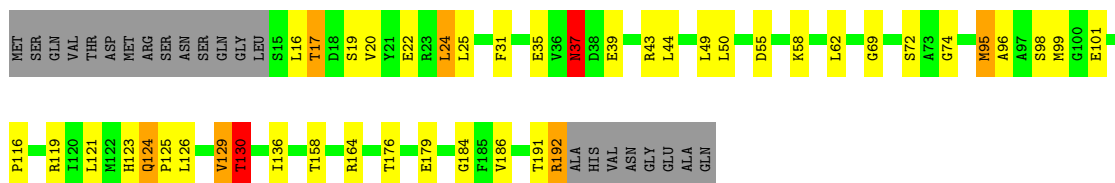
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



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

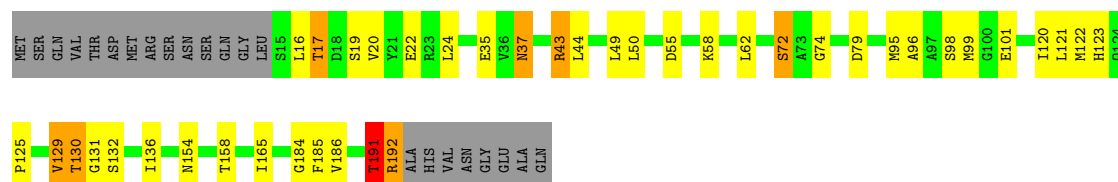


- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



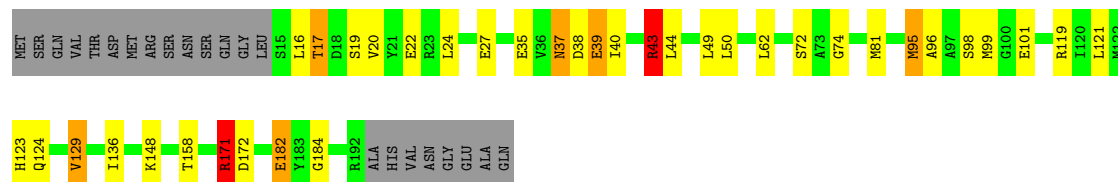
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1





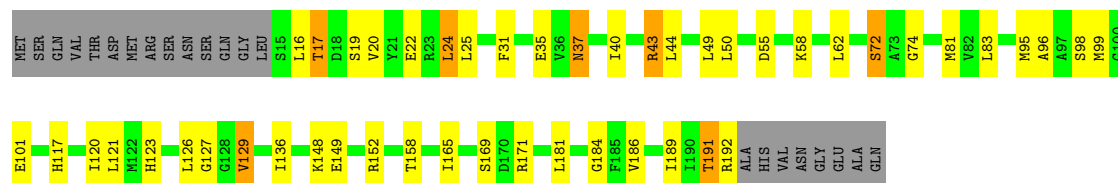
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain k: 70% 14% 11%



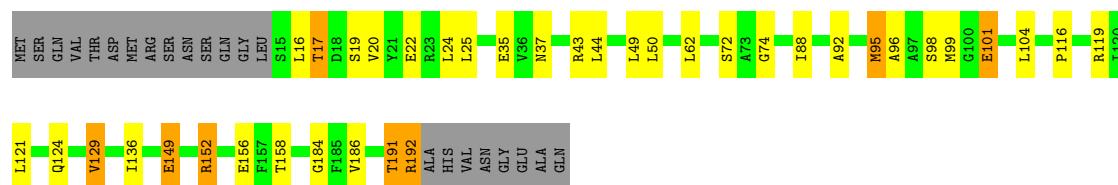
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain l: 65% 20% 11%



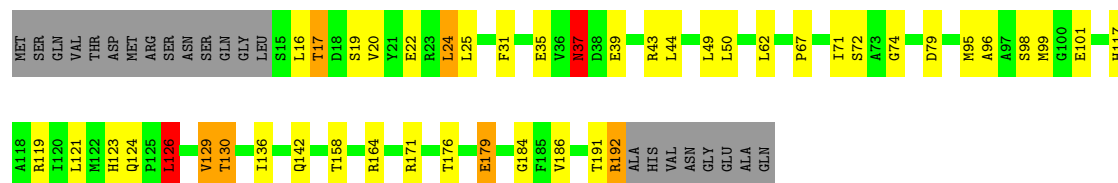
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain m: 70% 15% 11%



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

Chain n: 66% 18% 11%



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 72.24 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.2 (72.24-3.07) 93.2 (72.24-3.07)	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 (4.69%)	wwPDB-VP
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 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	1.21	0/1529	1.29	8/2068 (0.4%)
1	B	1.20	1/1555 (0.1%)	1.27	6/2104 (0.3%)
1	C	1.24	1/1529 (0.1%)	1.30	9/2068 (0.4%)
1	D	1.30	5/1529 (0.3%)	1.31	10/2068 (0.5%)
1	E	1.28	2/1555 (0.1%)	1.25	4/2104 (0.2%)
1	F	1.22	4/1529 (0.3%)	1.30	7/2068 (0.3%)
1	G	1.23	2/1523 (0.1%)	1.25	4/2060 (0.2%)
1	a	1.24	3/1534 (0.2%)	1.26	5/2075 (0.2%)
1	b	1.25	2/1555 (0.1%)	1.33	11/2104 (0.5%)
1	c	1.28	3/1534 (0.2%)	1.32	11/2075 (0.5%)
1	d	1.22	3/1529 (0.2%)	1.28	10/2068 (0.5%)
1	e	1.28	7/1555 (0.5%)	1.37	15/2104 (0.7%)
1	f	1.23	1/1529 (0.1%)	1.28	5/2068 (0.2%)
1	g	1.24	3/1529 (0.2%)	1.28	8/2068 (0.4%)
2	1	0.93	0/16	1.23	0/19
2	2	1.10	0/16	1.20	0/19
2	3	0.65	0/16	1.20	0/19
2	4	0.91	0/16	1.42	0/19
2	O	0.92	0/16	0.87	0/19
2	P	0.73	0/16	1.52	0/19
2	Q	0.70	0/16	1.08	0/19
2	R	0.84	0/16	1.28	0/19
2	S	0.47	0/16	1.60	0/19
2	T	0.99	0/16	1.04	0/19
2	U	0.73	0/16	0.87	0/19
2	V	0.62	0/16	1.48	0/19
2	W	1.06	0/16	1.11	0/19
2	X	0.83	0/16	0.86	0/19
2	Y	1.02	0/16	1.02	0/19
2	Z	1.35	0/16	1.52	0/19
2	o	0.68	0/16	1.54	0/19
2	p	0.58	0/16	1.24	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q	0.46	0/16	1.65	0/19
2	r	0.98	0/16	1.21	0/19
2	s	0.80	0/16	1.63	0/19
2	t	0.60	0/16	1.20	0/19
2	u	0.66	0/16	1.55	0/19
2	v	0.74	0/16	1.06	0/19
2	w	0.86	0/16	1.05	0/19
2	x	0.78	0/16	1.39	0/19
2	y	1.01	0/16	1.31	0/19
2	z	0.92	0/16	1.67	0/19
3	H	1.21	2/1379 (0.1%)	1.25	6/1864 (0.3%)
3	I	1.25	3/1379 (0.2%)	1.35	8/1864 (0.4%)
3	J	1.24	2/1379 (0.1%)	1.26	5/1864 (0.3%)
3	K	1.16	0/1379	1.23	3/1864 (0.2%)
3	L	1.17	1/1379 (0.1%)	1.23	4/1864 (0.2%)
3	M	1.13	1/1379 (0.1%)	1.24	6/1864 (0.3%)
3	N	1.14	0/1384	1.21	4/1871 (0.2%)
3	h	1.17	4/1379 (0.3%)	1.22	2/1864 (0.1%)
3	i	1.16	0/1379	1.26	6/1864 (0.3%)
3	j	1.15	1/1379 (0.1%)	1.31	8/1864 (0.4%)
3	k	1.18	1/1379 (0.1%)	1.23	4/1864 (0.2%)
3	l	1.17	1/1379 (0.1%)	1.21	3/1864 (0.2%)
3	m	1.18	0/1379	1.23	0/1864
3	n	1.21	0/1379	1.26	7/1864 (0.4%)
All	All	1.21	53/41273 (0.1%)	1.27	179/55737 (0.3%)

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	97	ARG	N-CA	7.49	1.55	1.46
1	G	80	GLY	C-O	-7.24	1.19	1.24
1	g	16	LEU	C-O	-7.14	1.19	1.25
1	e	94	GLN	CA-C	-6.92	1.43	1.52
1	e	94	GLN	CG-CD	-6.87	1.34	1.52

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	94	GLN	CA-CB-CG	-16.21	81.67	114.10
3	I	164	ARG	CB-CG-CD	11.72	138.25	111.30
3	h	26	SER	CB-CA-C	-11.70	88.98	110.63
3	I	163	GLU	CB-CG-CD	-11.32	93.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LEU	N-CA-C	-10.40	93.41	109.95

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	39	0
1	B	1534	0	1545	49	0
1	C	1508	0	1520	44	0
1	D	1508	0	1520	47	0
1	E	1534	0	1545	47	1
1	F	1508	0	1517	48	0
1	G	1502	0	1515	40	0
1	a	1513	0	1525	36	0
1	b	1534	0	1545	48	0
1	c	1513	0	1525	40	0
1	d	1508	0	1520	33	0
1	e	1534	0	1545	36	0
1	f	1508	0	1520	25	0
1	g	1508	0	1520	33	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	7	0
2	Q	25	0	27	4	0
2	R	25	0	27	2	0
2	S	25	0	27	5	0
2	T	25	0	27	1	0
2	U	25	0	27	5	0
2	V	25	0	27	2	0
2	W	25	0	27	2	0
2	X	25	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	25	0	27	1	0
2	Z	25	0	27	2	0
2	o	25	0	27	1	0
2	p	25	0	27	5	0
2	q	25	0	27	1	0
2	r	25	0	27	3	0
2	s	25	0	27	7	0
2	t	25	0	27	0	0
2	u	25	0	27	1	0
2	v	25	0	27	4	0
2	w	25	0	27	2	0
2	x	25	0	27	2	0
2	y	25	0	27	3	0
2	z	25	0	27	2	0
3	H	1357	0	1349	31	1
3	I	1357	0	1349	30	0
3	J	1357	0	1349	19	0
3	K	1357	0	1349	31	0
3	L	1357	0	1349	32	0
3	M	1357	0	1349	20	0
3	N	1362	0	1354	32	0
3	h	1357	0	1349	22	0
3	i	1357	0	1349	25	0
3	j	1357	0	1349	30	0
3	k	1357	0	1349	26	0
3	l	1357	0	1349	28	0
3	m	1357	0	1349	21	0
3	n	1357	0	1349	28	0
4	A	1	0	0	0	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	0	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
4	K	2	0	0	1	0
4	L	2	0	0	0	0
4	M	3	0	0	1	0
4	N	2	0	0	0	0
4	a	1	0	0	1	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	1	0
4	i	3	0	0	0	0
4	j	3	0	0	0	0
4	k	6	0	0	1	0
4	l	2	0	0	0	0
4	m	4	0	0	2	0
4	n	3	0	0	0	0
All	All	40976	0	41029	744	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 9.

The worst 5 of 744 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	1.21	1.34
1:E:98:ALA:O	1:F:208:LYS:HE2	1.40	1.17
1:E:97:ARG:C	1:F:208:LYS:CE	2.24	1.11
3:I:159:GLY:O	3:l:191:THR:CG2	2.00	1.10
1:c:142:VAL:HG22	3:j:130:THR:CG2	1.84	1.07

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%)	24	54
1	B	198/214 (92%)	191 (96%)	5 (2%)	2 (1%)	12	39
1	C	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	12	39
1	D	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	24	54
1	E	198/214 (92%)	190 (96%)	6 (3%)	2 (1%)	12	39
1	F	194/214 (91%)	187 (96%)	5 (3%)	2 (1%)	12	39
1	G	193/214 (90%)	186 (96%)	6 (3%)	1 (0%)	24	54
1	a	195/214 (91%)	189 (97%)	5 (3%)	1 (0%)	24	54
1	b	198/214 (92%)	189 (96%)	6 (3%)	3 (2%)	8	30
1	c	195/214 (91%)	189 (97%)	4 (2%)	2 (1%)	12	39
1	d	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	12	39
1	e	198/214 (92%)	188 (95%)	8 (4%)	2 (1%)	12	39
1	f	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	24	54
1	g	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	12	39
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%)	24	54

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%)	4	16
1	B	165/178 (93%)	140 (85%)	25 (15%)	3	11
1	C	163/178 (92%)	141 (86%)	22 (14%)	4	14
1	D	163/178 (92%)	143 (88%)	20 (12%)	4	18
1	E	165/178 (93%)	145 (88%)	20 (12%)	5	18
1	F	163/178 (92%)	139 (85%)	24 (15%)	3	12
1	G	162/178 (91%)	143 (88%)	19 (12%)	5	20
1	a	163/178 (92%)	142 (87%)	21 (13%)	4	16
1	b	165/178 (93%)	139 (84%)	26 (16%)	2	10
1	c	163/178 (92%)	144 (88%)	19 (12%)	5	20
1	d	163/178 (92%)	143 (88%)	20 (12%)	4	18
1	e	165/178 (93%)	142 (86%)	23 (14%)	3	14
1	f	163/178 (92%)	144 (88%)	19 (12%)	5	20
1	g	163/178 (92%)	142 (87%)	21 (13%)	4	16
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%)	1 (50%)	1 (50%)	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%)	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%)	1 (50%)	1 (50%)	0	0
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%)	118 (85%)	21 (15%)	3	12
3	I	139/157 (88%)	122 (88%)	17 (12%)	5	18
3	J	139/157 (88%)	120 (86%)	19 (14%)	3	14
3	K	139/157 (88%)	116 (84%)	23 (16%)	2	10
3	L	139/157 (88%)	120 (86%)	19 (14%)	3	14
3	M	139/157 (88%)	118 (85%)	21 (15%)	3	12
3	N	139/157 (88%)	122 (88%)	17 (12%)	5	18
3	h	139/157 (88%)	116 (84%)	23 (16%)	2	10
3	i	139/157 (88%)	118 (85%)	21 (15%)	3	12
3	j	139/157 (88%)	122 (88%)	17 (12%)	5	18
3	k	139/157 (88%)	118 (85%)	21 (15%)	3	12
3	l	139/157 (88%)	117 (84%)	22 (16%)	2	10
3	m	139/157 (88%)	116 (84%)	23 (16%)	2	10
3	n	139/157 (88%)	120 (86%)	19 (14%)	3	14
All	All	4291/4746 (90%)	3679 (86%)	612 (14%)	3	13

5 of 612 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	h	22	GLU
3	m	35	GLU
3	h	101	GLU
3	h	19	SER
3	j	186	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	31	ASN
1	d	31	ASN
3	n	124	GLN
3	k	124	GLN
1	a	59	GLN

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 oligosaccharides 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%)	-0.17	0 100 100	51, 66, 90, 117	0
1	B	200/214 (93%)	-0.16	1 (0%) 87 72	48, 64, 93, 118	0
1	C	196/214 (91%)	-0.18	1 (0%) 87 72	46, 60, 88, 100	0
1	D	196/214 (91%)	-0.25	1 (0%) 87 72	48, 60, 82, 102	0
1	E	200/214 (93%)	-0.21	0 100 100	48, 65, 92, 141	0
1	F	196/214 (91%)	-0.13	1 (0%) 87 72	57, 75, 92, 115	0
1	G	195/214 (91%)	-0.21	2 (1%) 79 59	55, 72, 93, 107	0
1	a	197/214 (92%)	-0.21	1 (0%) 87 72	52, 63, 91, 112	0
1	b	200/214 (93%)	-0.14	1 (0%) 87 72	50, 63, 93, 124	0
1	c	197/214 (92%)	-0.19	1 (0%) 87 72	50, 67, 92, 110	0
1	d	196/214 (91%)	-0.18	1 (0%) 87 72	48, 64, 91, 113	0
1	e	200/214 (93%)	-0.23	1 (0%) 87 72	47, 65, 93, 125	0
1	f	196/214 (91%)	-0.24	0 100 100	48, 67, 91, 111	0
1	g	196/214 (91%)	-0.27	1 (0%) 87 72	49, 66, 89, 109	0
2	1	2/3 (66%)	0.77	0 100 100	91, 91, 91, 97	0
2	2	2/3 (66%)	0.45	0 100 100	86, 86, 86, 112	0
2	3	2/3 (66%)	0.26	0 100 100	94, 94, 94, 100	0
2	4	2/3 (66%)	0.18	0 100 100	87, 87, 87, 88	0
2	O	2/3 (66%)	1.22	0 100 100	99, 99, 99, 99	0
2	P	2/3 (66%)	0.82	0 100 100	96, 96, 96, 101	0
2	Q	2/3 (66%)	0.72	0 100 100	92, 92, 92, 95	0
2	R	2/3 (66%)	-0.02	0 100 100	89, 89, 89, 95	0
2	S	2/3 (66%)	0.56	0 100 100	90, 90, 90, 112	0
2	T	2/3 (66%)	0.69	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%)	0.37	0 100 100	93, 93, 93, 105	0
2	V	2/3 (66%)	0.39	0 100 100	83, 83, 83, 89	0
2	W	2/3 (66%)	0.07	0 100 100	76, 76, 76, 84	0
2	X	2/3 (66%)	0.54	0 100 100	82, 82, 82, 91	0
2	Y	2/3 (66%)	0.13	0 100 100	85, 85, 85, 88	0
2	Z	2/3 (66%)	0.15	0 100 100	89, 89, 89, 103	0
2	o	2/3 (66%)	0.44	0 100 100	98, 98, 98, 100	0
2	p	2/3 (66%)	0.88	0 100 100	95, 95, 95, 102	0
2	q	2/3 (66%)	0.73	0 100 100	97, 97, 97, 109	0
2	r	2/3 (66%)	1.30	0 100 100	91, 91, 91, 100	0
2	s	2/3 (66%)	0.68	0 100 100	89, 89, 89, 98	0
2	t	2/3 (66%)	0.44	0 100 100	98, 98, 98, 105	0
2	u	2/3 (66%)	0.96	0 100 100	98, 98, 98, 108	0
2	v	2/3 (66%)	0.40	0 100 100	82, 82, 82, 88	0
2	w	2/3 (66%)	0.25	0 100 100	88, 88, 88, 89	0
2	x	2/3 (66%)	0.63	0 100 100	77, 77, 77, 97	0
2	y	2/3 (66%)	0.08	0 100 100	88, 88, 88, 90	0
2	z	2/3 (66%)	0.80	0 100 100	80, 80, 80, 95	0
3	H	178/200 (89%)	-0.24	1 (0%) 85 69	46, 61, 82, 117	0
3	I	178/200 (89%)	-0.25	0 100 100	44, 54, 81, 121	0
3	J	178/200 (89%)	-0.28	0 100 100	48, 53, 82, 96	0
3	K	178/200 (89%)	-0.24	0 100 100	45, 60, 87, 116	0
3	L	178/200 (89%)	-0.16	0 100 100	51, 71, 95, 104	0
3	M	178/200 (89%)	-0.16	0 100 100	53, 73, 91, 114	0
3	N	179/200 (89%)	-0.25	0 100 100	48, 67, 88, 110	0
3	h	178/200 (89%)	-0.29	0 100 100	46, 64, 86, 113	0
3	i	178/200 (89%)	-0.24	0 100 100	48, 67, 92, 118	0
3	j	178/200 (89%)	-0.29	0 100 100	49, 65, 94, 116	0
3	k	178/200 (89%)	-0.36	0 100 100	48, 61, 84, 101	0
3	l	178/200 (89%)	-0.29	0 100 100	46, 59, 80, 100	0
3	m	178/200 (89%)	-0.41	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%)	-0.40	0 100 100	45, 59, 85, 126	0
All	All	5310/5880 (90%)	-0.23	13 (0%) 91 83	44, 64, 91, 141	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	ILE	2.9
3	H	130	THR	2.8
1	a	15	ILE	2.8
1	g	15	ILE	2.6
1	G	209	LEU	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.