wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 11:40 AM 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

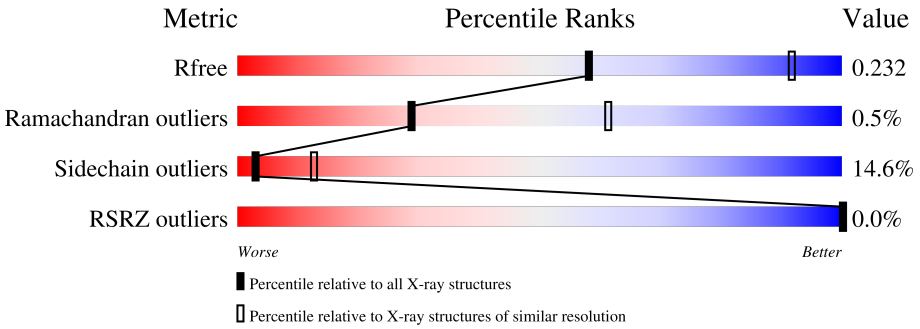
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	1447 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (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 <=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	79% 10% • 8%
1	B	214	79% 13% • 7%
1	C	214	78% 13% • 8%
1	D	214	79% 13% 8%
1	E	214	82% 11% 7%
1	F	214	76% 14% • 8%
1	G	214	80% 11% 9%

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Mol	Chain	Length	Quality of chain
1	a	214	82% 9% • 8%
1	b	214	79% 14% • 7%
1	c	214	78% 14% 8%
1	d	214	79% 11% • 8%
1	e	214	80% 12% • 7%
1	f	214	80% 12% 8%
1	g	214	78% 14% 8%
2	1	3	67% 33%
2	2	3	33% 67% 33%
2	3	3	67% 33%
2	4	3	67% 33%
2	O	3	100%
2	P	3	33% 67%
2	Q	3	100%
2	R	3	67% 33%
2	S	3	33% 33% 33%
2	T	3	33% 67%
2	U	3	100%
2	V	3	67% 33%
2	W	3	100%
2	X	3	67% 33%
2	Y	3	100%
2	Z	3	67% 33%
2	o	3	67% 33%
2	p	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	q	3	33% 33% 33%
2	r	3	67% 33%
2	s	3	33% 67%
2	t	3	100%
2	u	3	33% 67%
2	v	3	67% 33%
2	w	3	100%
2	x	3	33% 67%
2	y	3	100%
2	z	3	67% 33%
3	H	200	76% 12% • 11%
3	I	200	77% 11% • 11%
3	J	200	78% 10% • 11%
3	K	200	76% 10% • 11%
3	L	200	78% 10% • 11%
3	M	200	75% 13% • 11%
3	N	200	80% 9% • 10%
3	h	200	76% 13% 11%
3	i	200	75% 13% • 11%
3	j	200	78% 10% 11%
3	k	200	76% 12% • 11%
3	l	200	76% 12% • 11%
3	m	200	76% 12% • 11%
3	n	200	76% 12% • 11%

2 Entry composition (i)

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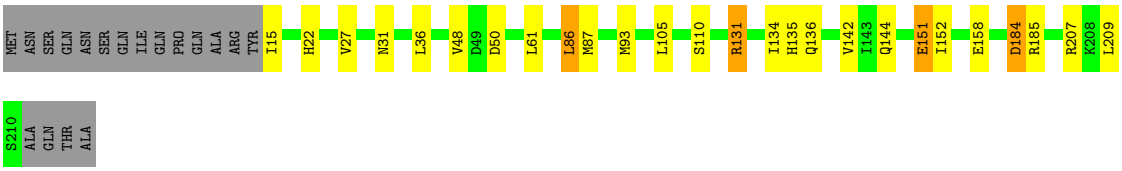
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	i	3	Total O 3 3	0	0
4	j	3	Total O 3 3	0	0
4	k	6	Total O 6 6	0	0
4	l	2	Total O 2 2	0	0
4	m	4	Total O 4 4	0	0
4	n	3	Total O 3 3	0	0

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.

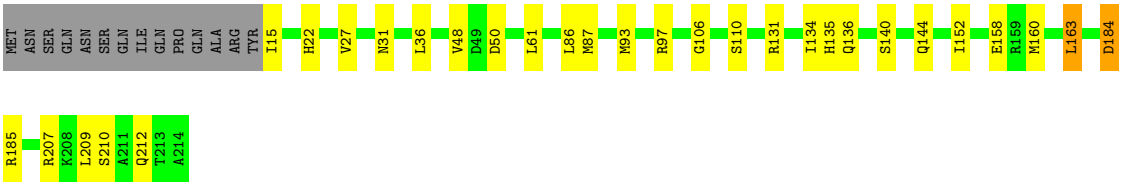
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A:



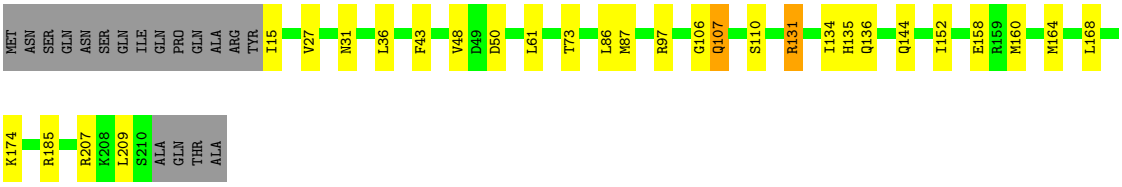
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



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

Chain C:



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

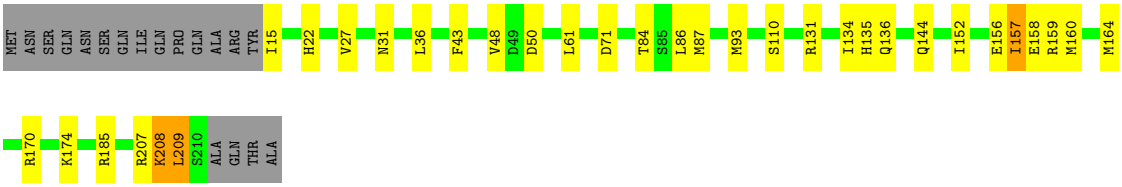
Chain D:

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

Chain E:

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

Chain F:



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

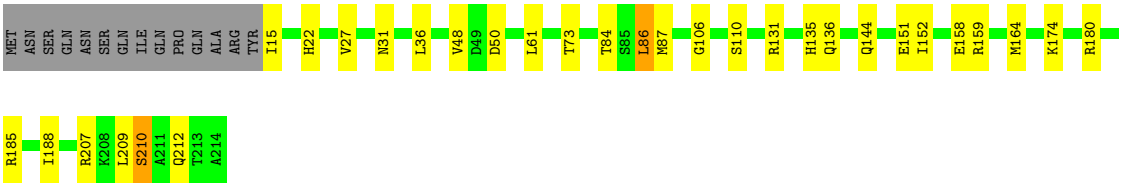
Chain G:

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

Chain a:

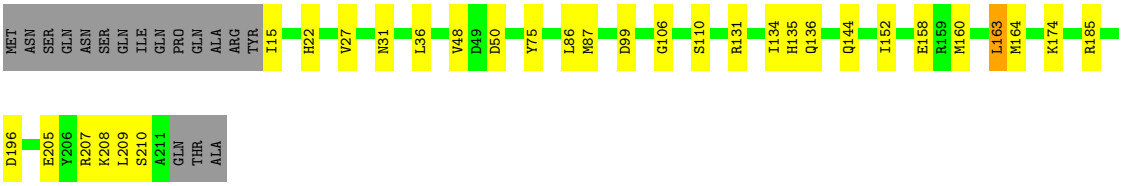
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain b:



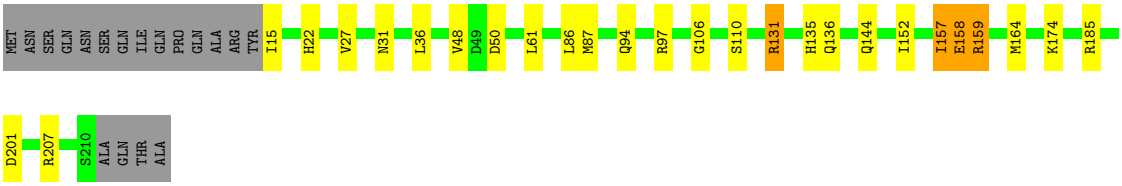
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain c:



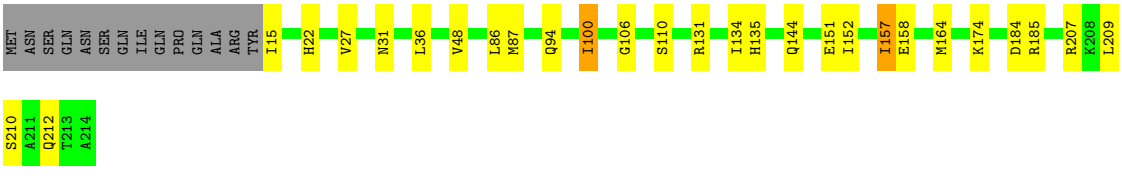
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain d:



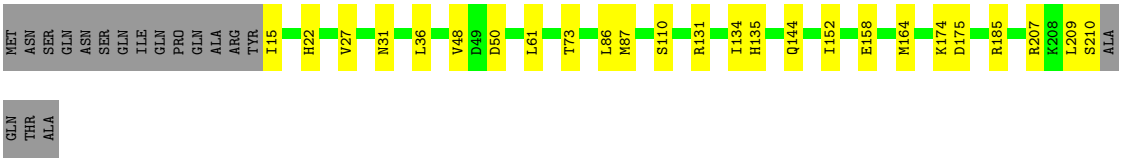
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain e:



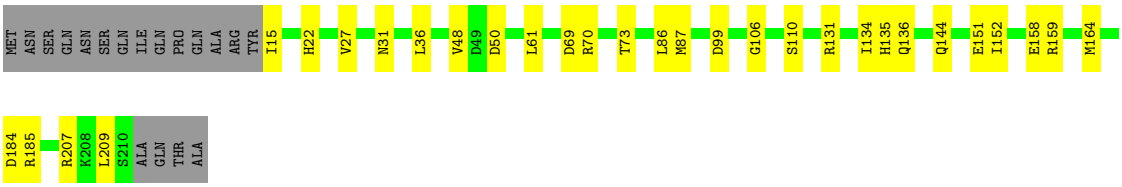
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f:



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

Chain g:



• Molecule 2: BEZ-LEU-LEU

Chain O:

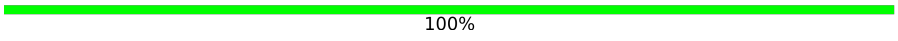
There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain P:

• Molecule 2: BEZ-LEU-LEU

Chain Q:



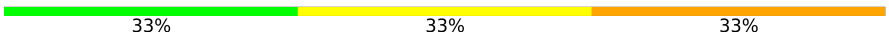
There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain R:

• Molecule 2: BEZ-LEU-LEU

Chain S:

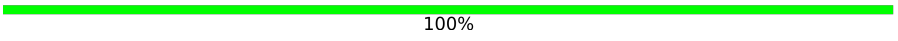


• Molecule 2: BEZ-LEU-LEU

Chain T:

• Molecule 2: BEZ-LEU-LEU

Chain U:



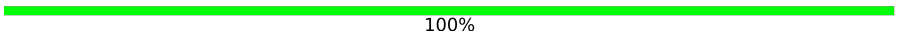
There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain V:

• Molecule 2: BEZ-LEU-LEU

Chain W:

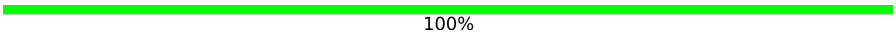


There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain X: 

• Molecule 2: BEZ-LEU-LEU

Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain Z: 

• Molecule 2: BEZ-LEU-LEU

Chain 1: 

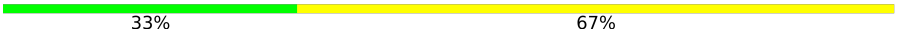
• Molecule 2: BEZ-LEU-LEU

Chain 2: 

• Molecule 2: BEZ-LEU-LEU

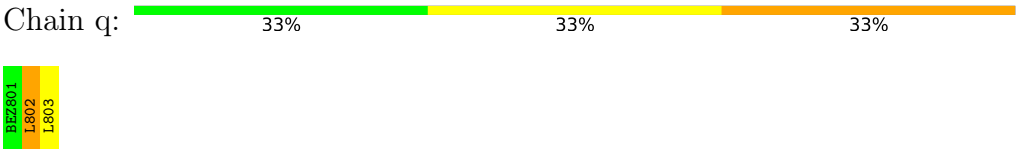
Chain o: 

• Molecule 2: BEZ-LEU-LEU

Chain p: 

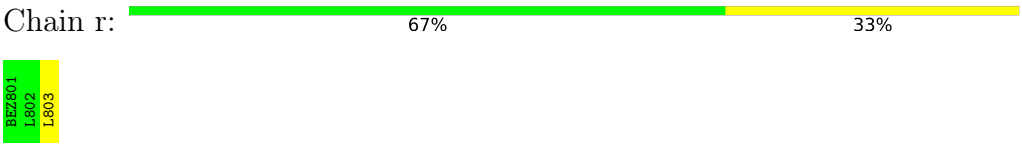
• Molecule 2: BEZ-LEU-LEU

Chain q:



• Molecule 2: BEZ-LEU-LEU

Chain r:

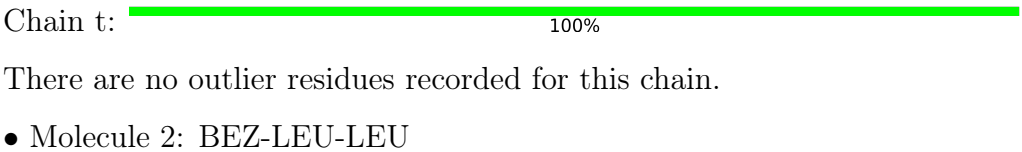


• Molecule 2: BEZ-LEU-LEU

Chain s:

• Molecule 2: BEZ-LEU-LEU

Chain t:



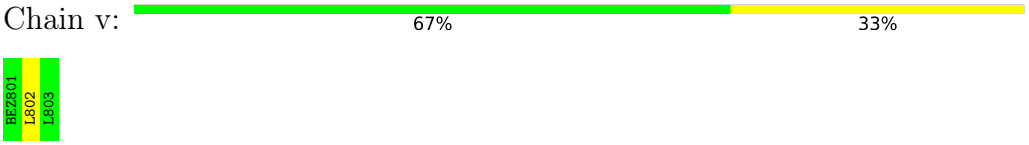
There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain u:

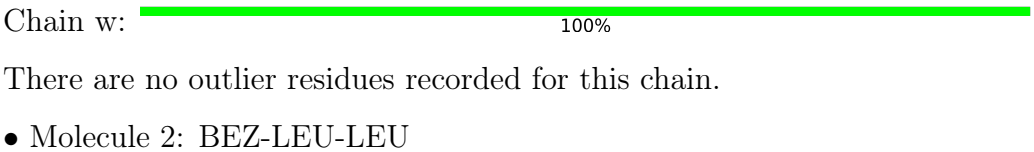
• Molecule 2: BEZ-LEU-LEU

Chain v:



• Molecule 2: BEZ-LEU-LEU

Chain w:



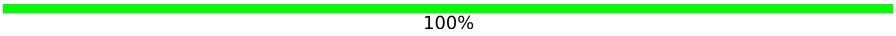
There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain x:

• Molecule 2: BEZ-LEU-LEU

Chain y:



There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain z:

• Molecule 2: BEZ-LEU-LEU

Chain 3:

• Molecule 2: BEZ-LEU-LEU

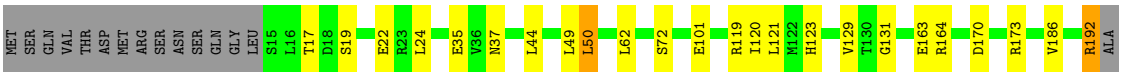
Chain 4:

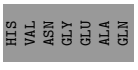
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain H:

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

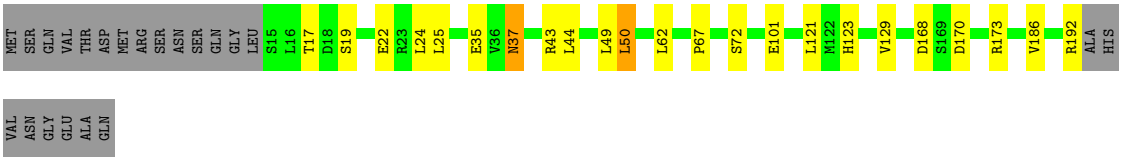
Chain I:





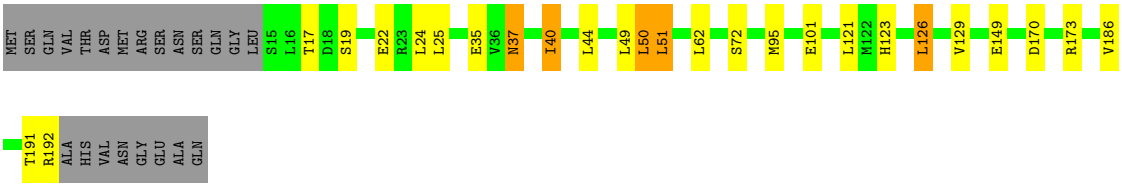
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain J:



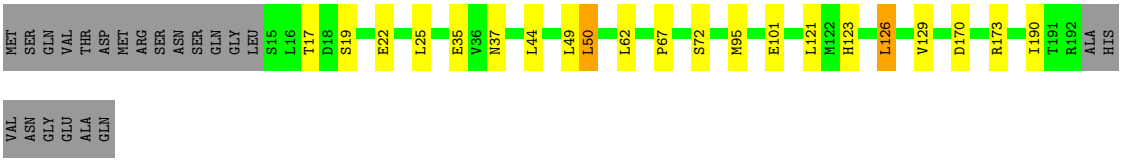
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain K:



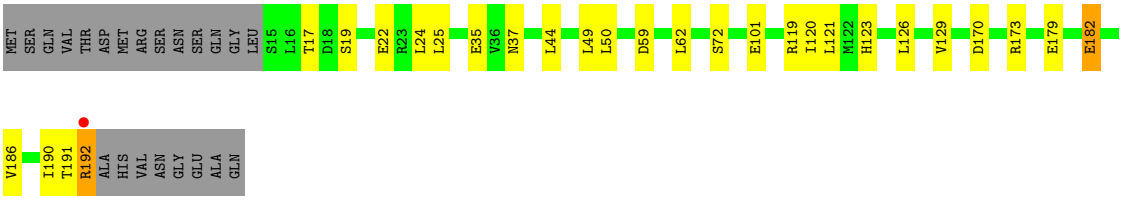
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain L:



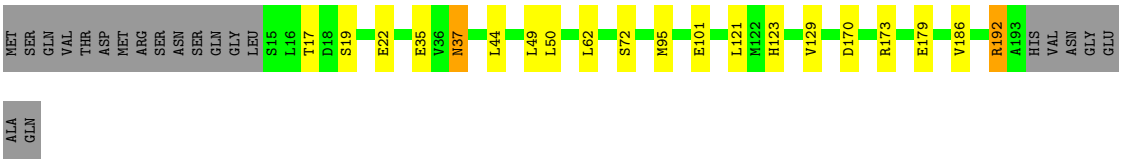
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain M:



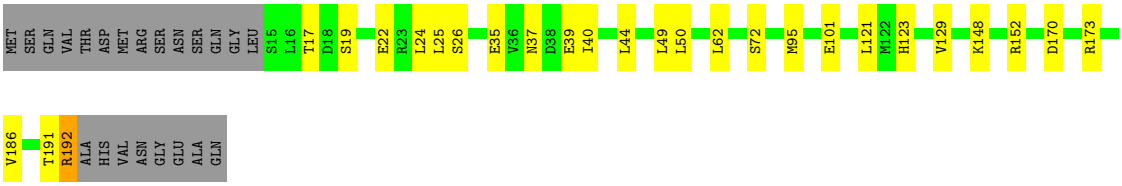
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



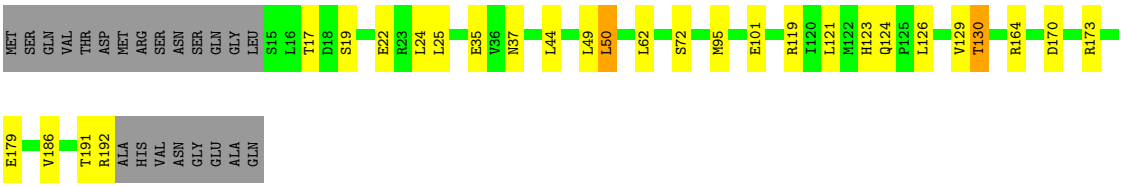
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain h:



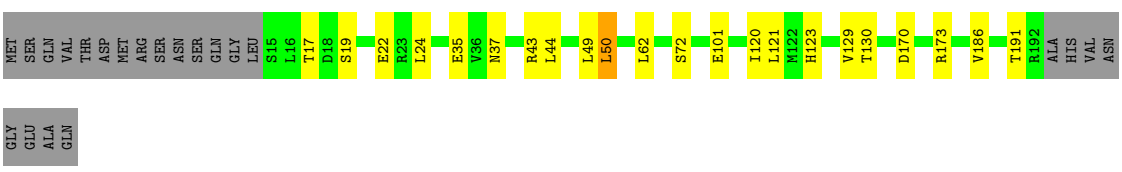
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain i:



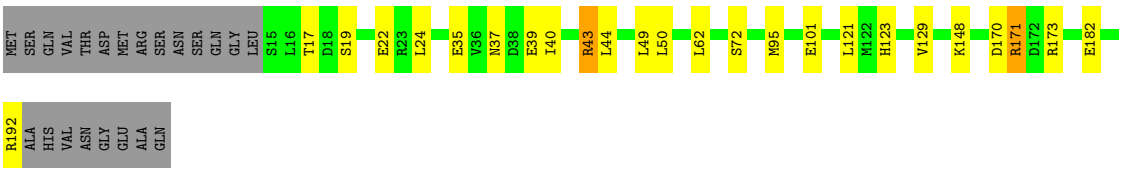
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain j:



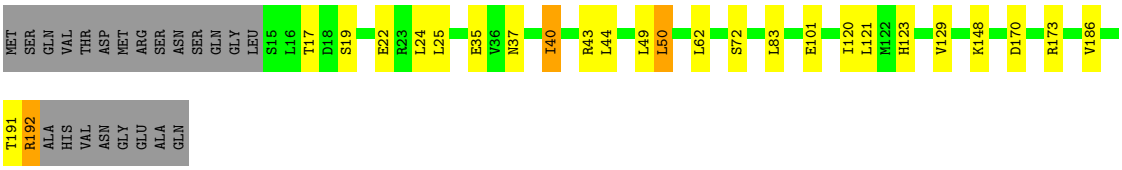
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain k:



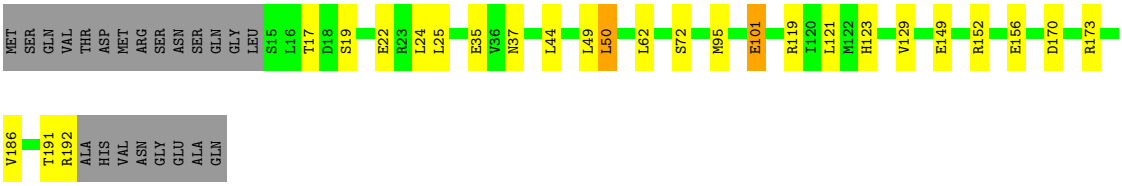
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain l:

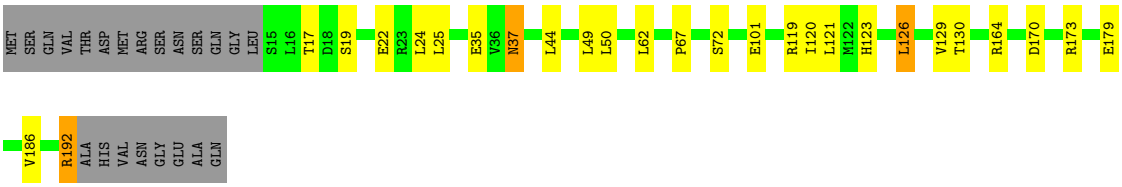


• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain m:



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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.03%)	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 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	29	61
1	B	198/214 (92%)	191 (96%)	5 (2%)	2 (1%)	15	47
1	C	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	15	47
1	D	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	29	61
1	E	198/214 (92%)	190 (96%)	6 (3%)	2 (1%)	15	47
1	F	194/214 (91%)	187 (96%)	5 (3%)	2 (1%)	15	47
1	G	193/214 (90%)	186 (96%)	6 (3%)	1 (0%)	29	61
1	a	195/214 (91%)	189 (97%)	5 (3%)	1 (0%)	29	61
1	b	198/214 (92%)	189 (96%)	6 (3%)	3 (2%)	10	37
1	c	195/214 (91%)	189 (97%)	4 (2%)	2 (1%)	15	47
1	d	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	15	47
1	e	198/214 (92%)	188 (95%)	8 (4%)	2 (1%)	15	47
1	f	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	29	61
1	g	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	15	47
2	1	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	61

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 (i)

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	17
1	B	165/178 (93%)	142 (86%)	23 (14%)	3	14
1	C	163/178 (92%)	140 (86%)	23 (14%)	3	14
1	D	163/178 (92%)	141 (86%)	22 (14%)	4	15
1	E	165/178 (93%)	145 (88%)	20 (12%)	5	19
1	F	163/178 (92%)	137 (84%)	26 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	162/178 (91%)	143 (88%)	19 (12%)	5 20
1	a	163/178 (92%)	143 (88%)	20 (12%)	4 18
1	b	165/178 (93%)	140 (85%)	25 (15%)	3 11
1	c	163/178 (92%)	142 (87%)	21 (13%)	4 17
1	d	163/178 (92%)	142 (87%)	21 (13%)	4 17
1	e	165/178 (93%)	145 (88%)	20 (12%)	5 19
1	f	163/178 (92%)	143 (88%)	20 (12%)	4 18
1	g	163/178 (92%)	142 (87%)	21 (13%)	4 17
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	2 10
3	I	139/157 (88%)	121 (87%)	18 (13%)	4 17
3	J	139/157 (88%)	119 (86%)	20 (14%)	3 13
3	K	139/157 (88%)	114 (82%)	25 (18%)	1 7
3	L	139/157 (88%)	120 (86%)	19 (14%)	3 15
3	M	139/157 (88%)	117 (84%)	22 (16%)	2 10
3	N	139/157 (88%)	121 (87%)	18 (13%)	4 17
3	h	139/157 (88%)	115 (83%)	24 (17%)	2 8
3	i	139/157 (88%)	116 (84%)	23 (16%)	2 9
3	j	139/157 (88%)	121 (87%)	18 (13%)	4 17
3	k	139/157 (88%)	117 (84%)	22 (16%)	2 10
3	l	139/157 (88%)	116 (84%)	23 (16%)	2 9
3	m	139/157 (88%)	115 (83%)	24 (17%)	2 8
3	n	139/157 (88%)	118 (85%)	21 (15%)	3 11
All	All	4291/4746 (90%)	3663 (85%)	628 (15%)	3 13

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

Mol	Chain	Res	Type
1	g	185	ARG
3	l	123	HIS
3	h	44	LEU
1	g	184	ASP
3	j	35	GLU

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

Mol	Chain	Res	Type
1	b	94	GLN

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Mol	Chain	Res	Type
3	i	37	ASN
1	b	146	GLN
1	f	94	GLN
3	j	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	-0.15	0	100	100	51, 66, 90, 117	0
1	B	200/214 (93%)	-0.19	0	100	100	48, 64, 93, 118	0
1	C	196/214 (91%)	-0.15	0	100	100	46, 60, 88, 100	0
1	D	196/214 (91%)	-0.24	0	100	100	48, 60, 82, 102	0
1	E	200/214 (93%)	-0.11	0	100	100	48, 65, 92, 141	0
1	F	196/214 (91%)	0.02	0	100	100	57, 75, 92, 115	0
1	G	195/214 (91%)	-0.02	0	100	100	55, 72, 93, 107	0
1	a	197/214 (92%)	-0.13	0	100	100	52, 63, 91, 112	0
1	b	200/214 (93%)	-0.19	0	100	100	50, 63, 93, 124	0
1	c	197/214 (92%)	-0.20	0	100	100	50, 67, 92, 110	0
1	d	196/214 (91%)	-0.20	0	100	100	48, 64, 91, 113	0
1	e	200/214 (93%)	-0.12	0	100	100	47, 65, 93, 125	0
1	f	196/214 (91%)	-0.07	0	100	100	48, 67, 91, 111	0
1	g	196/214 (91%)	-0.07	0	100	100	49, 66, 89, 109	0
2	1	2/3 (66%)	0.39	0	100	100	91, 91, 91, 97	0
2	2	2/3 (66%)	1.16	1 (50%)	0	0	86, 86, 86, 112	0
2	3	2/3 (66%)	0.84	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%)	0.36	0	100	100	99, 99, 99, 99	0
2	P	2/3 (66%)	0.01	0	100	100	96, 96, 96, 101	0
2	Q	2/3 (66%)	-0.03	0	100	100	92, 92, 92, 95	0
2	R	2/3 (66%)	0.61	0	100	100	89, 89, 89, 95	0
2	S	2/3 (66%)	0.32	0	100	100	90, 90, 90, 112	0
2	T	2/3 (66%)	1.44	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%)	0.47	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%)	-0.23	0	100	100	85, 85, 85, 88	0
2	Z	2/3 (66%)	0.67	0	100	100	89, 89, 89, 103	0
2	o	2/3 (66%)	-0.10	0	100	100	98, 98, 98, 100	0
2	p	2/3 (66%)	0.10	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%)	0.51	0	100	100	91, 91, 91, 100	0
2	s	2/3 (66%)	0.35	0	100	100	89, 89, 89, 98	0
2	t	2/3 (66%)	1.01	0	100	100	98, 98, 98, 105	0
2	u	2/3 (66%)	0.44	0	100	100	98, 98, 98, 108	0
2	v	2/3 (66%)	-0.23	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%)	0.29	0	100	100	77, 77, 77, 97	0
2	y	2/3 (66%)	-0.12	0	100	100	88, 88, 88, 90	0
2	z	2/3 (66%)	1.02	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%)	0.01	0	100	100	45, 60, 87, 116	0
3	L	178/200 (89%)	-0.00	0	100	100	51, 71, 95, 104	0
3	M	178/200 (89%)	0.10	1 (0%)	89	77	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%)	-0.14	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%)	-0.09	0	100	100	49, 65, 94, 116	0
3	k	178/200 (89%)	-0.08	0	100	100	48, 61, 84, 101	0
3	l	178/200 (89%)	-0.08	0	100	100	46, 59, 80, 100	0
3	m	178/200 (89%)	-0.17	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%)	-0.05	0 100 100	45, 59, 85, 126	0
All	All	5310/5880 (90%)	-0.11	2 (0%) 100 100	44, 64, 91, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	803	LEU	2.0
3	M	192	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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.