wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 12:56 PM EDT

PDB ID	:	5E0S
Title	:	crystal structure of the active form of the proteolytic complex clpP1 and clpP2
Authors	:	LI, M.; Wlodawer, A.; Maurizi, M.
Deposited on	:	2015-09-29
Resolution	:	2.90 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 (i)) were used in the production of this report:

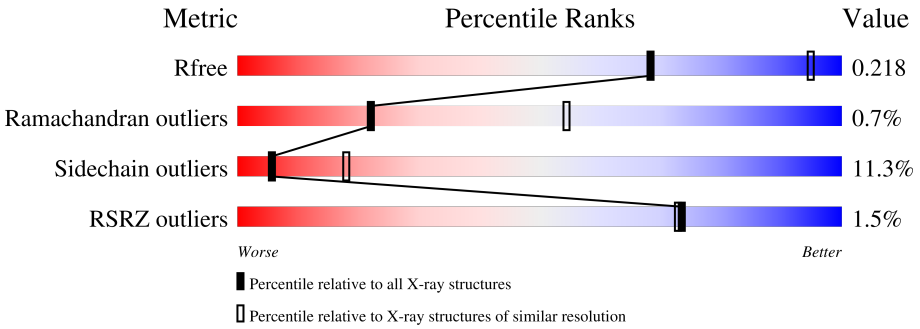
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	2% 84% 8% 8%
1	B	214	4% 85% 9% 6%
1	C	214	% 81% 9% 8%
1	D	214	80% 11% 8%
1	E	214	% 85% 8% 7%
1	F	214	2% 79% 12% 8%
1	G	214	% 83% 9% 8%

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Mol	Chain	Length	Quality of chain
1	a	214	84% 8% 7%
1	b	214	82% 10% • 6%
1	c	214	82% 9% • 7%
1	d	214	81% 10% • 8%
1	e	214	82% 10% 7%
1	f	214	82% 9% 8%
1	g	214	81% 10% • 8%
2	H	200	80% 12% • 7%
2	I	200	79% 10% 11%
2	J	200	78% 10% 11%
2	K	200	78% 10% • 11%
2	L	200	79% 10% 11%
2	M	200	78% 10% • 11%
2	N	200	82% 10% 8%
2	h	200	80% 10% 8%
2	i	200	78% 12% • 10%
2	j	200	80% 9% 11%
2	k	200	78% 10% 11%
2	l	200	78% 10% 11%
2	m	200	79% 10% 11%
2	n	200	80% 12% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40670 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	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	B	201	Total	C	N	O	S	0	0	0
			1546	972	263	303	8			
1	C	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	D	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	E	199	Total	C	N	O	S	0	0	0
			1534	965	261	300	8			
1	F	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	G	196	Total	C	N	O	S	0	0	0
			1514	954	257	295	8			
1	a	198	Total	C	N	O	S	0	0	0
			1525	960	259	298	8			
1	b	201	Total	C	N	O	S	0	0	0
			1546	972	263	303	8			
1	c	198	Total	C	N	O	S	0	0	0
			1525	960	259	298	8			
1	d	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	e	199	Total	C	N	O	S	0	0	0
			1534	965	261	300	8			
1	f	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			
1	g	197	Total	C	N	O	S	0	0	0
			1520	957	258	297	8			

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	186	Total	C	N	O	S	0	0	0
			1417	892	242	273	10			
2	I	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	J	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	K	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	L	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	M	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	N	184	Total	C	N	O	S	0	0	0
			1400	883	238	270	9			
2	h	183	Total	C	N	O	S	0	0	0
			1391	878	237	267	9			
2	i	181	Total	C	N	O	S	0	0	0
			1379	872	234	264	9			
2	j	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	k	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	l	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	m	178	Total	C	N	O	S	0	0	0
			1357	858	229	261	9			
2	n	184	Total	C	N	O	S	0	0	0
			1400	883	238	270	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	2	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			1	1		
3	G	3	Total	O	0	0
			3	3		
3	H	4	Total	O	0	0
			4	4		

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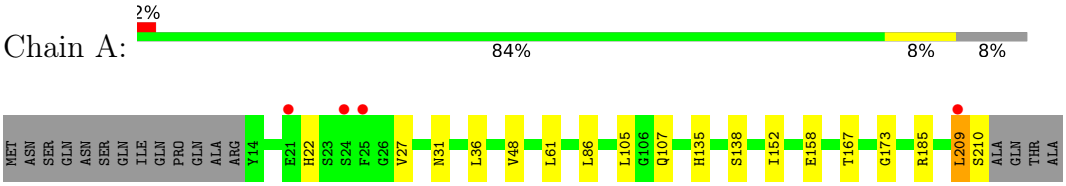
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O 1 1	0	0
3	J	1	Total O 1 1	0	0
3	K	2	Total O 2 2	0	0
3	L	2	Total O 2 2	0	0
3	N	4	Total O 4 4	0	0
3	a	8	Total O 8 8	0	0
3	b	11	Total O 11 11	0	0
3	c	9	Total O 9 9	0	0
3	d	5	Total O 5 5	0	0
3	e	1	Total O 1 1	0	0
3	g	8	Total O 8 8	0	0
3	h	5	Total O 5 5	0	0
3	i	5	Total O 5 5	0	0
3	j	4	Total O 4 4	0	0
3	k	2	Total O 2 2	0	0
3	l	1	Total O 1 1	0	0
3	m	7	Total O 7 7	0	0
3	n	10	Total O 10 10	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

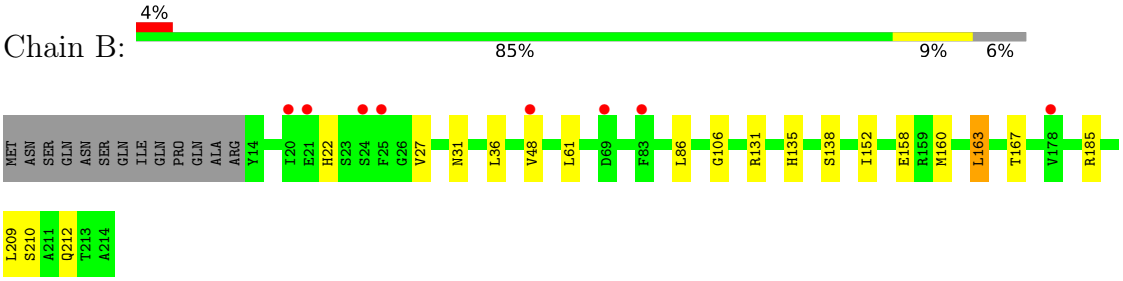
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A:



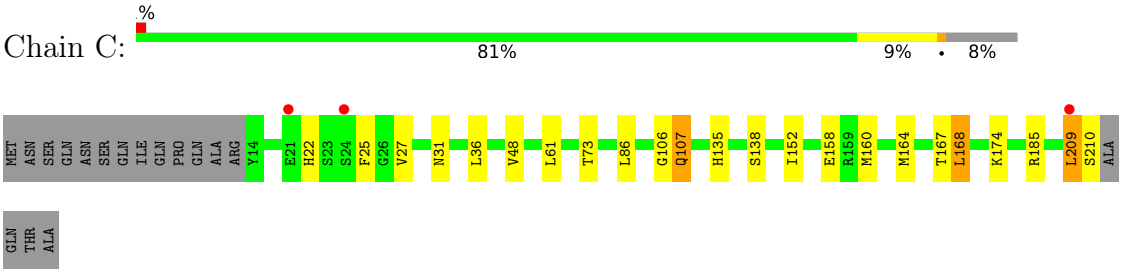
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



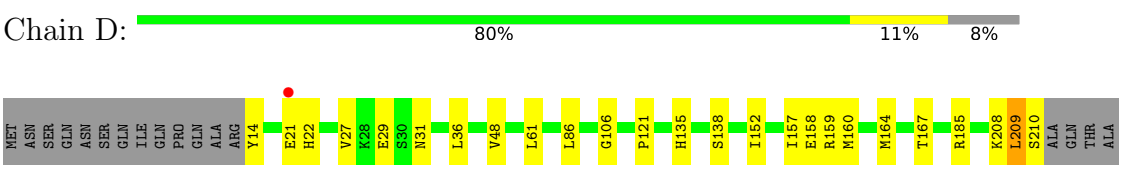
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain C:



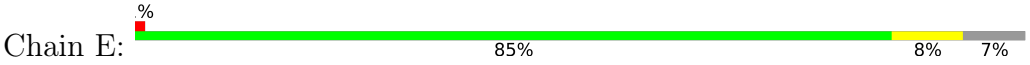
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

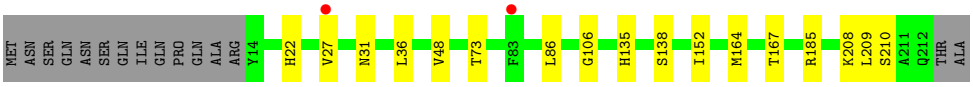
Chain D:



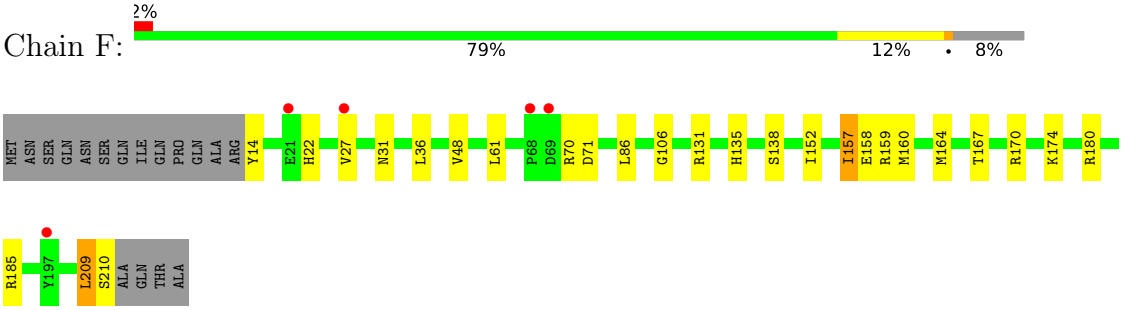
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E:

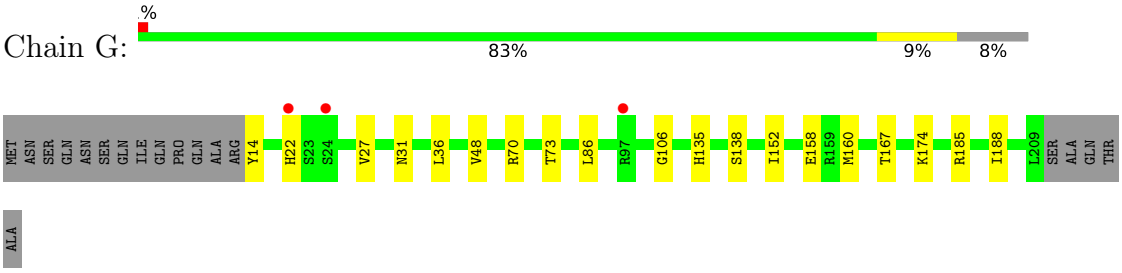




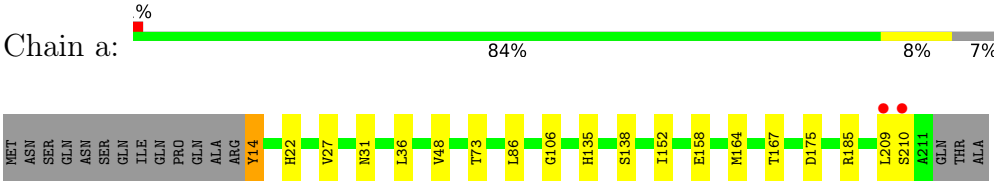
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



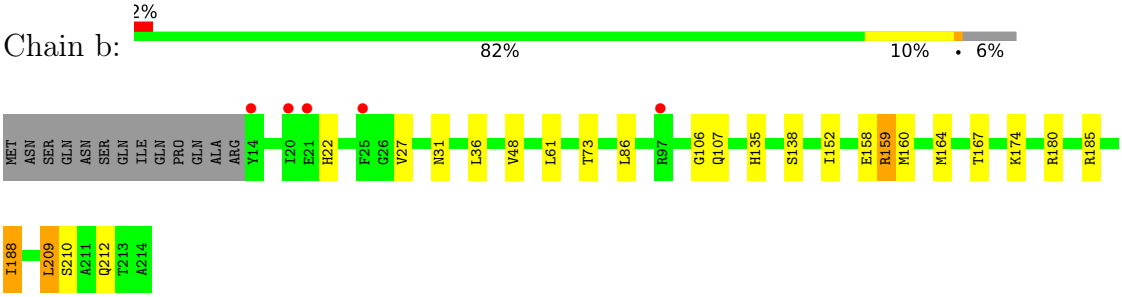
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



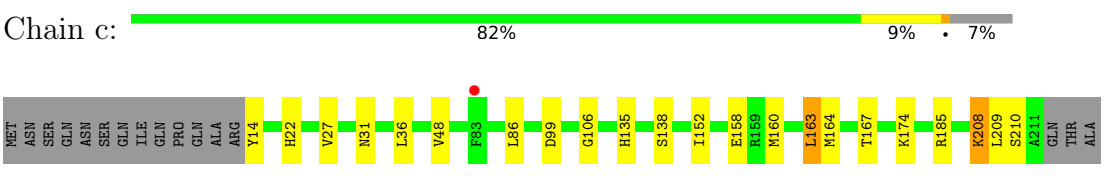
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



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

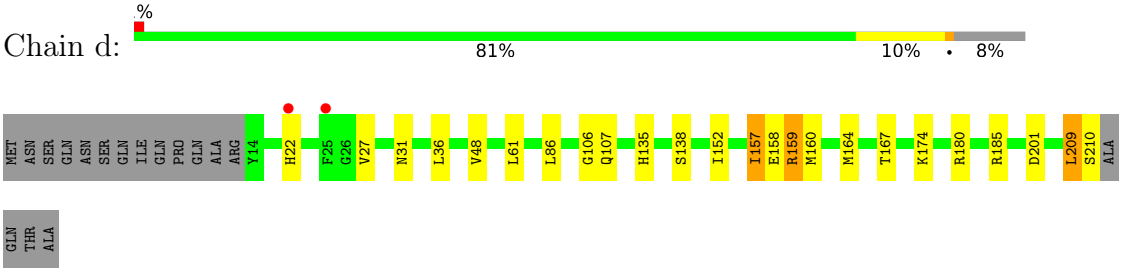


• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



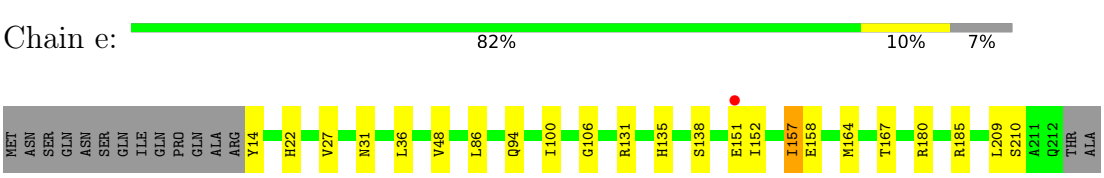
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain d:



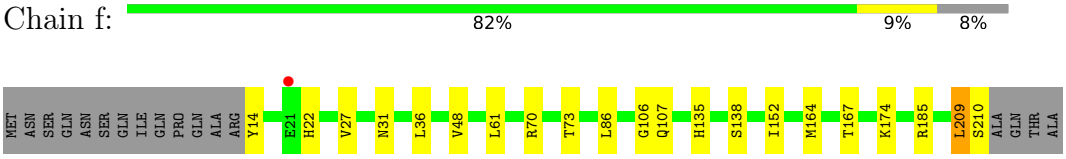
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain e:



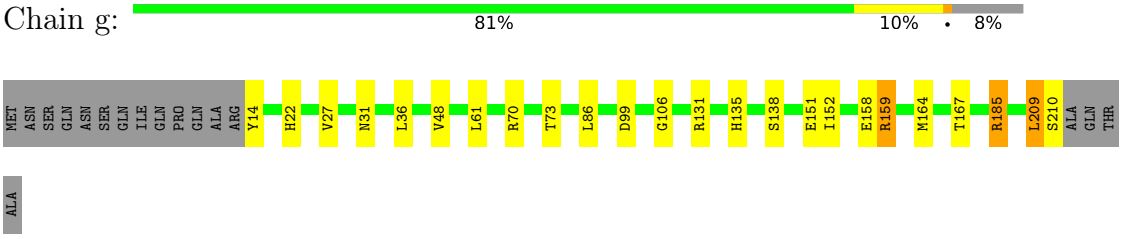
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f:



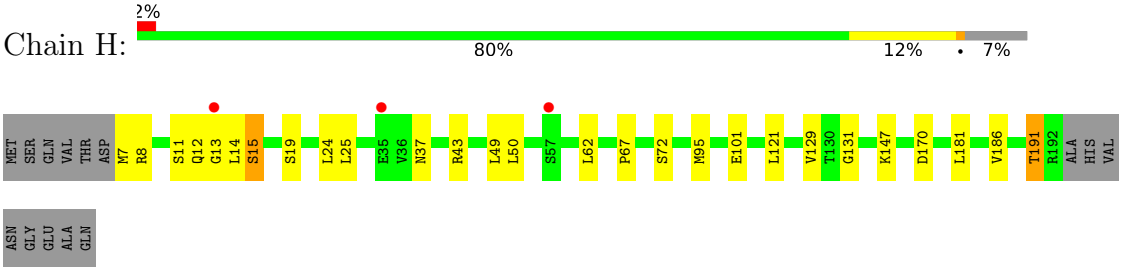
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain g:



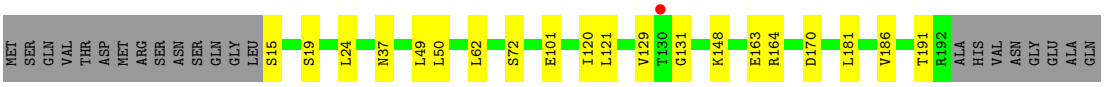
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain H:



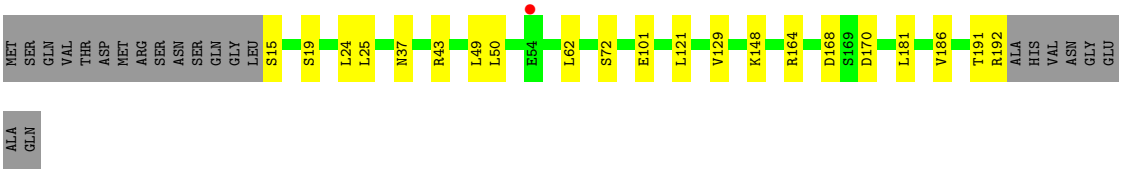
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain I:



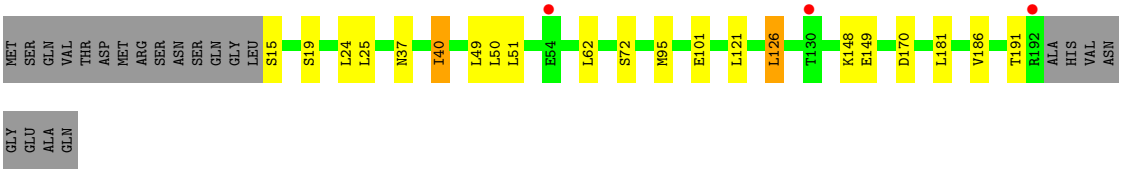
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain J:



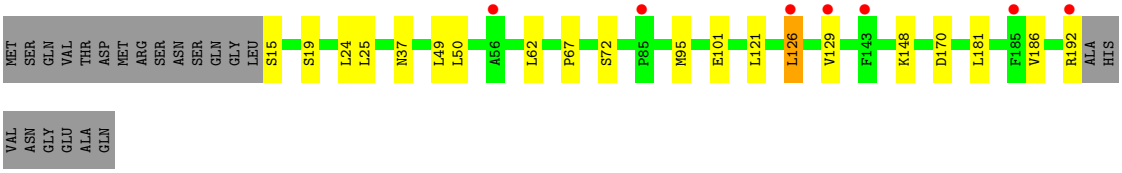
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain K:



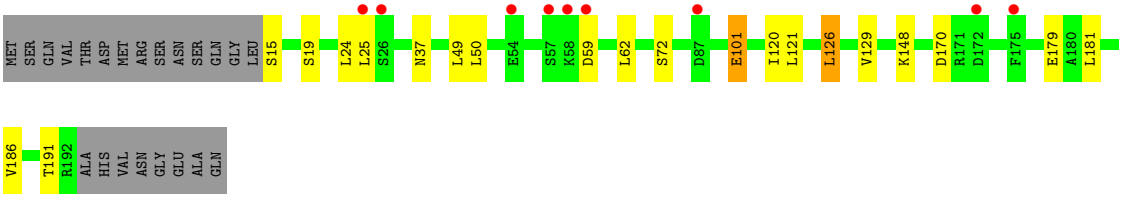
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain L:



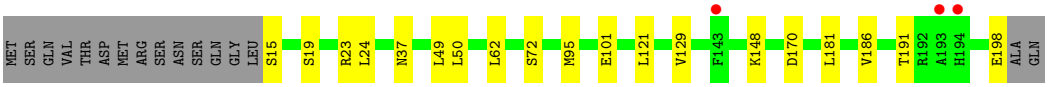
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain M:



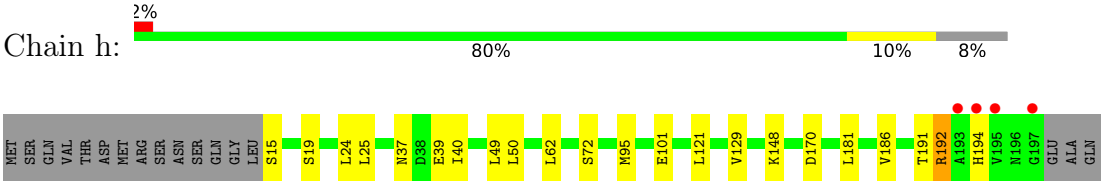
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



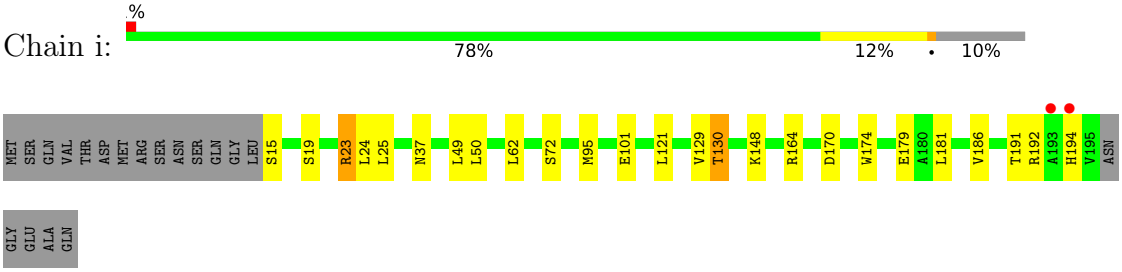
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain h:



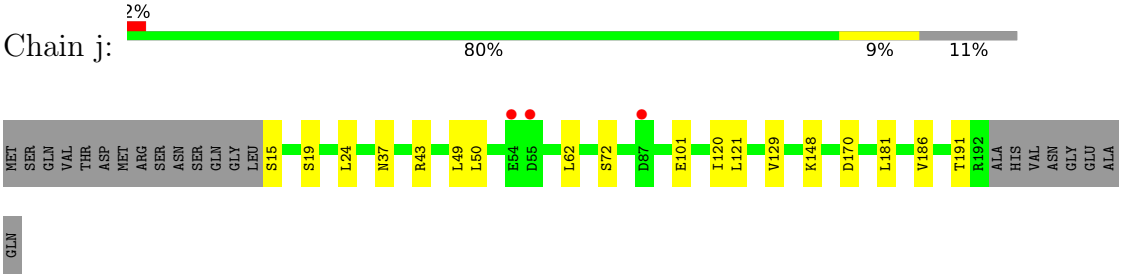
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain i:



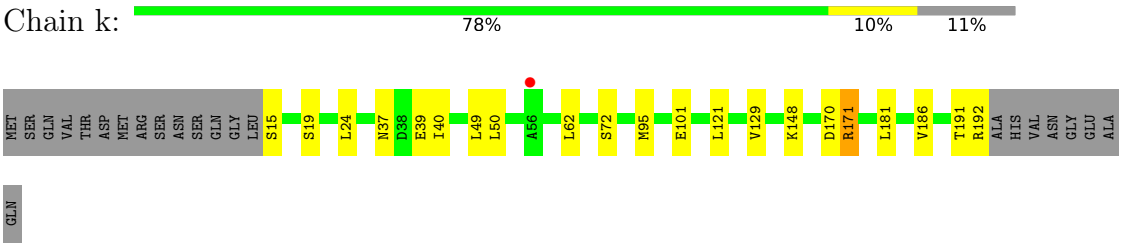
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain j:



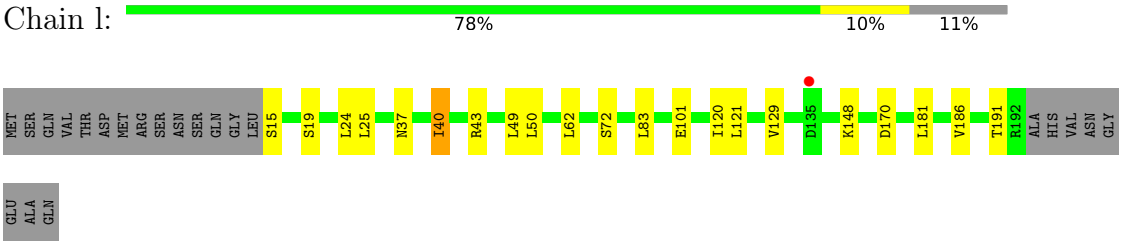
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain k:



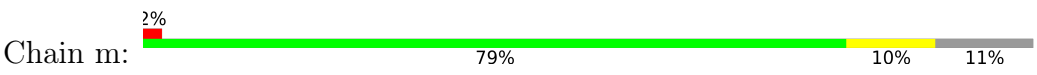
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

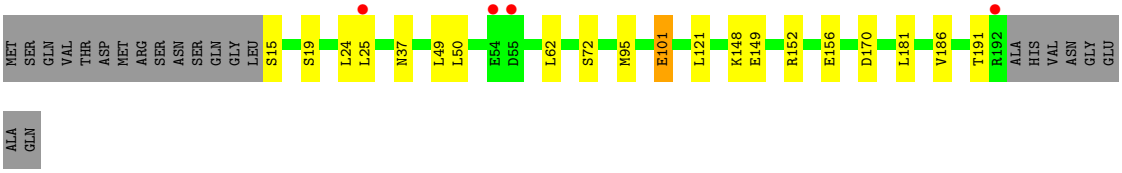
Chain l:



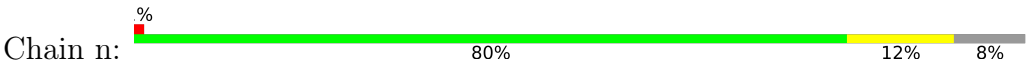
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

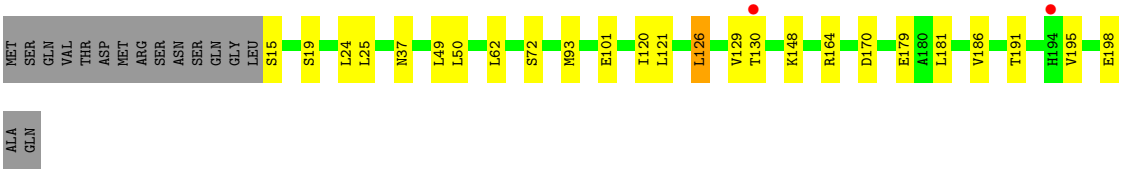
Chain m:





• Molecule 2: 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	205.18Å 183.54Å 188.37Å 90.00° 94.53° 90.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.22 – 2.88	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.27-2.90) 93.8 (49.22-2.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.204 , 0.236 0.200 , 0.218	Depositor DCC
R_{free} test set	7424 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40670	wwPDB-VP
Average B, all atoms (Å^2)	80.0	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 36.52 % 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 4.9322e-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)

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	0.81	0/1542	1.04	3/2086 (0.1%)
1	B	0.81	0/1568	1.05	4/2122 (0.2%)
1	C	0.84	0/1542	1.08	5/2086 (0.2%)
1	D	0.87	1/1542 (0.1%)	1.09	6/2086 (0.3%)
1	E	0.84	0/1556	1.04	1/2105 (0.0%)
1	F	0.82	0/1542	1.09	8/2086 (0.4%)
1	G	0.81	0/1536	1.07	6/2078 (0.3%)
1	a	0.85	0/1547	1.07	5/2093 (0.2%)
1	b	0.88	0/1568	1.15	10/2122 (0.5%)
1	c	0.88	0/1547	1.18	7/2093 (0.3%)
1	d	0.87	0/1542	1.14	9/2086 (0.4%)
1	e	0.92	1/1556 (0.1%)	1.17	7/2105 (0.3%)
1	f	0.84	0/1542	1.06	4/2086 (0.2%)
1	g	0.89	1/1542 (0.1%)	1.23	11/2086 (0.5%)
2	H	0.84	1/1439 (0.1%)	1.04	4/1943 (0.2%)
2	I	0.87	1/1379 (0.1%)	1.08	6/1864 (0.3%)
2	J	0.86	0/1379	1.07	5/1864 (0.3%)
2	K	0.81	0/1379	0.99	3/1864 (0.2%)
2	L	0.80	0/1379	0.98	3/1864 (0.2%)
2	M	0.80	0/1379	1.02	8/1864 (0.4%)
2	N	0.79	0/1423	1.02	5/1924 (0.3%)
2	h	0.84	0/1414	1.01	2/1912 (0.1%)
2	i	0.85	1/1402 (0.1%)	1.05	7/1896 (0.4%)
2	j	0.84	0/1379	1.00	4/1864 (0.2%)
2	k	0.85	0/1379	1.02	3/1864 (0.2%)
2	l	0.83	0/1379	1.03	5/1864 (0.3%)
2	m	0.86	1/1379 (0.1%)	1.01	2/1864 (0.1%)
2	n	0.86	0/1423	1.04	7/1924 (0.4%)
All	All	0.85	7/41184 (0.0%)	1.07	150/55695 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	a	0	1
1	b	0	1
2	H	0	1
2	I	0	1
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	94	GLN	CG-CD	-8.51	1.31	1.51
2	I	163	GLU	CD-OE1	-8.02	1.16	1.25
2	H	15	SER	CB-OG	-7.53	1.32	1.42
1	g	151	GLU	CD-OE2	6.75	1.33	1.25
2	m	101	GLU	CD-OE1	-5.57	1.19	1.25

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	99	ASP	CB-CG-OD2	17.94	134.44	118.30
1	g	99	ASP	CB-CG-OD2	17.61	134.15	118.30
1	c	99	ASP	CB-CG-OD1	-16.25	103.67	118.30
1	g	99	ASP	CB-CG-OD1	-16.25	103.67	118.30
1	e	94	GLN	CA-CB-CG	-14.34	81.85	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	212	GLN	Peptide
2	H	13	GLY	Peptide
2	I	191	THR	Peptide
1	a	14	TYR	Peptide
1	b	212	GLN	Peptide

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	195/214 (91%)	185 (95%)	8 (4%)	2 (1%)	15	45
1	B	199/214 (93%)	188 (94%)	9 (4%)	2 (1%)	15	45
1	C	195/214 (91%)	185 (95%)	7 (4%)	3 (2%)	10	34
1	D	195/214 (91%)	185 (95%)	7 (4%)	3 (2%)	10	34
1	E	197/214 (92%)	187 (95%)	8 (4%)	2 (1%)	15	45
1	F	195/214 (91%)	184 (94%)	8 (4%)	3 (2%)	10	34
1	G	194/214 (91%)	185 (95%)	7 (4%)	2 (1%)	15	45
1	a	196/214 (92%)	187 (95%)	7 (4%)	2 (1%)	15	45
1	b	199/214 (93%)	190 (96%)	7 (4%)	2 (1%)	15	45
1	c	196/214 (92%)	187 (95%)	7 (4%)	2 (1%)	15	45
1	d	195/214 (91%)	185 (95%)	7 (4%)	3 (2%)	10	34
1	e	197/214 (92%)	187 (95%)	8 (4%)	2 (1%)	15	45
1	f	195/214 (91%)	185 (95%)	7 (4%)	3 (2%)	10	34
1	g	195/214 (91%)	184 (94%)	8 (4%)	3 (2%)	10	34
2	H	184/200 (92%)	175 (95%)	8 (4%)	1 (0%)	29	61
2	I	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
2	J	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	K	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	L	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	M	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	N	182/200 (91%)	176 (97%)	6 (3%)	0	100	100
2	h	181/200 (90%)	174 (96%)	6 (3%)	1 (1%)	25	58
2	i	179/200 (90%)	174 (97%)	5 (3%)	0	100	100
2	j	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	k	176/200 (88%)	172 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	m	176/200 (88%)	172 (98%)	4 (2%)	0	100	100
2	n	182/200 (91%)	175 (96%)	6 (3%)	1 (0%)	29	61
All	All	5235/5796 (90%)	5025 (96%)	173 (3%)	37 (1%)	22	54

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	h	192	ARG
2	n	195	VAL
1	A	48	VAL
1	B	48	VAL
1	C	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	164/178 (92%)	151 (92%)	13 (8%)	12	34
1	B	166/178 (93%)	152 (92%)	14 (8%)	11	31
1	C	164/178 (92%)	146 (89%)	18 (11%)	6	19
1	D	164/178 (92%)	145 (88%)	19 (12%)	5	16
1	E	165/178 (93%)	151 (92%)	14 (8%)	10	31
1	F	164/178 (92%)	145 (88%)	19 (12%)	5	16
1	G	163/178 (92%)	151 (93%)	12 (7%)	13	38
1	a	164/178 (92%)	151 (92%)	13 (8%)	12	34
1	b	166/178 (93%)	148 (89%)	18 (11%)	6	20
1	c	164/178 (92%)	148 (90%)	16 (10%)	8	24
1	d	164/178 (92%)	146 (89%)	18 (11%)	6	19
1	e	165/178 (93%)	149 (90%)	16 (10%)	8	25
1	f	164/178 (92%)	148 (90%)	16 (10%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	g	164/178 (92%)	147 (90%)	17 (10%)	7 21
2	H	146/157 (93%)	124 (85%)	22 (15%)	3 9
2	I	139/157 (88%)	125 (90%)	14 (10%)	7 23
2	J	139/157 (88%)	122 (88%)	17 (12%)	5 15
2	K	139/157 (88%)	119 (86%)	20 (14%)	3 9
2	L	139/157 (88%)	120 (86%)	19 (14%)	3 11
2	M	139/157 (88%)	121 (87%)	18 (13%)	4 13
2	N	143/157 (91%)	127 (89%)	16 (11%)	6 18
2	h	142/157 (90%)	121 (85%)	21 (15%)	3 9
2	i	141/157 (90%)	120 (85%)	21 (15%)	3 9
2	j	139/157 (88%)	124 (89%)	15 (11%)	6 20
2	k	139/157 (88%)	120 (86%)	19 (14%)	3 11
2	l	139/157 (88%)	121 (87%)	18 (13%)	4 13
2	m	139/157 (88%)	120 (86%)	19 (14%)	3 11
2	n	143/157 (91%)	124 (87%)	19 (13%)	4 11
All	All	4267/4690 (91%)	3786 (89%)	481 (11%)	6 18

5 of 481 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	181	LEU
2	m	15	SER
1	d	86	LEU
2	l	129	VAL
2	n	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	f	135	HIS
2	k	123	HIS
1	g	31	ASN
2	i	37	ASN
2	m	123	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	197/214 (92%)	-0.09	4 (2%)	65	63	61, 81, 123, 146	0
1	B	201/214 (93%)	0.00	8 (3%)	38	33	59, 80, 122, 149	0
1	C	197/214 (92%)	-0.02	3 (1%)	73	73	55, 77, 115, 138	0
1	D	197/214 (92%)	-0.07	1 (0%)	91	91	54, 77, 112, 149	0
1	E	199/214 (92%)	-0.03	2 (1%)	82	82	63, 83, 114, 133	0
1	F	197/214 (92%)	0.03	5 (2%)	57	55	69, 94, 121, 144	0
1	G	196/214 (91%)	0.09	3 (1%)	73	73	63, 90, 126, 148	0
1	a	198/214 (92%)	-0.11	2 (1%)	82	82	52, 72, 111, 128	0
1	b	201/214 (93%)	-0.05	5 (2%)	57	55	51, 71, 108, 128	0
1	c	198/214 (92%)	-0.11	1 (0%)	91	91	51, 75, 113, 132	0
1	d	197/214 (92%)	-0.12	2 (1%)	82	82	49, 71, 109, 139	0
1	e	199/214 (92%)	-0.12	1 (0%)	91	91	51, 71, 110, 139	0
1	f	197/214 (92%)	-0.08	1 (0%)	91	91	53, 74, 108, 133	0
1	g	197/214 (92%)	-0.13	0	100	100	52, 73, 106, 132	0
2	H	186/200 (93%)	0.04	3 (1%)	72	71	60, 75, 117, 175	0
2	I	178/200 (89%)	-0.20	1 (0%)	89	89	54, 68, 99, 124	0
2	J	178/200 (89%)	-0.10	1 (0%)	89	89	53, 68, 99, 114	0
2	K	178/200 (89%)	-0.09	3 (1%)	70	69	58, 77, 107, 182	0
2	L	178/200 (89%)	0.05	7 (3%)	39	35	66, 86, 112, 139	0
2	M	178/200 (89%)	0.10	9 (5%)	28	24	72, 89, 112, 130	0
2	N	184/200 (92%)	-0.10	3 (1%)	72	71	64, 82, 111, 164	0
2	h	183/200 (91%)	0.04	4 (2%)	62	59	50, 67, 102, 188	0
2	i	181/200 (90%)	-0.16	2 (1%)	80	80	55, 71, 107, 194	0
2	j	178/200 (89%)	-0.06	3 (1%)	70	69	54, 69, 102, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	k	178/200 (89%)	-0.22	1 (0%)	89	89	52, 67, 97, 164	0
2	l	178/200 (89%)	-0.15	1 (0%)	89	89	53, 66, 93, 127	0
2	m	178/200 (89%)	-0.28	4 (2%)	62	59	50, 63, 94, 131	0
2	n	184/200 (92%)	-0.24	2 (1%)	80	80	50, 65, 100, 176	0
All	All	5291/5796 (91%)	-0.08	82 (1%)	73	73	49, 75, 112, 194	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	i	193	ALA	5.1
2	h	194	HIS	4.3
2	i	194	HIS	4.0
2	K	192	ARG	4.0
1	a	209	LEU	3.9

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.