Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

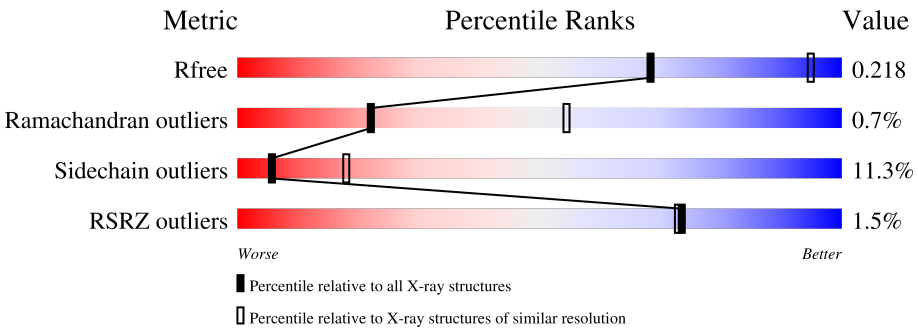
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	2%, 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	2%, 80%, 12%, 7%
2	I	200	79%, 10%, 11%
2	J	200	78%, 10%, 11%
2	K	200	2%, 78%, 10%, 11%
2	L	200	4%, 79%, 10%, 11%
2	M	200	4%, 78%, 10%, 11%
2	N	200	2%, 82%, 10%, 8%
2	h	200	2%, 80%, 10%, 8%
2	i	200	%, 78%, 12%, 10%
2	j	200	2%, 80%, 9%, 11%
2	k	200	78%, 10%, 11%
2	l	200	78%, 10%, 11%
2	m	200	2%, 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
			Total	C	N	O	S			
1	A	197	1520	957	258	297	8	0	0	0
1	B	201	1546	972	263	303	8	0	0	0
1	C	197	1520	957	258	297	8	0	0	0
1	D	197	1520	957	258	297	8	0	0	0
1	E	199	1534	965	261	300	8	0	0	0
1	F	197	1520	957	258	297	8	0	0	0
1	G	196	1514	954	257	295	8	0	0	0
1	a	198	1525	960	259	298	8	0	0	0
1	b	201	1546	972	263	303	8	0	0	0
1	c	198	1525	960	259	298	8	0	0	0
1	d	197	1520	957	258	297	8	0	0	0
1	e	199	1534	965	261	300	8	0	0	0
1	f	197	1520	957	258	297	8	0	0	0
1	g	197	1520	957	258	297	8	0	0	0

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

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

- Molecule 3 is water.

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

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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 (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: 2% 84% 8% 8%

MET ASN SER GLN ASN SER GLN ILE GLN PRO GLN ALA ARG Y14 E21 H22 S23 S24 F25 G26 V27 N31 L36 V48 L61 L86 L105 G106 Q107 H135 S138 I152 E158 T167 G173 R185 L209 S210 ALA GLN THR ALA

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

Chain B: 4% 85% 9% 6%

MET ASN SER GLN ASN SER GLN ILE GLN PRO GLN ALA ARG Y14 I20 E21 H22 S23 S24 F25 G26 V27 N31 L36 V48 L61 D69 F83 L86 G106 R131 H135 S138 I152 E158 R159 M160 L163 T167 V178 R185

L209 S210 A211 Q212 T213 A214

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

Chain C: % 81% 9% • 8%

MET ASN SER GLN ASN SER GLN ILE GLN PRO GLN ALA ARG Y14 E21 H22 S23 S24 F25 G26 V27 N31 L36 V48 L61 T73 L86 G106 Q107 H135 S138 I152 E158 R159 M160 M164 T167 L168 K174 R185 L209 S210 ALA

GLN THR ALA

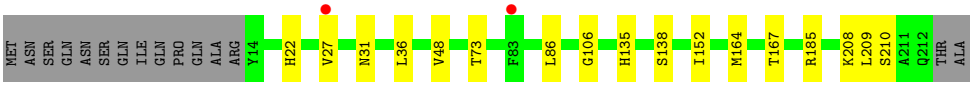
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D: 80% 11% 8%

MET ASN SER GLN ASN SER GLN ILE GLN PRO GLN ALA ARG Y14 E21 H22 V27 K28 E29 S30 N31 L36 V48 L61 L86 G106 P121 H135 S138 I152 I157 E158 R159 M160 M164 T167 R185 K208 L209 S210 ALA GLN THR ALA

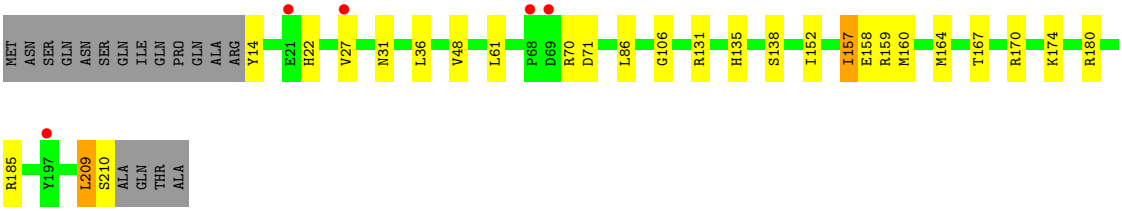
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E: % 85% 8% 7%



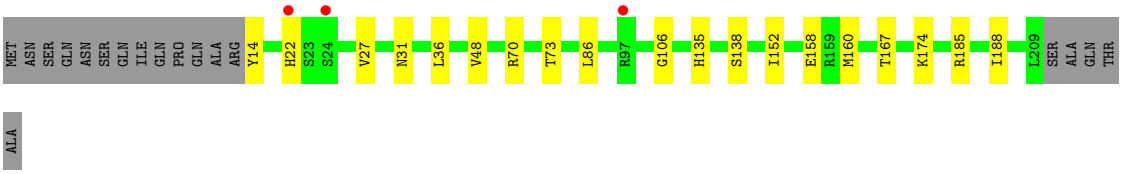
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F:



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

Chain G:

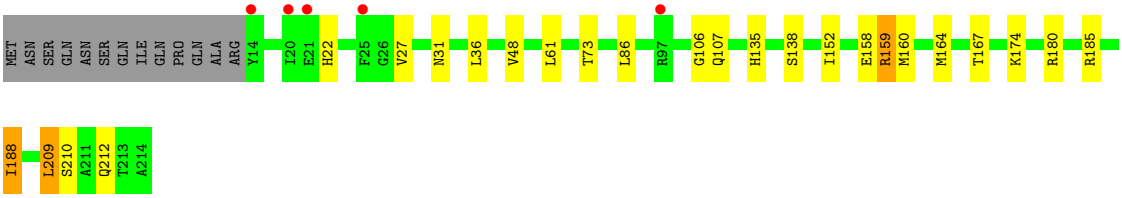


• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain a:

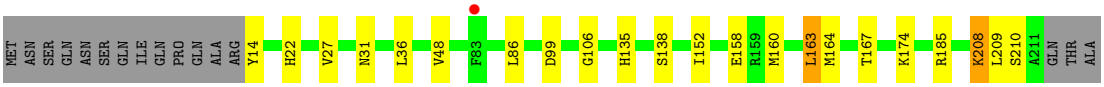
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain b:



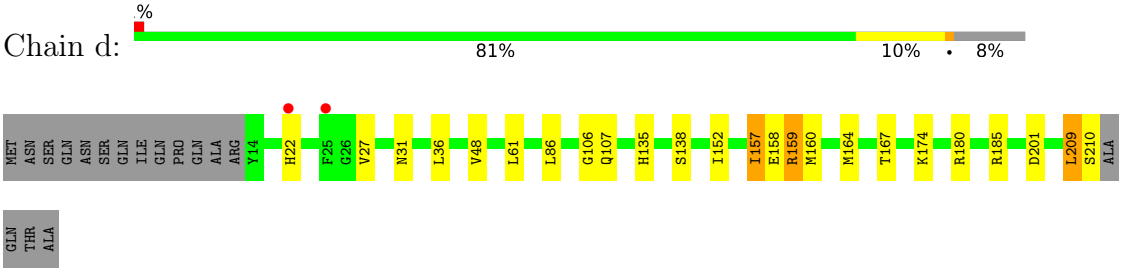
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain c:



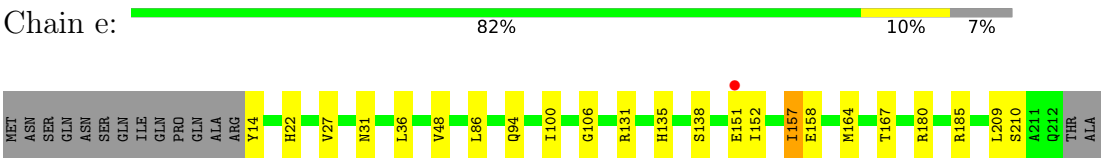
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain d:



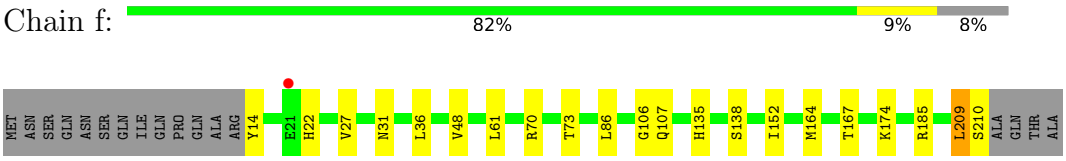
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain e:



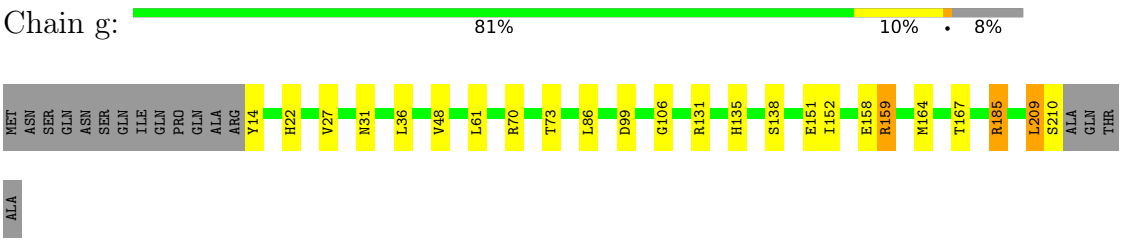
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f:



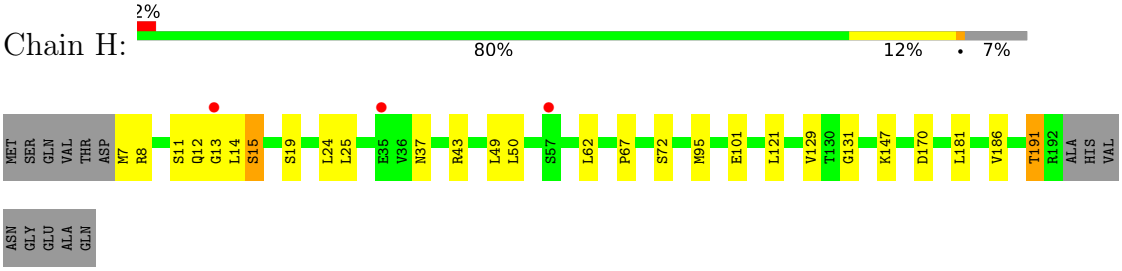
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain g:



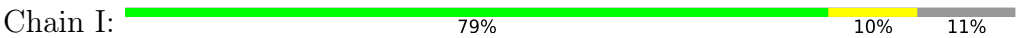
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

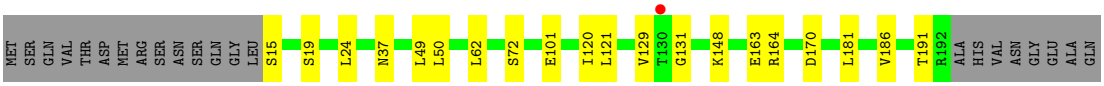
Chain H:



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

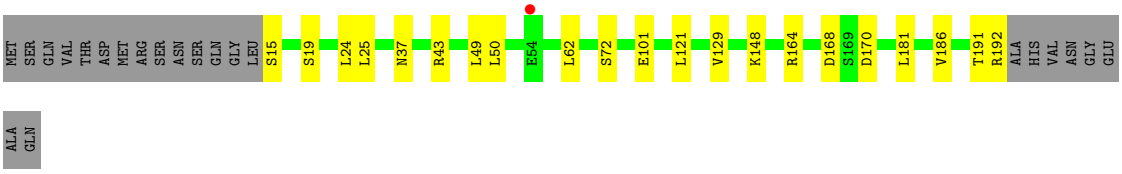
Chain I:





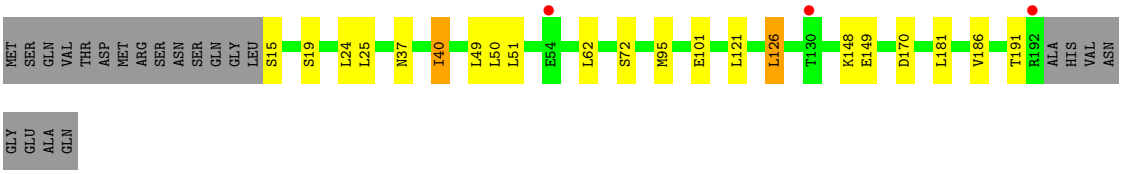
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain J:



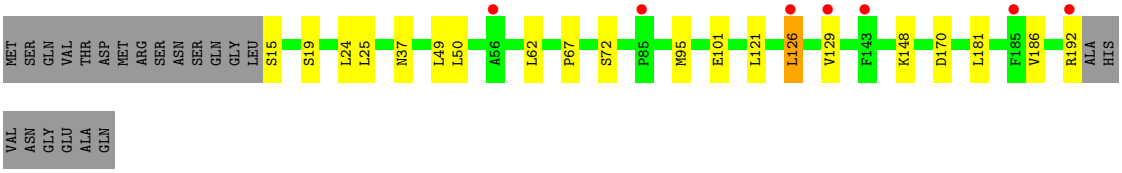
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain K:



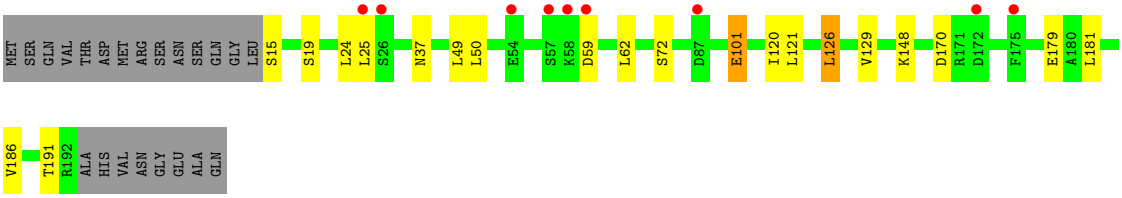
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain L:



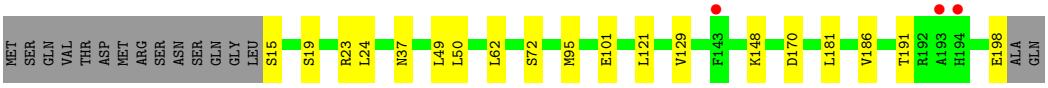
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain M:



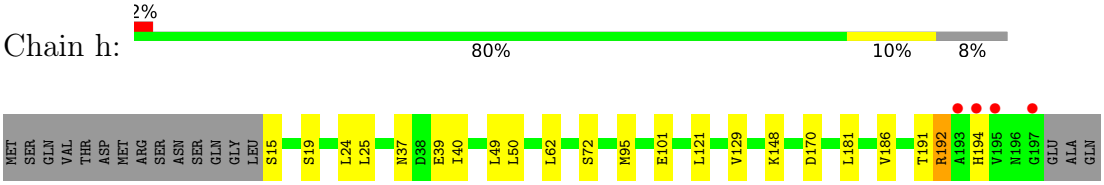
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



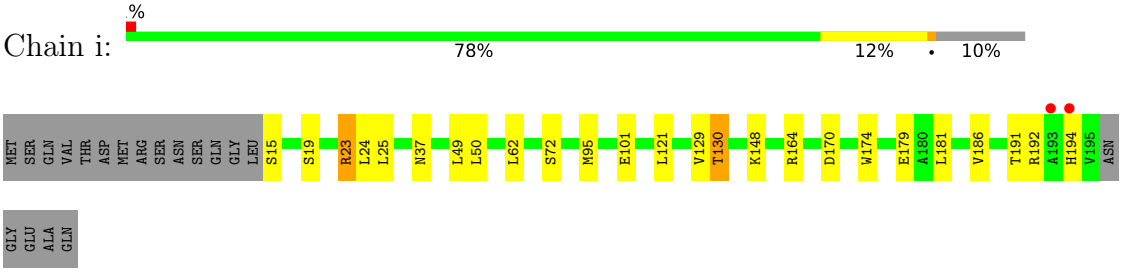
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain h:



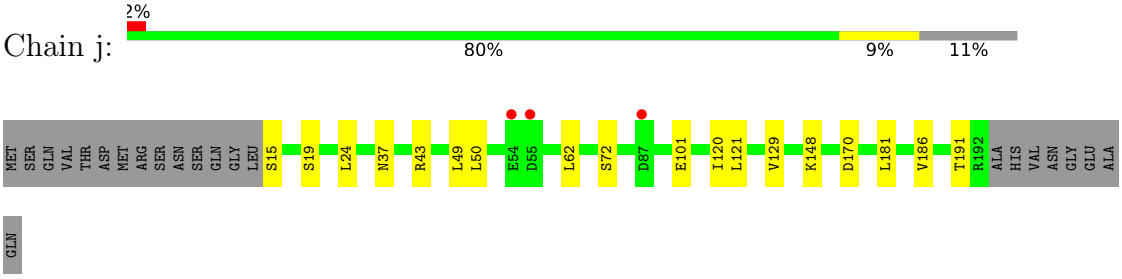
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain i:



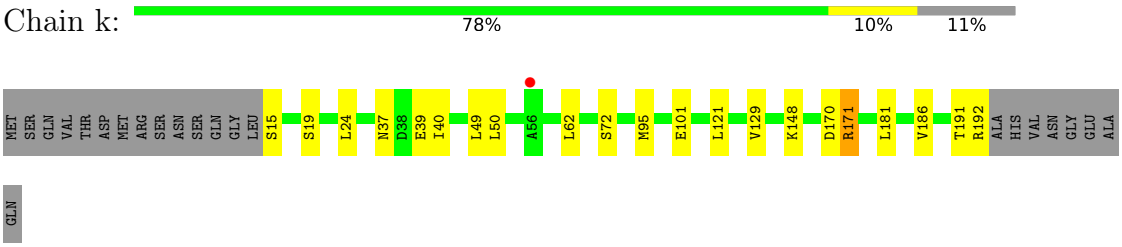
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain j:



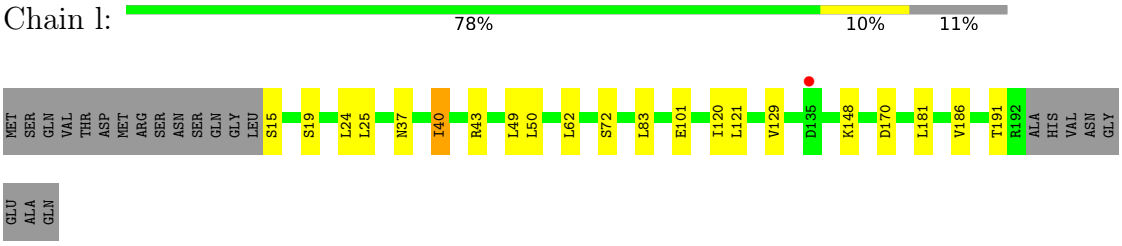
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

Chain k:



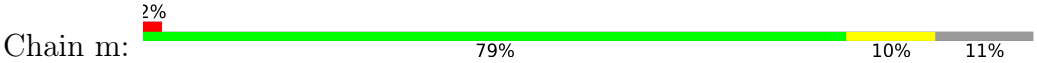
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1

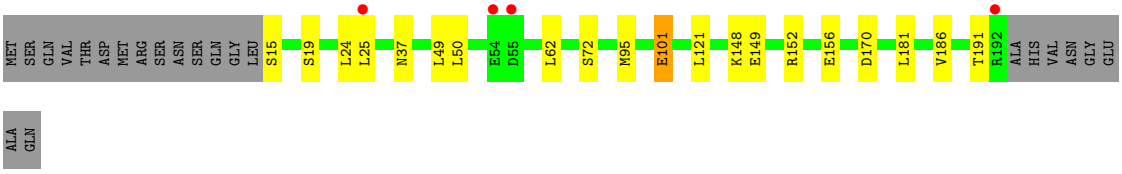
Chain l:



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

Chain m:





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

Chain n:

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

All (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
2	i	174	TRP	CB-CG	-5.17	1.41	1.50
1	D	29	GLU	CD-OE2	-5.03	1.20	1.25

All (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
2	J	168	ASP	CB-CG-OD1	13.88	130.79	118.30
1	e	100	ILE	CG1-CB-CG2	-12.82	83.19	111.40
2	I	164	ARG	CB-CG-CD	11.65	141.88	111.60
1	b	209	LEU	CA-CB-CG	10.90	140.38	115.30
1	e	31	ASN	CB-CA-C	-9.12	92.17	110.40
2	n	164	ARG	CG-CD-NE	9.04	130.78	111.80
1	A	31	ASN	CB-CA-C	-9.01	92.39	110.40
1	g	31	ASN	CB-CA-C	-8.93	92.54	110.40
1	a	31	ASN	CB-CA-C	-8.92	92.57	110.40
1	f	31	ASN	CB-CA-C	-8.87	92.66	110.40
1	C	31	ASN	CB-CA-C	-8.87	92.66	110.40
1	E	31	ASN	CB-CA-C	-8.84	92.72	110.40
2	m	170	ASP	CB-CG-OD1	8.66	126.09	118.30
1	D	31	ASN	CB-CA-C	-8.65	93.10	110.40
1	d	31	ASN	CB-CA-C	-8.59	93.21	110.40
1	B	31	ASN	CB-CA-C	-8.51	93.39	110.40
2	I	170	ASP	CB-CG-OD1	8.49	125.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	31	ASN	CB-CA-C	-8.47	93.46	110.40
1	G	31	ASN	CB-CA-C	-8.35	93.70	110.40
1	b	31	ASN	CB-CA-C	-8.27	93.86	110.40
2	h	170	ASP	CB-CG-OD1	8.24	125.72	118.30
1	d	201	ASP	CB-CG-OD2	8.18	125.66	118.30
1	c	31	ASN	CB-CA-C	-8.16	94.08	110.40
2	N	170	ASP	CB-CG-OD1	8.14	125.63	118.30
2	J	170	ASP	CB-CG-OD1	8.08	125.57	118.30
2	i	164	ARG	CG-CD-NE	7.93	128.46	111.80
1	f	70	ARG	NE-CZ-NH2	-7.93	116.34	120.30
2	i	170	ASP	CB-CG-OD1	7.78	125.30	118.30
2	k	171	ARG	CA-CB-CG	7.69	130.32	113.40
1	b	174	LYS	CA-CB-CG	7.63	130.18	113.40
2	h	170	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	F	70	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	f	70	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	86	LEU	CB-CG-CD1	7.24	123.31	111.00
1	d	174	LYS	CA-CB-CG	7.16	129.16	113.40
1	d	159	ARG	N-CA-CB	7.14	123.45	110.60
1	A	105	LEU	N-CA-C	-7.06	91.94	111.00
1	F	70	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	a	175	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	b	86	LEU	CB-CG-CD1	6.92	122.76	111.00
1	a	86	LEU	CB-CG-CD1	6.91	122.75	111.00
2	m	170	ASP	CB-CG-OD2	-6.85	112.13	118.30
2	I	163	GLU	CB-CG-CD	-6.79	95.86	114.20
1	d	160	MET	CG-SD-CE	6.78	111.05	100.20
2	i	170	ASP	CB-CG-OD2	-6.77	112.21	118.30
2	l	170	ASP	CB-CG-OD2	6.76	124.39	118.30
2	J	170	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	d	201	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	b	159	ARG	CD-NE-CZ	6.68	132.96	123.60
2	I	170	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	d	159	ARG	CG-CD-NE	-6.67	97.80	111.80
1	B	163	LEU	CA-CB-CG	6.59	130.46	115.30
2	M	126	LEU	CB-CA-C	6.55	122.65	110.20
1	D	21	GLU	CG-CD-OE2	-6.52	105.27	118.30
1	G	160	MET	CG-SD-CE	6.50	110.60	100.20
2	j	120	ILE	CG1-CB-CG2	-6.46	97.20	111.40
2	i	23	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	a	14	TYR	CA-CB-CG	-6.39	101.25	113.40
1	g	70	ARG	NE-CZ-NH2	-6.39	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	GLN	CB-CA-C	-6.38	97.63	110.40
1	g	159	ARG	CD-NE-CZ	6.38	132.53	123.60
2	k	170	ASP	CB-CG-OD2	6.38	124.04	118.30
1	g	159	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	J	168	ASP	OD1-CG-OD2	-6.36	111.21	123.30
1	d	159	ARG	CA-CB-CG	6.36	127.39	113.40
1	C	160	MET	CG-SD-CE	6.34	110.35	100.20
2	n	170	ASP	CB-CG-OD2	6.34	124.01	118.30
1	D	160	MET	CG-SD-CE	6.34	110.34	100.20
1	a	175	ASP	CB-CG-OD2	6.34	124.00	118.30
2	N	24	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	G	70	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	e	94	GLN	CG-CD-OE1	-6.27	109.06	121.60
1	c	160	MET	CG-SD-CE	6.26	110.21	100.20
2	N	170	ASP	CB-CG-OD2	-6.24	112.68	118.30
2	j	170	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	g	70	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	G	70	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	c	163	LEU	CA-CB-CG	6.18	129.50	115.30
1	g	159	ARG	CG-CD-NE	6.18	124.77	111.80
1	e	131	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	N	23	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	H	147	LYS	CB-CG-CD	6.12	127.51	111.60
2	n	120	ILE	CG1-CB-CG2	-6.10	97.99	111.40
2	j	170	ASP	CB-CG-OD2	6.04	123.73	118.30
2	M	170	ASP	CB-CG-OD2	6.04	123.73	118.30
2	M	120	ILE	CA-CB-CG1	-6.02	99.57	111.00
2	H	170	ASP	CB-CG-OD2	5.98	123.68	118.30
1	b	160	MET	CG-SD-CE	5.98	109.77	100.20
1	F	160	MET	CG-SD-CE	5.91	109.66	100.20
1	B	160	MET	CG-SD-CE	5.89	109.63	100.20
1	b	159	ARG	CG-CD-NE	5.85	124.08	111.80
1	b	209	LEU	CB-CG-CD2	5.82	120.89	111.00
1	g	131	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	n	179	GLU	CG-CD-OE2	5.79	129.88	118.30
2	N	24	LEU	CB-CG-CD1	5.79	120.84	111.00
2	M	179	GLU	CG-CD-OE2	5.78	129.86	118.30
2	I	120	ILE	CA-CB-CG1	-5.73	100.11	111.00
2	H	131	GLY	N-CA-C	5.72	127.41	113.10
1	b	188	ILE	N-CA-CB	5.69	123.89	110.80
1	D	21	GLU	CG-CD-OE1	5.68	129.67	118.30
1	D	29	GLU	CG-CD-OE1	5.67	129.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	130	THR	CB-CA-C	-5.61	96.46	111.60
2	k	192	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	l	120	ILE	CA-CB-CG1	-5.59	100.38	111.00
2	L	170	ASP	CB-CG-OD2	5.52	123.27	118.30
1	e	157	ILE	CB-CA-C	5.51	122.63	111.60
1	b	159	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	j	43	ARG	CG-CD-NE	5.50	123.34	111.80
2	l	40	ILE	CG1-CB-CG2	-5.48	99.34	111.40
2	M	179	GLU	CG-CD-OE1	-5.48	107.35	118.30
1	B	131	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	i	179	GLU	CG-CD-OE1	-5.35	107.61	118.30
2	n	179	GLU	CG-CD-OE1	-5.31	107.68	118.30
2	L	170	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	D	29	GLU	CG-CD-OE2	-5.29	107.71	118.30
1	F	14	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	I	131	GLY	N-CA-C	5.29	126.32	113.10
1	F	157	ILE	CB-CA-C	5.28	122.16	111.60
2	i	179	GLU	CG-CD-OE2	5.28	128.86	118.30
1	F	131	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	L	126	LEU	CA-CB-CG	5.24	127.35	115.30
2	M	101	GLU	CG-CD-OE2	5.21	128.72	118.30
1	f	174	LYS	CD-CE-NZ	5.21	123.68	111.70
1	c	208	LYS	CA-CB-CG	5.21	124.86	113.40
1	G	174	LYS	CD-CE-NZ	5.18	123.62	111.70
1	e	151	GLU	CG-CD-OE2	5.15	128.61	118.30
1	g	151	GLU	CG-CD-OE1	-5.15	107.99	118.30
2	K	40	ILE	CG1-CB-CG2	-5.15	100.06	111.40
2	M	126	LEU	CB-CG-CD1	5.12	119.71	111.00
2	J	43	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	n	126	LEU	CA-CB-CG	5.12	127.06	115.30
1	F	174	LYS	CD-CE-NZ	5.11	123.44	111.70
1	d	157	ILE	CB-CA-C	5.10	121.80	111.60
2	n	130	THR	CB-CA-C	-5.08	97.89	111.60
2	H	43	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	14	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	l	43	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	l	170	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	C	168	LEU	CA-CB-CG	5.05	126.92	115.30
2	K	170	ASP	CB-CG-OD2	5.05	122.84	118.30
1	c	174	LYS	CD-CE-NZ	5.05	123.31	111.70
2	M	170	ASP	CB-CG-OD1	-5.04	113.77	118.30
2	K	126	LEU	CA-CB-CG	5.03	126.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	PHE	CB-CG-CD1	5.02	124.31	120.80
1	g	185	ARG	NE-CZ-NH1	5.02	122.81	120.30

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	D	48	VAL
1	E	48	VAL
1	F	48	VAL
1	F	209	LEU
1	G	48	VAL
2	H	191	THR

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Mol	Chain	Res	Type
1	a	48	VAL
1	b	48	VAL
1	c	48	VAL
1	d	48	VAL
1	e	48	VAL
1	f	48	VAL
1	g	48	VAL
1	D	209	LEU
1	A	209	LEU
1	C	106	GLY
1	F	106	GLY
1	d	209	LEU
1	B	106	GLY
1	C	209	LEU
1	D	106	GLY
1	E	106	GLY
1	G	106	GLY
1	a	106	GLY
1	b	106	GLY
1	c	106	GLY
1	d	106	GLY
1	e	106	GLY
1	f	106	GLY
1	f	209	LEU
1	g	106	GLY
1	g	209	LEU

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (481) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	27	VAL
1	A	36	LEU
1	A	61	LEU
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	135	HIS
1	A	138	SER
1	A	152	ILE
1	A	158	GLU
1	A	167	THR
1	A	185	ARG
1	A	209	LEU
1	A	210	SER
1	B	22	HIS
1	B	27	VAL
1	B	36	LEU
1	B	61	LEU
1	B	86	LEU
1	B	135	HIS
1	B	138	SER
1	B	152	ILE
1	B	158	GLU
1	B	163	LEU
1	B	167	THR
1	B	185	ARG
1	B	209	LEU
1	B	210	SER
1	C	22	HIS
1	C	27	VAL
1	C	36	LEU
1	C	61	LEU
1	C	73	THR
1	C	86	LEU
1	C	107	GLN
1	C	135	HIS
1	C	138	SER
1	C	152	ILE
1	C	158	GLU
1	C	164	MET
1	C	167	THR
1	C	168	LEU
1	C	174	LYS
1	C	185	ARG
1	C	209	LEU
1	C	210	SER
1	D	14	TYR
1	D	22	HIS

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Mol	Chain	Res	Type
1	D	27	VAL
1	D	36	LEU
1	D	61	LEU
1	D	86	LEU
1	D	121	PRO
1	D	135	HIS
1	D	138	SER
1	D	152	ILE
1	D	157	ILE
1	D	158	GLU
1	D	159	ARG
1	D	164	MET
1	D	167	THR
1	D	185	ARG
1	D	208	LYS
1	D	209	LEU
1	D	210	SER
1	E	22	HIS
1	E	27	VAL
1	E	36	LEU
1	E	73	THR
1	E	86	LEU
1	E	135	HIS
1	E	138	SER
1	E	152	ILE
1	E	164	MET
1	E	167	THR
1	E	185	ARG
1	E	208	LYS
1	E	209	LEU
1	E	210	SER
1	F	22	HIS
1	F	27	VAL
1	F	36	LEU
1	F	61	LEU
1	F	71	ASP
1	F	86	LEU
1	F	135	HIS
1	F	138	SER
1	F	152	ILE
1	F	157	ILE
1	F	158	GLU

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Mol	Chain	Res	Type
1	F	159	ARG
1	F	164	MET
1	F	167	THR
1	F	170	ARG
1	F	180	ARG
1	F	185	ARG
1	F	209	LEU
1	F	210	SER
1	G	22	HIS
1	G	27	VAL
1	G	36	LEU
1	G	73	THR
1	G	86	LEU
1	G	135	HIS
1	G	138	SER
1	G	152	ILE
1	G	158	GLU
1	G	167	THR
1	G	185	ARG
1	G	188	ILE
2	H	7	MET
2	H	8	ARG
2	H	11	SER
2	H	12	GLN
2	H	14	LEU
2	H	15	SER
2	H	19	SER
2	H	24	LEU
2	H	25	LEU
2	H	37	ASN
2	H	49	LEU
2	H	50	LEU
2	H	62	LEU
2	H	67	PRO
2	H	72	SER
2	H	95	MET
2	H	101	GLU
2	H	121	LEU
2	H	129	VAL
2	H	181	LEU
2	H	186	VAL
2	H	191	THR

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Mol	Chain	Res	Type
2	I	15	SER
2	I	19	SER
2	I	24	LEU
2	I	37	ASN
2	I	49	LEU
2	I	50	LEU
2	I	62	LEU
2	I	72	SER
2	I	101	GLU
2	I	121	LEU
2	I	129	VAL
2	I	148	LYS
2	I	181	LEU
2	I	186	VAL
2	J	15	SER
2	J	19	SER
2	J	24	LEU
2	J	25	LEU
2	J	37	ASN
2	J	49	LEU
2	J	50	LEU
2	J	62	LEU
2	J	72	SER
2	J	101	GLU
2	J	121	LEU
2	J	129	VAL
2	J	148	LYS
2	J	181	LEU
2	J	186	VAL
2	J	191	THR
2	J	192	ARG
2	K	15	SER
2	K	19	SER
2	K	24	LEU
2	K	25	LEU
2	K	37	ASN
2	K	40	ILE
2	K	49	LEU
2	K	50	LEU
2	K	51	LEU
2	K	62	LEU
2	K	72	SER

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Mol	Chain	Res	Type
2	K	95	MET
2	K	101	GLU
2	K	121	LEU
2	K	126	LEU
2	K	148	LYS
2	K	149	GLU
2	K	181	LEU
2	K	186	VAL
2	K	191	THR
2	L	15	SER
2	L	19	SER
2	L	24	LEU
2	L	25	LEU
2	L	37	ASN
2	L	49	LEU
2	L	50	LEU
2	L	62	LEU
2	L	67	PRO
2	L	72	SER
2	L	95	MET
2	L	101	GLU
2	L	121	LEU
2	L	126	LEU
2	L	129	VAL
2	L	148	LYS
2	L	181	LEU
2	L	186	VAL
2	L	192	ARG
2	M	15	SER
2	M	19	SER
2	M	24	LEU
2	M	25	LEU
2	M	37	ASN
2	M	49	LEU
2	M	50	LEU
2	M	59	ASP
2	M	62	LEU
2	M	72	SER
2	M	101	GLU
2	M	121	LEU
2	M	126	LEU
2	M	129	VAL

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Mol	Chain	Res	Type
2	M	148	LYS
2	M	181	LEU
2	M	186	VAL
2	M	191	THR
2	N	15	SER
2	N	19	SER
2	N	37	ASN
2	N	49	LEU
2	N	50	LEU
2	N	62	LEU
2	N	72	SER
2	N	95	MET
2	N	101	GLU
2	N	121	LEU
2	N	129	VAL
2	N	148	LYS
2	N	181	LEU
2	N	186	VAL
2	N	191	THR
2	N	198	GLU
1	a	22	HIS
1	a	27	VAL
1	a	36	LEU
1	a	73	THR
1	a	135	HIS
1	a	138	SER
1	a	152	ILE
1	a	158	GLU
1	a	164	MET
1	a	167	THR
1	a	185	ARG
1	a	209	LEU
1	a	210	SER
1	b	22	HIS
1	b	27	VAL
1	b	36	LEU
1	b	61	LEU
1	b	73	THR
1	b	107	GLN
1	b	135	HIS
1	b	138	SER
1	b	152	ILE

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Mol	Chain	Res	Type
1	b	158	GLU
1	b	159	ARG
1	b	164	MET
1	b	167	THR
1	b	180	ARG
1	b	185	ARG
1	b	188	ILE
1	b	209	LEU
1	b	210	SER
1	c	14	TYR
1	c	22	HIS
1	c	27	VAL
1	c	36	LEU
1	c	86	LEU
1	c	135	HIS
1	c	138	SER
1	c	152	ILE
1	c	158	GLU
1	c	163	LEU
1	c	164	MET
1	c	167	THR
1	c	185	ARG
1	c	208	LYS
1	c	209	LEU
1	c	210	SER
1	d	22	HIS
1	d	27	VAL
1	d	36	LEU
1	d	61	LEU
1	d	86	LEU
1	d	107	GLN
1	d	135	HIS
1	d	138	SER
1	d	152	ILE
1	d	157	ILE
1	d	158	GLU
1	d	159	ARG
1	d	164	MET
1	d	167	THR
1	d	180	ARG
1	d	185	ARG
1	d	209	LEU

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Mol	Chain	Res	Type
1	d	210	SER
1	e	14	TYR
1	e	22	HIS
1	e	27	VAL
1	e	36	LEU
1	e	86	LEU
1	e	135	HIS
1	e	138	SER
1	e	152	ILE
1	e	157	ILE
1	e	158	GLU
1	e	164	MET
1	e	167	THR
1	e	180	ARG
1	e	185	ARG
1	e	209	LEU
1	e	210	SER
1	f	14	TYR
1	f	22	HIS
1	f	27	VAL
1	f	36	LEU
1	f	61	LEU
1	f	73	THR
1	f	86	LEU
1	f	107	GLN
1	f	135	HIS
1	f	138	SER
1	f	152	ILE
1	f	164	MET
1	f	167	THR
1	f	185	ARG
1	f	209	LEU
1	f	210	SER
1	g	14	TYR
1	g	22	HIS
1	g	27	VAL
1	g	36	LEU
1	g	61	LEU
1	g	73	THR
1	g	86	LEU
1	g	135	HIS
1	g	138	SER

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Mol	Chain	Res	Type
1	g	152	ILE
1	g	158	GLU
1	g	159	ARG
1	g	164	MET
1	g	167	THR
1	g	185	ARG
1	g	209	LEU
1	g	210	SER
2	h	15	SER
2	h	19	SER
2	h	24	LEU
2	h	25	LEU
2	h	37	ASN
2	h	39	GLU
2	h	40	ILE
2	h	49	LEU
2	h	50	LEU
2	h	62	LEU
2	h	72	SER
2	h	95	MET
2	h	101	GLU
2	h	121	LEU
2	h	129	VAL
2	h	148	LYS
2	h	181	LEU
2	h	186	VAL
2	h	191	THR
2	h	192	ARG
2	h	194	HIS
2	i	15	SER
2	i	19	SER
2	i	23	ARG
2	i	24	LEU
2	i	25	LEU
2	i	37	ASN
2	i	49	LEU
2	i	50	LEU
2	i	62	LEU
2	i	72	SER
2	i	95	MET
2	i	101	GLU
2	i	121	LEU

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Mol	Chain	Res	Type
2	i	129	VAL
2	i	130	THR
2	i	148	LYS
2	i	181	LEU
2	i	186	VAL
2	i	191	THR
2	i	192	ARG
2	i	194	HIS
2	j	15	SER
2	j	19	SER
2	j	24	LEU
2	j	37	ASN
2	j	49	LEU
2	j	50	LEU
2	j	62	LEU
2	j	72	SER
2	j	101	GLU
2	j	121	LEU
2	j	129	VAL
2	j	148	LYS
2	j	181	LEU
2	j	186	VAL
2	j	191	THR
2	k	15	SER
2	k	19	SER
2	k	24	LEU
2	k	37	ASN
2	k	39	GLU
2	k	40	ILE
2	k	49	LEU
2	k	50	LEU
2	k	62	LEU
2	k	72	SER
2	k	95	MET
2	k	101	GLU
2	k	121	LEU
2	k	129	VAL
2	k	148	LYS
2	k	171	ARG
2	k	181	LEU
2	k	186	VAL
2	k	191	THR

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Mol	Chain	Res	Type
2	l	15	SER
2	l	19	SER
2	l	24	LEU
2	l	25	LEU
2	l	37	ASN
2	l	40	ILE
2	l	49	LEU
2	l	50	LEU
2	l	62	LEU
2	l	72	SER
2	l	83	LEU
2	l	101	GLU
2	l	121	LEU
2	l	129	VAL
2	l	148	LYS
2	l	181	LEU
2	l	186	VAL
2	l	191	THR
2	m	15	SER
2	m	19	SER
2	m	24	LEU
2	m	25	LEU
2	m	37	ASN
2	m	49	LEU
2	m	50	LEU
2	m	62	LEU
2	m	72	SER
2	m	95	MET
2	m	101	GLU
2	m	121	LEU
2	m	148	LYS
2	m	149	GLU
2	m	152	ARG
2	m	156	GLU
2	m	181	LEU
2	m	186	VAL
2	m	191	THR
2	n	15	SER
2	n	19	SER
2	n	24	LEU
2	n	25	LEU
2	n	37	ASN

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Mol	Chain	Res	Type
2	n	49	LEU
2	n	50	LEU
2	n	62	LEU
2	n	72	SER
2	n	93	MET
2	n	101	GLU
2	n	121	LEU
2	n	126	LEU
2	n	129	VAL
2	n	148	LYS
2	n	181	LEU
2	n	186	VAL
2	n	191	THR
2	n	198	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	135	HIS
1	A	136	GLN
1	B	31	ASN
1	B	135	HIS
1	C	31	ASN
1	C	47	GLN
1	C	135	HIS
1	C	144	GLN
1	D	22	HIS
1	D	31	ASN
1	D	135	HIS
1	D	136	GLN
1	E	31	ASN
1	E	135	HIS
1	F	31	ASN
1	F	135	HIS
1	F	171	HIS
1	G	31	ASN
1	G	135	HIS
1	G	136	GLN
2	H	12	GLN
2	H	37	ASN
2	H	123	HIS

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Mol	Chain	Res	Type
2	I	37	ASN
2	I	65	ASN
2	I	123	HIS
2	J	37	ASN
2	J	65	ASN
2	J	123	HIS
2	K	37	ASN
2	K	123	HIS
2	L	37	ASN
2	L	123	HIS
2	M	37	ASN
2	M	65	ASN
2	M	123	HIS
2	N	37	ASN
2	N	117	HIS
2	N	123	HIS
2	N	196	ASN
1	a	31	ASN
1	a	135	HIS
1	a	136	GLN
1	a	144	GLN
1	b	31	ASN
1	b	135	HIS
1	b	146	GLN
1	c	31	ASN
1	c	135	HIS
1	d	31	ASN
1	d	135	HIS
1	d	136	GLN
1	e	31	ASN
1	e	135	HIS
1	e	136	GLN
1	f	31	ASN
1	f	135	HIS
1	f	136	GLN
1	g	31	ASN
1	g	47	GLN
1	g	135	HIS
1	g	136	GLN
2	h	37	ASN
2	h	123	HIS
2	i	37	ASN

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Mol	Chain	Res	Type
2	i	65	ASN
2	i	123	HIS
2	j	37	ASN
2	j	123	HIS
2	k	37	ASN
2	k	123	HIS
2	l	37	ASN
2	l	123	HIS
2	m	37	ASN
2	m	123	HIS
2	n	37	ASN
2	n	123	HIS

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	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

All (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
2	h	195	VAL	3.8
1	B	25	PHE	3.7
2	j	54	GLU	3.6
2	h	193	ALA	3.6
1	F	21	GLU	3.5
1	A	209	LEU	3.4
2	K	54	GLU	3.3
1	A	24	SER	3.3
1	F	69	ASP	3.3
2	M	87	ASP	3.2
2	M	54	GLU	3.2
2	K	130	THR	3.1
2	M	57	SER	3.1
1	G	97	ARG	3.1
1	A	21	GLU	3.0
2	N	193	ALA	3.0
1	B	83	PHE	3.0
1	b	14	TYR	2.9
1	B	24	SER	2.9
2	n	194	HIS	2.9
1	d	22	HIS	2.8
1	G	24	SER	2.8
1	C	209	LEU	2.8
1	b	97	ARG	2.8
2	M	59	ASP	2.8
2	M	25	LEU	2.8
1	B	21	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	57	SER	2.7
1	b	20	ILE	2.7
1	B	20	ILE	2.6
1	D	21	GLU	2.6
2	H	13	GLY	2.6
1	E	83	PHE	2.6
2	L	126	LEU	2.6
2	m	54	GLU	2.5
2	N	143	PHE	2.5
2	H	35	GLU	2.5
1	f	21	GLU	2.4
1	B	48	VAL	2.4
1	A	25	PHE	2.4
1	F	68	PRO	2.4
2	L	129	VAL	2.3
1	c	83	PHE	2.3
2	h	197	GLY	2.3
2	M	58	LYS	2.3
2	L	143	PHE	2.3
2	L	56	ALA	2.3
2	L	192	ARG	2.2
2	l	135	ASP	2.2
2	j	87	ASP	2.2
1	e	151	GLU	2.2
1	B	69	ASP	2.2
1	E	27	VAL	2.2
2	J	54	GLU	2.2
1	B	178	VAL	2.2
2	L	185	PHE	2.2
2	n	130	THR	2.2
1	F	197	TYR	2.2
1	F	27	VAL	2.1
1	b	21	GLU	2.1
2	N	194	HIS	2.1
1	d	25	PHE	2.1
1	C	24	SER	2.1
1	a	210	SER	2.1
1	b	25	PHE	2.1
2	L	85	PRO	2.1
2	I	130	THR	2.1
2	M	172	ASP	2.1
1	G	22	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	m	25	LEU	2.0
2	j	55	ASP	2.0
1	C	21	GLU	2.0
2	k	56	ALA	2.0
2	M	175	PHE	2.0
2	m	55	ASP	2.0
2	M	26	SER	2.0
2	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.