Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2016 – 07:27 PM EDT

PDB ID	:	5DZK
Title	:	Crystal structure of the active form of the proteolytic complex clpP1 and clpP2
Authors	:	LI, M.; Wlodawer, A.; Maurizi, M.
Deposited on	:	2015-09-25
Resolution	:	3.07 Å(reported)

This is a 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

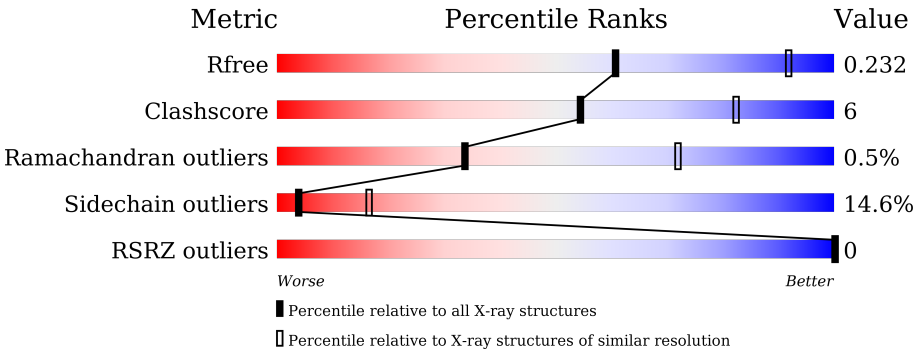
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (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}	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	64% 21% 6% • 8%
1	B	214	62% 24% 6% • 7%
1	C	214	60% 25% 7% 8%
1	D	214	62% 25% • 8%
1	E	214	64% 24% 5% 7%
1	F	214	62% 24% 5% • 8%

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Mol	Chain	Length	Quality of chain
1	G	214	66% 20% 5% 9%
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	33% 67%
2	2	3	67% 33%
2	3	3	67% 33%
2	4	3	67% 33%
2	O	3	33% 67%
2	P	3	33% 67%
2	Q	3	67% 33%
2	R	3	33% 33% 33%
2	S	3	33% 33% 33%
2	T	3	33% 33% 33%
2	U	3	33% 67%
2	V	3	67% 33%
2	W	3	67% 33%
2	X	3	33% 67%
2	Y	3	67% 33%
2	Z	3	67% 33%
2	o	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	p	3	33% 67%
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	66% 18% 5% 11%
3	I	200	64% 22% 11%
3	J	200	65% 20% 11%
3	K	200	67% 16% 6% 11%
3	L	200	65% 20% 11%
3	M	200	66% 19% 11%
3	N	200	63% 23% 11%
3	h	200	76% 13% 11%
3	i	200	75% 13% 11%
3	j	200	78% 11% 11%
3	k	200	77% 12% 11%
3	l	200	76% 12% 11%
3	m	200	76% 12% 11%
3	n	200	76% 12% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40976 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

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

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

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

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

- Molecule 4 is water.

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

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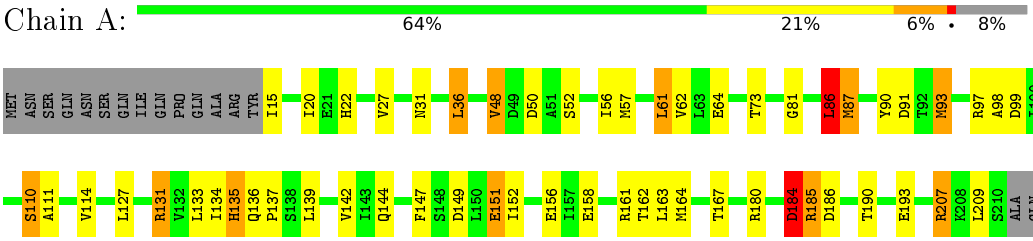
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	i	3	Total O 3 3	0	0
4	j	3	Total O 3 3	0	0
4	k	6	Total O 6 6	0	0
4	l	2	Total O 2 2	0	0
4	m	4	Total O 4 4	0	0
4	n	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

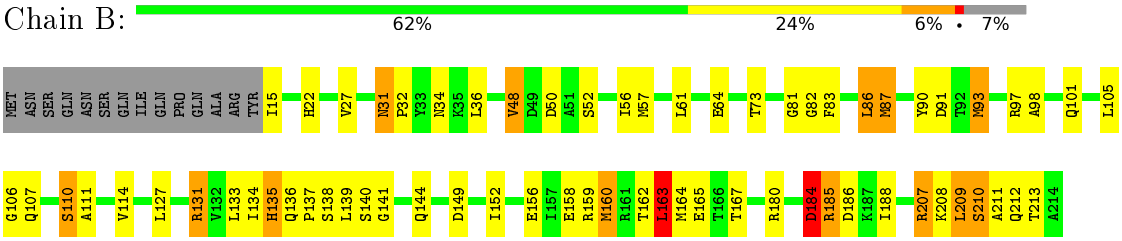
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A:



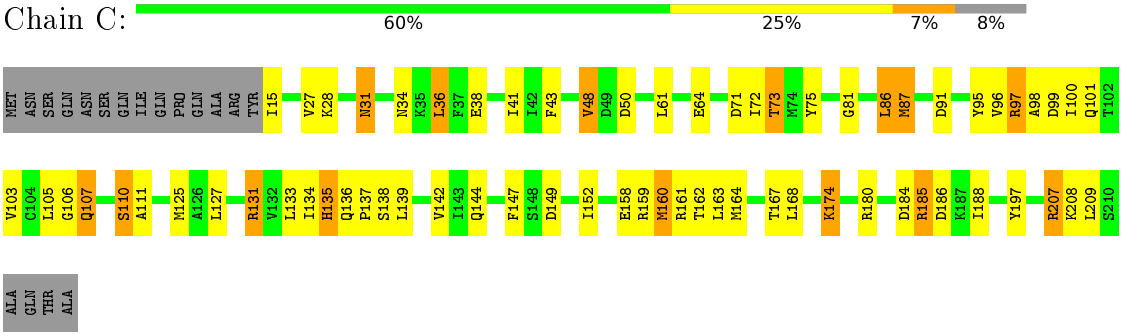
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



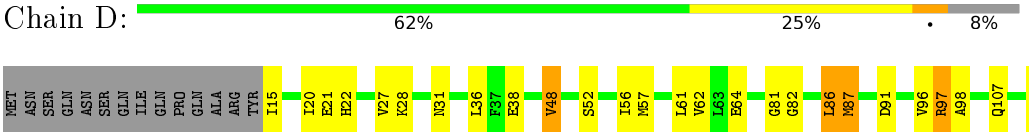
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain C:



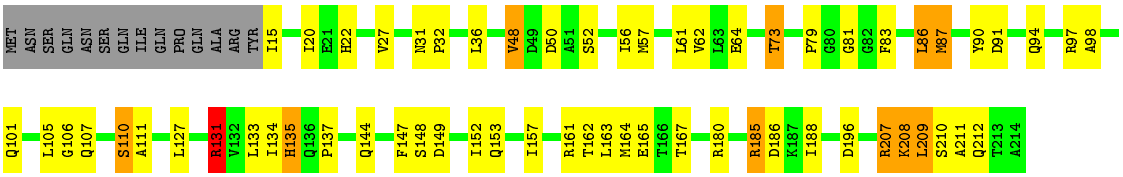
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D:



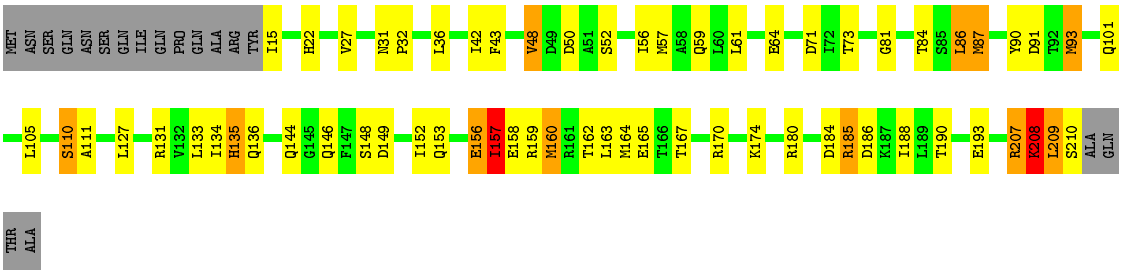
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E:



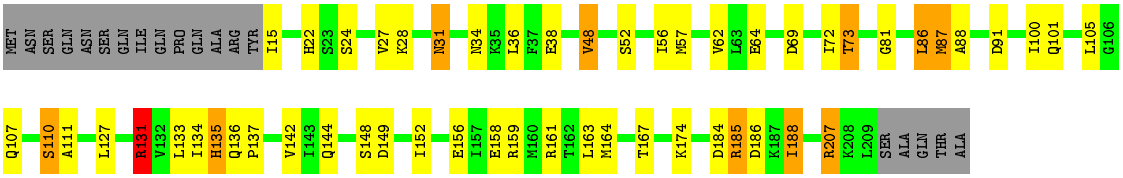
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F:



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

Chain G:



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

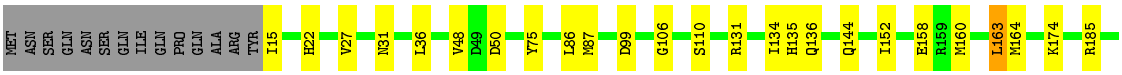
Chain a:

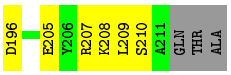
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain b:

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

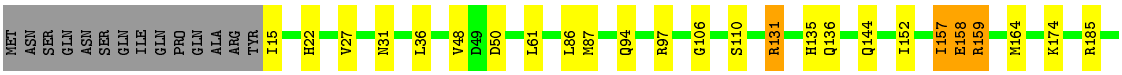
Chain c:

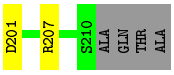




• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

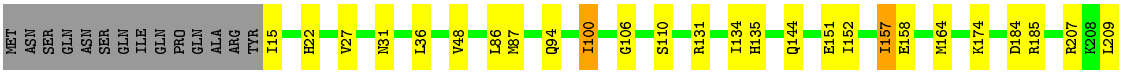
Chain d:





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

Chain e:

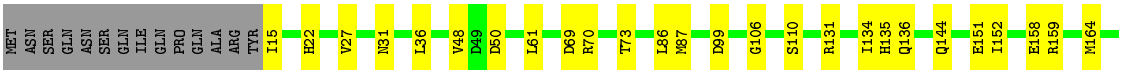


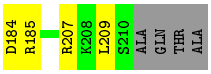
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain f:

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

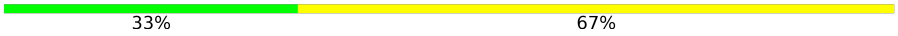
Chain g:





• Molecule 2: BEZ-LEU-LEU

Chain O:



• Molecule 2: BEZ-LEU-LEU

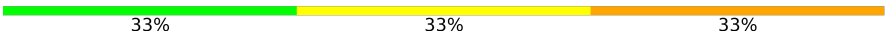
Chain P:

• Molecule 2: BEZ-LEU-LEU

Chain Q:

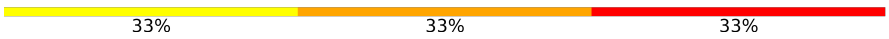
• Molecule 2: BEZ-LEU-LEU

Chain R:



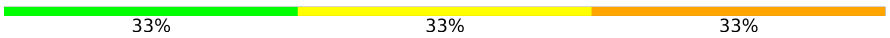
• Molecule 2: BEZ-LEU-LEU

Chain S:



• Molecule 2: BEZ-LEU-LEU

Chain T:



• Molecule 2: BEZ-LEU-LEU

Chain U:

- Molecule 2: BEZ-LEU-LEU

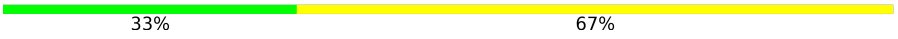
Chain V:

- Molecule 2: BEZ-LEU-LEU

Chain W:

- Molecule 2: BEZ-LEU-LEU

Chain X:



- Molecule 2: BEZ-LEU-LEU

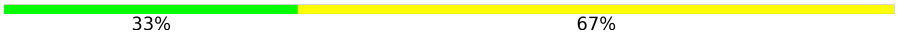
Chain Y:

- Molecule 2: BEZ-LEU-LEU

Chain Z:

- Molecule 2: BEZ-LEU-LEU

Chain 1:



- Molecule 2: BEZ-LEU-LEU

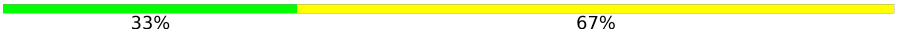
Chain 2:

- Molecule 2: BEZ-LEU-LEU

Chain o:

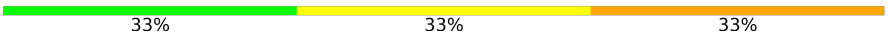
• Molecule 2: BEZ-LEU-LEU

Chain p:



• Molecule 2: BEZ-LEU-LEU

Chain q:

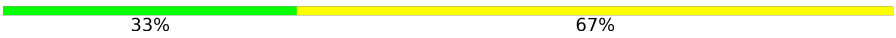


• Molecule 2: BEZ-LEU-LEU

Chain r:

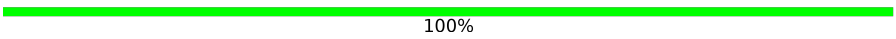
• Molecule 2: BEZ-LEU-LEU

Chain s:



• Molecule 2: BEZ-LEU-LEU

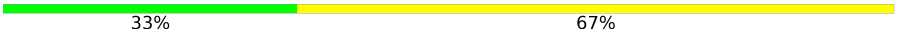
Chain t:



There are no outlier residues recorded for this chain.

• Molecule 2: BEZ-LEU-LEU

Chain u:



• Molecule 2: BEZ-LEU-LEU

Chain v:

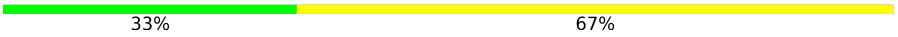
• Molecule 2: BEZ-LEU-LEU

Chain w:

There are no outlier residues recorded for this chain.

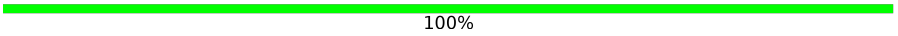
• Molecule 2: BEZ-LEU-LEU

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

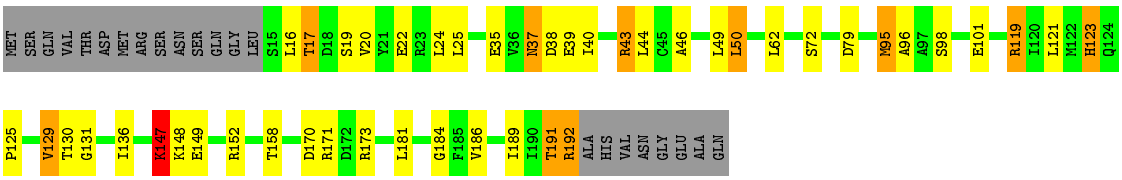
Chain 3:

• Molecule 2: BEZ-LEU-LEU

Chain 4:

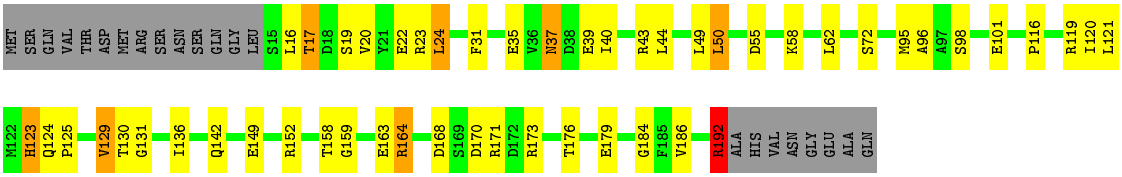
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain H:



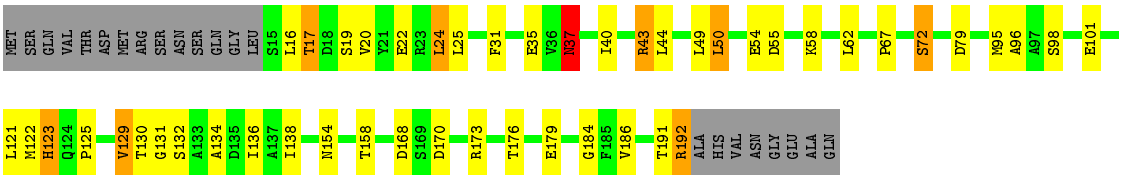
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain I:



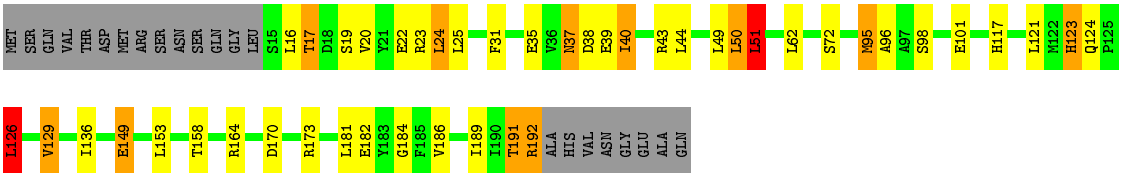
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain J:



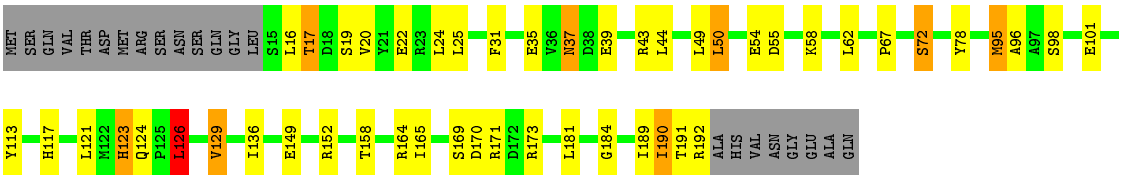
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain K:



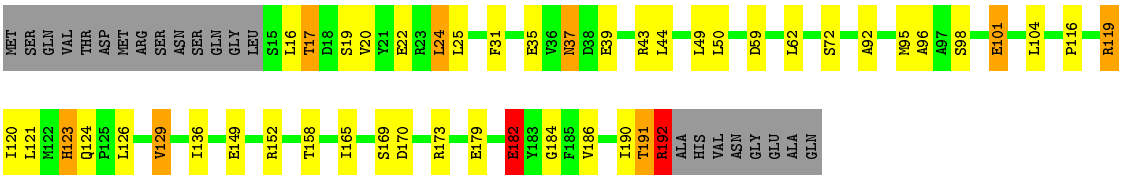
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain L:



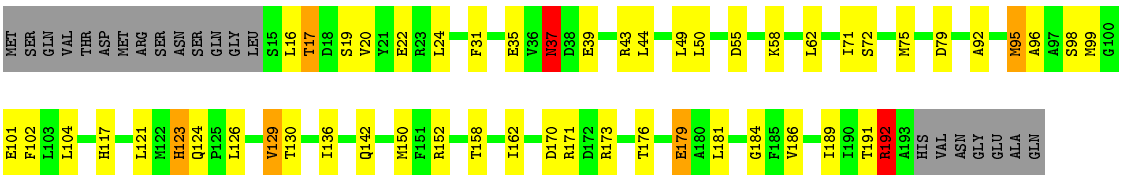
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain M:



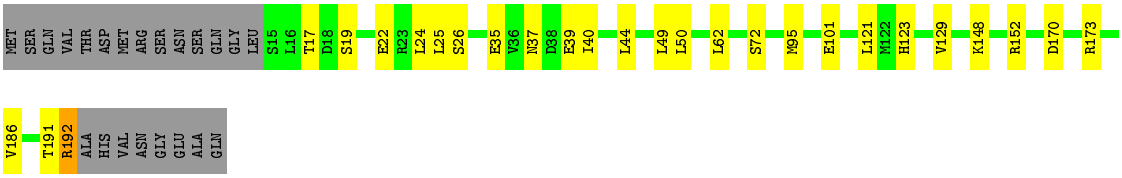
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



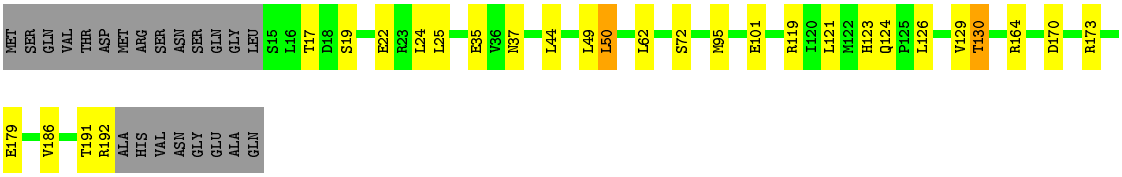
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain h:



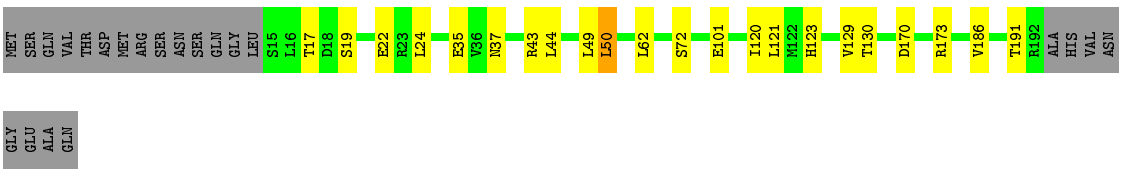
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain i:



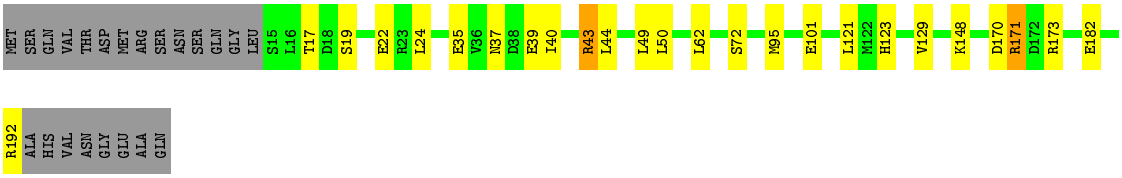
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain j:



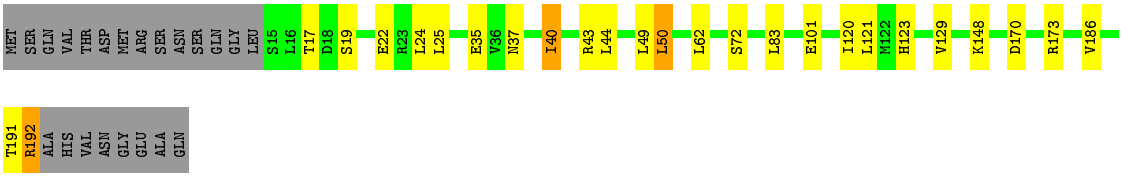
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain k:



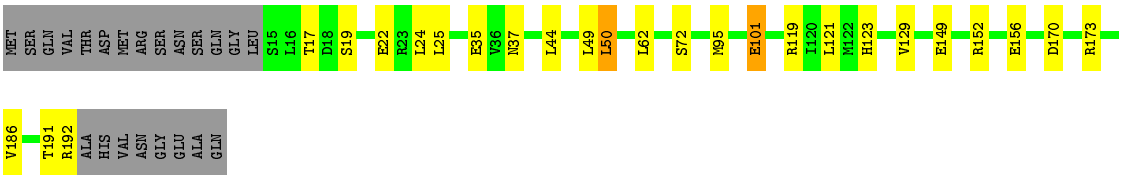
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain l:



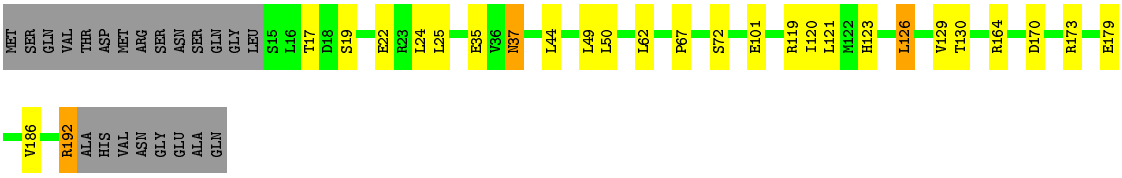
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain m:



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

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	205.94Å 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 (5.30%)	DCC
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	7 of 121114 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	40976	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

All (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
3	M	179	GLU	CD-OE1	-6.38	1.18	1.25
3	h	192	ARG	N-CA	6.00	1.58	1.46
1	D	21	GLU	CD-OE2	-5.70	1.19	1.25
1	f	158	GLU	CD-OE2	-5.63	1.19	1.25
3	m	101	GLU	CD-OE1	-5.53	1.19	1.25
3	I	163	GLU	CD-OE1	-5.48	1.19	1.25
1	c	205	GLU	CD-OE1	5.42	1.31	1.25
1	g	151	GLU	CD-OE1	-5.38	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	i	179	GLU	CD-OE1	-5.30	1.19	1.25
1	d	94	GLN	CD-OE1	5.01	1.34	1.24

All (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
1	e	94	GLN	CA-CB-CG	-14.42	81.67	113.40
3	J	168	ASP	CB-CG-OD1	14.32	131.19	118.30
1	e	174	LYS	CD-CE-NZ	12.95	141.49	111.70
1	D	174	LYS	CD-CE-NZ	12.53	140.53	111.70
1	e	100	ILE	CG1-CB-CG2	-12.44	84.03	111.40
3	h	26	SER	CB-CA-C	-11.12	88.98	110.10
3	N	170	ASP	CB-CG-OD1	10.96	128.16	118.30
3	i	119	ARG	NE-CZ-NH1	10.51	125.55	120.30
3	I	164	ARG	CB-CG-CD	10.25	138.25	111.60
3	J	170	ASP	CB-CG-OD1	10.03	127.33	118.30
3	i	170	ASP	CB-CG-OD1	9.90	127.21	118.30
3	m	170	ASP	CB-CG-OD1	9.89	127.20	118.30
3	h	170	ASP	CB-CG-OD2	-9.72	109.56	118.30
3	I	170	ASP	CB-CG-OD1	9.48	126.83	118.30
3	L	126	LEU	CA-CB-CG	9.20	136.47	115.30
3	n	119	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	b	86	LEU	CB-CG-CD1	9.04	126.36	111.00
3	I	170	ASP	CB-CG-OD2	-8.92	110.28	118.30
3	K	126	LEU	CA-CB-CG	8.87	135.71	115.30
3	n	126	LEU	CA-CB-CG	8.74	135.40	115.30
1	a	86	LEU	CB-CG-CD1	8.66	125.72	111.00
3	m	170	ASP	CB-CG-OD2	-8.59	110.57	118.30
3	j	43	ARG	CG-CD-NE	8.58	129.81	111.80
3	J	170	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	B	160	MET	CG-SD-CE	8.49	113.78	100.20
3	h	170	ASP	CB-CG-OD1	8.29	125.76	118.30
1	d	201	ASP	CB-CG-OD2	8.26	125.73	118.30
1	C	160	MET	CG-SD-CE	8.24	113.39	100.20
1	c	205	GLU	CG-CD-OE2	-8.22	101.86	118.30
1	A	86	LEU	CB-CG-CD1	8.17	124.88	111.00
1	c	160	MET	CG-SD-CE	8.15	113.25	100.20
1	F	160	MET	CG-SD-CE	8.02	113.03	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	107	GLN	CB-CA-C	-7.94	94.52	110.40
3	k	171	ARG	CA-CB-CG	7.90	130.78	113.40
3	i	124	GLN	CB-CA-C	-7.89	94.62	110.40
1	c	205	GLU	CG-CD-OE1	7.74	133.79	118.30
3	I	163	GLU	CB-CG-CD	-7.72	93.36	114.20
1	C	107	GLN	CB-CA-C	-7.69	95.01	110.40
3	J	168	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	B	163	LEU	CA-CB-CG	7.55	132.67	115.30
3	i	164	ARG	CG-CD-NE	7.55	127.66	111.80
3	n	164	ARG	CG-CD-NE	7.55	127.65	111.80
3	l	170	ASP	CB-CG-OD2	7.47	125.03	118.30
3	M	126	LEU	CB-CA-C	7.35	124.17	110.20
1	b	131	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	c	163	LEU	CA-CB-CG	7.30	132.09	115.30
3	H	119	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	B	31	ASN	CB-CA-C	-7.16	96.07	110.40
1	d	159	ARG	CG-CD-NE	-7.16	96.77	111.80
3	N	170	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	a	31	ASN	CB-CA-C	-7.05	96.30	110.40
3	i	170	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	C	31	ASN	CB-CA-C	-7.02	96.37	110.40
1	f	31	ASN	CB-CA-C	-6.99	96.42	110.40
1	e	31	ASN	CB-CA-C	-6.88	96.65	110.40
1	A	31	ASN	CB-CA-C	-6.84	96.71	110.40
3	K	51	LEU	CB-CG-CD1	-6.82	99.40	111.00
3	N	179	GLU	CG-CD-OE1	6.80	131.90	118.30
3	I	119	ARG	CG-CD-NE	6.79	126.06	111.80
1	E	31	ASN	CB-CA-C	-6.78	96.84	110.40
3	M	170	ASP	CB-CG-OD2	6.78	124.40	118.30
3	l	192	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	d	201	ASP	CB-CG-OD1	-6.74	112.23	118.30
3	n	170	ASP	CB-CG-OD2	6.71	124.34	118.30
3	n	120	ILE	CG1-CB-CG2	-6.70	96.67	111.40
1	b	31	ASN	CB-CA-C	-6.68	97.04	110.40
1	D	31	ASN	CB-CA-C	-6.66	97.09	110.40
1	A	105	LEU	N-CA-C	-6.51	93.41	111.00
3	M	192	ARG	NE-CZ-NH1	6.49	123.55	120.30
3	j	120	ILE	CG1-CB-CG2	-6.49	97.12	111.40
1	g	31	ASN	CB-CA-C	-6.46	97.49	110.40
2	z	803	LEU	CA-CB-CG	6.45	130.14	115.30
1	e	131	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	q	802	LEU	CA-CB-CG	6.42	130.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	131	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	F	157	ILE	CB-CA-C	6.36	124.32	111.60
3	i	50	LEU	CA-CB-CG	6.35	129.91	115.30
3	I	192	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	d	157	ILE	CB-CA-C	6.28	124.17	111.60
1	F	31	ASN	CB-CA-C	-6.28	97.83	110.40
3	i	130	THR	CB-CA-C	-6.27	94.67	111.60
1	d	158	GLU	OE1-CD-OE2	-6.26	115.78	123.30
1	d	31	ASN	CB-CA-C	-6.23	97.94	110.40
3	j	130	THR	CB-CA-C	-6.22	94.81	111.60
3	k	170	ASP	CB-CG-OD2	6.22	123.90	118.30
3	N	179	GLU	CG-CD-OE2	-6.20	105.91	118.30
3	m	50	LEU	CA-CB-CG	6.19	129.55	115.30
2	Z	803	LEU	CA-CB-CG	6.17	129.50	115.30
1	G	31	ASN	CB-CA-C	-6.14	98.11	110.40
3	n	192	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	a	131	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	L	50	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	174	LYS	CA-CB-CG	6.04	126.68	113.40
3	l	50	LEU	CA-CB-CG	6.02	129.15	115.30
3	M	126	LEU	CB-CG-CD2	6.01	121.21	111.00
3	I	120	ILE	CA-CB-CG1	-6.01	99.59	111.00
3	n	179	GLU	CG-CD-OE2	5.99	130.29	118.30
1	D	157	ILE	CB-CA-C	5.99	123.58	111.60
3	j	170	ASP	CB-CG-OD2	5.99	123.69	118.30
3	I	50	LEU	CA-CB-CG	5.98	129.05	115.30
3	L	170	ASP	CB-CG-OD2	5.95	123.66	118.30
1	c	31	ASN	CB-CA-C	-5.91	98.59	110.40
1	f	134	ILE	CB-CA-C	-5.90	99.79	111.60
3	H	131	GLY	N-CA-C	5.90	127.85	113.10
3	N	192	ARG	NE-CZ-NH1	5.90	123.25	120.30
3	l	120	ILE	CA-CB-CG1	-5.89	99.80	111.00
3	H	50	LEU	CA-CB-CG	5.88	128.83	115.30
1	b	174	LYS	CA-CB-CG	5.88	126.34	113.40
1	e	151	GLU	CG-CD-OE2	5.88	130.05	118.30
3	j	50	LEU	CA-CB-CG	5.87	128.80	115.30
3	H	170	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	134	ILE	CB-CA-C	-5.84	99.92	111.60
1	E	131	ARG	NE-CZ-NH2	-5.84	117.38	120.30
3	J	50	LEU	CA-CB-CG	5.81	128.66	115.30
1	e	151	GLU	CG-CD-OE1	-5.81	106.68	118.30
3	n	119	ARG	CD-NE-CZ	5.80	131.72	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	40	ILE	CG1-CB-CG2	-5.79	98.66	111.40
3	i	179	GLU	CG-CD-OE2	5.79	129.88	118.30
3	M	120	ILE	CA-CB-CG1	-5.79	100.01	111.00
1	g	151	GLU	CG-CD-OE1	-5.78	106.74	118.30
3	M	179	GLU	CG-CD-OE2	5.78	129.86	118.30
3	l	40	ILE	CG1-CB-CG2	-5.76	98.72	111.40
1	b	151	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	B	134	ILE	CB-CA-C	-5.75	100.11	111.60
3	K	50	LEU	CA-CB-CG	5.73	128.47	115.30
3	H	119	ARG	CG-CD-NE	5.72	123.81	111.80
3	k	192	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	f	174	LYS	CD-CE-NZ	5.70	124.82	111.70
3	K	170	ASP	CB-CG-OD2	5.68	123.41	118.30
1	e	157	ILE	CB-CA-C	5.67	122.94	111.60
3	M	119	ARG	CG-CD-NE	5.67	123.71	111.80
1	B	93	MET	CG-SD-CE	-5.67	91.13	100.20
1	C	131	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	V	803	LEU	CA-CB-CG	5.63	128.24	115.30
3	L	190	ILE	CA-CB-CG1	5.60	121.64	111.00
1	g	134	ILE	CB-CA-C	-5.58	100.43	111.60
3	j	43	ARG	CB-CG-CD	-5.58	97.11	111.60
2	4	803	LEU	CA-CB-CG	5.56	128.10	115.30
3	k	43	ARG	CG-CD-NE	5.55	123.45	111.80
1	g	151	GLU	CG-CD-OE2	5.54	129.38	118.30
1	g	131	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	93	MET	CG-SD-CE	-5.52	91.37	100.20
1	G	131	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	M	182	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	A	134	ILE	CB-CA-C	-5.46	100.68	111.60
3	h	40	ILE	CG1-CB-CG2	-5.46	99.39	111.40
3	K	37	ASN	CB-CA-C	-5.41	99.57	110.40
3	k	40	ILE	CG1-CB-CG2	-5.41	99.49	111.40
3	i	119	ARG	CD-NE-CZ	5.38	131.13	123.60
1	G	174	LYS	CD-CE-NZ	5.37	124.04	111.70
1	d	174	LYS	CA-CB-CG	5.35	125.18	113.40
1	F	93	MET	CG-SD-CE	-5.35	91.64	100.20
1	F	174	LYS	CD-CE-NZ	5.35	124.00	111.70
1	g	70	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	134	ILE	CB-CA-C	-5.34	100.92	111.60
1	c	196	ASP	CB-CG-OD2	5.33	123.10	118.30
3	H	147	LYS	CB-CG-CD	5.33	125.45	111.60
1	F	208	LYS	CD-CE-NZ	5.32	123.94	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	174	LYS	CD-CE-NZ	5.32	123.94	111.70
3	M	179	GLU	CG-CD-OE1	-5.31	107.68	118.30
3	l	43	ARG	CG-CD-NE	5.31	122.94	111.80
1	G	134	ILE	CB-CA-C	-5.30	101.00	111.60
1	e	134	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	184	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	131	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	n	37	ASN	CB-CA-C	-5.28	99.85	110.40
1	E	134	ILE	CB-CA-C	-5.27	101.06	111.60
3	N	37	ASN	CB-CA-C	-5.26	99.87	110.40
3	J	43	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	H	43	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	c	75	TYR	CB-CG-CD1	5.25	124.15	121.00
3	i	179	GLU	CG-CD-OE1	-5.25	107.80	118.30
3	m	119	ARG	CG-CD-NE	5.25	122.83	111.80
1	d	159	ARG	CA-CB-CG	5.23	124.91	113.40
1	B	184	ASP	CB-CG-OD2	5.22	123.00	118.30
1	f	158	GLU	OE1-CD-OE2	-5.22	117.04	123.30
3	J	37	ASN	CB-CA-C	-5.21	99.98	110.40
3	J	43	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	n	130	THR	N-CA-CB	5.18	120.15	110.30
3	n	130	THR	CB-CA-C	-5.14	97.73	111.60
1	G	69	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	d	131	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	M	190	ILE	CA-CB-CG1	5.10	120.68	111.00
3	I	131	GLY	N-CA-C	5.10	125.84	113.10
1	D	134	ILE	CB-CA-C	-5.09	101.41	111.60
3	H	43	ARG	CG-CD-NE	5.09	122.50	111.80
1	A	151	GLU	CA-CB-CG	5.09	124.59	113.40
2	x	802	LEU	CA-CB-CG	5.08	126.98	115.30
2	S	802	LEU	CA-CB-CG	5.08	126.97	115.30
3	n	179	GLU	CG-CD-OE1	-5.08	108.15	118.30
3	k	43	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	k	43	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	g	69	ASP	CB-CG-OD1	-5.03	113.78	118.30
3	h	192	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	F	156	GLU	CG-CD-OE1	5.02	128.35	118.30
1	c	134	ILE	CB-CA-C	-5.02	101.56	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1508	0	1520	52	0
1	B	1534	0	1545	72	0
1	C	1508	0	1520	60	0
1	D	1508	0	1520	58	0
1	E	1534	0	1545	63	1
1	F	1508	0	1517	54	0
1	G	1502	0	1515	48	0
1	a	1513	0	1525	0	0
1	b	1534	0	1545	0	0
1	c	1513	0	1525	0	0
1	d	1508	0	1520	0	0
1	e	1534	0	1545	0	0
1	f	1508	0	1520	0	0
1	g	1508	0	1520	0	0
2	1	25	0	27	4	0
2	2	25	0	27	2	0
2	3	25	0	27	4	0
2	4	25	0	27	2	0
2	O	25	0	27	4	0
2	P	25	0	27	11	0
2	Q	25	0	27	4	0
2	R	25	0	27	5	0
2	S	25	0	27	8	0
2	T	25	0	27	1	0
2	U	25	0	27	5	0
2	V	25	0	27	4	0
2	W	25	0	27	2	0
2	X	25	0	27	3	0
2	Y	25	0	27	3	0
2	Z	25	0	27	3	0
2	o	25	0	27	0	0
2	p	25	0	27	0	0
2	q	25	0	27	0	0
2	r	25	0	27	0	0
2	s	25	0	27	0	0
2	t	25	0	27	0	0
2	u	25	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	v	25	0	27	0	0
2	w	25	0	27	0	0
2	x	25	0	27	0	0
2	y	25	0	27	0	0
2	z	25	0	27	0	0
3	H	1357	0	1349	37	1
3	I	1357	0	1349	39	0
3	J	1357	0	1349	35	0
3	K	1357	0	1349	37	0
3	L	1357	0	1349	39	0
3	M	1357	0	1349	29	0
3	N	1362	0	1354	49	0
3	h	1357	0	1349	0	0
3	i	1357	0	1349	0	0
3	j	1357	0	1349	0	0
3	k	1357	0	1349	0	0
3	l	1357	0	1349	0	0
3	m	1357	0	1349	0	0
3	n	1357	0	1349	0	0
4	A	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	G	2	0	0	1	0
4	H	2	0	0	1	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
4	K	2	0	0	2	0
4	L	2	0	0	0	0
4	M	3	0	0	3	0
4	N	2	0	0	0	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
4	d	2	0	0	0	0
4	e	1	0	0	0	0
4	h	4	0	0	0	0
4	i	3	0	0	0	0
4	j	3	0	0	0	0
4	k	6	0	0	0	0
4	l	2	0	0	0	0
4	m	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	n	3	0	0	0	0
All	All	40976	0	41029	528	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:159:GLY:O	3:L:191:THR:HG21	93.36	1.34
1:E:98:ALA:O	1:F:208:LYS:HE2	1.40	1.17
3:I:159:GLY:O	3:L:191:THR:CG2	92.56	1.10
1:C:142:VAL:HG22	3:J:130:THR:CG2	3.52	1.07
1:E:97:ARG:C	1:F:208:LYS:CE	2.24	1.06
1:E:98:ALA:N	1:F:208:LYS:NZ	2.07	1.03
1:E:97:ARG:C	1:F:208:LYS:HE3	1.81	1.02
1:E:97:ARG:O	1:F:208:LYS:HE3	1.60	1.01
1:C:64:GLU:OE2	1:D:207:ARG:NH1	1.96	0.98
3:M:98:SER:HB3	2:1:803:LEU:OXT	1.62	0.98
1:C:98:ALA:O	1:D:208:LYS:HE2	1.66	0.93
3:H:43:ARG:HD2	3:N:17:THR:HG23	1.52	0.91
3:H:38:ASP:OD2	4:H:301:HOH:O	18.64	0.91
1:G:142:VAL:HG22	3:N:130:THR:CG2	3.41	0.90
1:B:137:PRO:HD3	1:B:164:MET:HE3	1.52	0.89
1:G:161:ARG:NH1	4:G:301:HOH:O	2.04	0.88
3:K:17:THR:HG23	3:L:43:ARG:HD2	3.86	0.86
1:F:90:TYR:HA	1:F:93:MET:HE2	1.56	0.86
3:J:17:THR:HG23	3:K:43:ARG:HD2	2.32	0.86
1:C:103:VAL:HG22	1:C:125:MET:HE2	1.57	0.86
1:B:90:TYR:HA	1:B:93:MET:HE2	1.56	0.85
1:G:111:ALA:N	2:U:801:BEZ:H5	1.92	0.85
3:H:98:SER:HB3	2:V:803:LEU:OXT	1.82	0.84
1:A:90:TYR:HA	1:A:93:MET:HE2	1.57	0.84
3:H:79:ASP:OD2	3:N:117:HIS:HD2	1.61	0.83
1:C:98:ALA:O	1:D:208:LYS:CE	2.26	0.82
1:A:156:GLU:CD	1:B:188:ILE:HD13	4.64	0.81
1:C:142:VAL:HG22	3:J:130:THR:HG21	3.17	0.81
1:C:184:ASP:OD2	3:I:171:ARG:NH1	2.15	0.80
1:D:162:THR:HG22	1:D:180:ARG:HH12	4.74	0.80
1:A:99:ASP:OD2	1:B:210:SER:OG	1.99	0.79
1:F:162:THR:HG22	1:F:180:ARG:HH12	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ALA:N	1:F:208:LYS:CE	2.44	0.77
1:B:139:LEU:O	3:I:130:THR:O	2.02	0.77
3:I:17:THR:HG23	3:J:43:ARG:HD2	1.65	0.76
1:A:137:PRO:HD3	1:A:164:MET:HE3	1.68	0.76
1:E:162:THR:HG22	1:E:180:ARG:HH12	4.76	0.76
1:F:184:ASP:OD2	3:L:171:ARG:NH1	5.43	0.76
1:D:159:ARG:HG3	1:D:159:ARG:HH11	1.49	0.75
3:H:119:ARG:HH11	3:I:142:GLN:CG	1.99	0.75
3:K:38:ASP:OD2	4:K:301:HOH:O	3.34	0.75
1:B:184:ASP:OD2	3:H:171:ARG:NH1	2.19	0.75
1:B:110:SER:OG	2:P:801:BEZ:H6	1.87	0.74
3:J:98:SER:HB3	2:X:803:LEU:OXT	2.50	0.73
1:A:184:ASP:OD2	3:N:171:ARG:NH1	4.92	0.73
1:B:162:THR:HG22	1:B:180:ARG:HH12	4.76	0.72
1:D:158:GLU:OE1	1:D:180:ARG:NH2	2.93	0.72
1:G:137:PRO:HD3	1:G:164:MET:HE1	1.72	0.72
3:H:119:ARG:HH11	3:I:142:GLN:HG2	1.55	0.72
3:K:39:GLU:CA	3:K:39:GLU:OE1	4.32	0.71
1:B:83:PHE:CE2	1:B:160:MET:HG2	2.26	0.71
3:K:38:ASP:OD1	4:K:301:HOH:O	2.07	0.70
1:E:83:PHE:HD2	2:S:801:BEZ:H3	1.55	0.70
1:E:98:ALA:C	1:F:208:LYS:HE2	2.12	0.70
3:H:119:ARG:NH1	3:I:142:GLN:HG2	2.06	0.70
1:A:139:LEU:O	3:H:130:THR:O	2.10	0.70
2:S:802:LEU:C	2:S:803:LEU:HD23	2.51	0.69
3:H:98:SER:HB3	2:V:803:LEU:C	2.26	0.69
1:E:110:SER:OG	2:S:801:BEZ:H6	1.92	0.69
1:B:83:PHE:HE2	1:B:160:MET:HG2	1.57	0.68
1:A:86:LEU:HD23	1:A:87:MET:SD	2.34	0.68
1:F:42:ILE:HG12	1:F:59:GLN:HE21	1.59	0.68
3:L:98:SER:HB3	2:Z:803:LEU:C	2.20	0.67
1:D:153:GLN:O	1:D:157:ILE:HG23	1.94	0.67
3:H:17:THR:HG22	3:I:43:ARG:HG3	1.94	0.67
1:C:133:LEU:HD12	1:C:188:ILE:CD1	3.94	0.67
1:D:133:LEU:C	1:D:133:LEU:HD23	2.24	0.67
1:F:153:GLN:O	1:F:157:ILE:HG23	1.95	0.67
1:E:153:GLN:O	1:E:157:ILE:HG23	5.63	0.66
1:D:159:ARG:CG	1:D:159:ARG:HH11	2.07	0.66
3:N:191:THR:O	3:N:192:ARG:C	4.28	0.66
1:A:133:LEU:C	1:A:133:LEU:HD23	2.16	0.65
1:F:133:LEU:HD12	1:F:188:ILE:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:39:GLU:O	3:K:39:GLU:OE1	5.55	0.65
3:M:98:SER:HB3	2:1:803:LEU:C	2.18	0.64
3:H:43:ARG:HG3	3:N:17:THR:HG22	1.90	0.64
1:G:142:VAL:HG22	3:N:130:THR:HG22	3.62	0.64
3:M:98:SER:CB	2:1:803:LEU:OXT	2.43	0.64
1:E:161:ARG:NH1	4:E:301:HOH:O	2.29	0.64
3:N:123:HIS:CE1	3:N:126:LEU:HD21	4.21	0.64
1:C:137:PRO:HB3	2:Q:803:LEU:HD21	1.80	0.63
1:F:133:LEU:HD23	1:F:133:LEU:C	2.23	0.63
1:E:133:LEU:HD12	1:E:188:ILE:CD1	3.94	0.63
1:B:133:LEU:HD23	1:B:133:LEU:C	2.18	0.63
1:B:133:LEU:HD12	1:B:188:ILE:CD1	2.29	0.63
3:I:23:ARG:NH2	3:J:54:GLU:OE2	2.32	0.63
3:K:95:MET:HG3	3:K:96:ALA:N	2.14	0.63
1:C:142:VAL:HA	3:J:130:THR:HG22	4.92	0.62
1:D:133:LEU:HD12	1:D:188:ILE:CD1	3.98	0.62
3:H:43:ARG:HD2	3:N:17:THR:CG2	2.28	0.62
3:K:98:SER:HB3	2:Y:803:LEU:C	2.19	0.62
1:C:64:GLU:CD	1:D:207:ARG:NH1	2.53	0.62
3:K:123:HIS:CE1	3:K:126:LEU:HD21	2.34	0.62
1:C:98:ALA:O	1:D:208:LYS:NZ	2.32	0.62
1:G:133:LEU:HD23	1:G:133:LEU:C	2.20	0.61
1:B:86:LEU:HD23	1:B:87:MET:SD	5.88	0.61
1:C:133:LEU:HD12	1:C:188:ILE:HD13	4.11	0.61
1:G:133:LEU:HD12	1:G:188:ILE:CD1	6.13	0.61
1:D:98:ALA:O	1:E:208:LYS:HE2	2.00	0.61
3:H:191:THR:O	3:H:192:ARG:HG2	3.03	0.61
3:K:17:THR:CG2	3:L:43:ARG:HD2	4.46	0.61
3:L:123:HIS:CE1	3:L:126:LEU:HD21	2.35	0.61
4:M:303:HOH:O	2:1:803:LEU:HD11	2.01	0.61
1:A:156:GLU:OE1	1:B:188:ILE:CD1	4.43	0.61
1:A:20:ILE:HD12	1:G:28:LYS:HD2	1.83	0.60
3:I:95:MET:HG3	3:I:96:ALA:N	2.16	0.60
1:C:133:LEU:HD23	1:C:133:LEU:C	2.22	0.60
1:A:161:ARG:NH1	4:A:301:HOH:O	2.87	0.60
3:L:191:THR:O	3:L:192:ARG:HB2	2.01	0.60
1:A:91:ASP:HB3	1:B:127:LEU:HD13	1.92	0.60
1:C:174:LYS:HE2	1:C:197:TYR:O	2.01	0.60
1:D:86:LEU:HD13	1:D:87:MET:SD	2.42	0.60
1:E:86:LEU:HD13	1:E:87:MET:SD	2.42	0.60
1:G:148:SER:H	3:N:124:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LEU:HD12	1:E:188:ILE:HD13	4.12	0.60
1:F:133:LEU:HD12	1:F:188:ILE:HD13	1.83	0.60
3:L:17:THR:HG22	3:M:43:ARG:HG3	1.98	0.59
1:G:86:LEU:HD13	1:G:87:MET:SD	2.44	0.59
3:K:17:THR:HG22	3:L:43:ARG:HG3	1.84	0.59
1:F:156:GLU:OE2	1:G:188:ILE:HD13	2.02	0.59
3:K:39:GLU:C	3:K:39:GLU:OE1	4.99	0.59
3:H:98:SER:CB	2:V:803:LEU:OXT	2.64	0.59
1:E:91:ASP:HB3	1:F:127:LEU:HD13	1.84	0.59
3:H:79:ASP:OD2	3:N:117:HIS:CD2	2.51	0.59
1:A:57:MET:CE	1:B:105:LEU:HD13	2.42	0.59
1:B:133:LEU:HD12	1:B:188:ILE:HD13	1.84	0.59
1:C:28:LYS:HZ1	1:C:38:GLU:CD	2.05	0.59
1:C:28:LYS:HD2	1:D:20:ILE:HD12	1.84	0.59
1:E:133:LEU:C	1:E:133:LEU:HD23	2.26	0.59
1:G:133:LEU:HD12	1:G:188:ILE:HD13	5.72	0.59
3:M:182:GLU:HG2	3:M:182:GLU:O	2.02	0.59
1:A:105:LEU:HD13	1:G:57:MET:CE	2.34	0.59
1:C:86:LEU:HD13	1:C:87:MET:SD	2.43	0.58
3:J:17:THR:CG2	3:K:43:ARG:HD2	3.05	0.58
3:M:17:THR:HG22	3:N:43:ARG:HG3	1.85	0.58
3:L:95:MET:HG3	3:L:96:ALA:N	2.25	0.58
3:J:95:MET:HG3	3:J:96:ALA:N	2.23	0.58
1:A:156:GLU:OE1	1:B:188:ILE:HD13	5.02	0.58
1:F:148:SER:H	3:M:124:GLN:HE22	2.83	0.58
1:F:86:LEU:HD13	1:F:87:MET:SD	2.44	0.58
3:H:119:ARG:NH1	3:I:142:GLN:CG	2.65	0.58
1:E:137:PRO:HB3	2:S:803:LEU:HD21	2.09	0.57
1:C:100:ILE:HG12	1:D:208:LYS:NZ	2.19	0.57
1:B:86:LEU:HD13	1:B:87:MET:SD	2.44	0.57
3:K:182:GLU:HG2	3:K:182:GLU:O	4.63	0.57
1:A:190:THR:HG22	1:A:193:GLU:CD	5.02	0.57
1:D:133:LEU:HD12	1:D:188:ILE:HD13	4.14	0.57
1:D:162:THR:HG22	1:D:180:ARG:NH1	4.49	0.57
1:C:160:MET:CE	2:Q:803:LEU:HD22	2.35	0.56
3:M:152:ARG:O	3:M:152:ARG:HD2	5.42	0.56
1:D:139:LEU:HB2	2:R:803:LEU:CD1	5.33	0.56
1:A:127:LEU:HD13	1:G:91:ASP:HB3	1.86	0.56
1:D:148:SER:H	3:K:124:GLN:HE22	2.83	0.56
3:N:95:MET:HG3	3:N:96:ALA:N	2.20	0.56
3:I:98:SER:HB3	2:W:803:LEU:C	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:VAL:HB	1:C:81:GLY:HA3	1.87	0.56
1:E:48:VAL:HB	1:E:81:GLY:HA3	1.88	0.56
2:S:803:LEU:HD23	2:S:803:LEU:N	2.21	0.56
1:B:64:GLU:OE2	1:C:207:ARG:NH1	2.49	0.56
1:D:91:ASP:HB3	1:E:127:LEU:HD13	1.88	0.56
1:F:190:THR:HG22	1:F:193:GLU:CD	2.25	0.56
1:E:98:ALA:H	1:F:208:LYS:NZ	1.97	0.56
1:D:48:VAL:HB	1:D:81:GLY:HA3	1.87	0.56
1:E:148:SER:H	3:L:124:GLN:HE22	1.54	0.56
3:I:124:GLN:HB3	3:I:125:PRO:HD2	3.51	0.56
1:C:41:ILE:HG21	1:C:75:TYR:CE1	3.36	0.55
1:B:137:PRO:HB3	2:P:803:LEU:HD21	2.25	0.55
1:E:107:GLN:HG3	1:E:131:ARG:NH1	5.08	0.55
1:F:208:LYS:O	1:F:210:SER:N	2.38	0.55
1:B:165:GLU:OE1	1:B:180:ARG:NH1	5.11	0.55
3:H:149:GLU:OE2	3:N:117:HIS:HD2	5.89	0.55
1:F:48:VAL:HB	1:F:81:GLY:HA3	1.91	0.55
2:U:803:LEU:N	2:U:803:LEU:HD23	3.44	0.55
1:D:57:MET:CE	1:E:105:LEU:HD13	2.37	0.55
1:E:147:PHE:CD1	3:L:126:LEU:O	5.98	0.55
1:E:64:GLU:OE2	1:F:207:ARG:NH1	2.40	0.55
1:G:28:LYS:HZ1	1:G:38:GLU:CD	2.08	0.55
1:F:57:MET:CE	1:G:105:LEU:HD13	2.37	0.54
3:I:98:SER:HB3	2:W:803:LEU:OXT	2.21	0.54
1:B:208:LYS:O	1:B:211:ALA:HB2	5.27	0.54
1:C:41:ILE:HG21	1:C:75:TYR:CD1	3.39	0.54
1:D:135:HIS:HB2	1:D:186:ASP:OD1	2.09	0.54
1:C:139:LEU:O	3:J:131:GLY:N	2.96	0.54
1:C:161:ARG:NH1	4:C:301:HOH:O	2.34	0.54
1:F:91:ASP:HB3	1:G:127:LEU:HD13	1.90	0.54
1:A:147:PHE:HB3	3:H:147:LYS:HE2	1.89	0.54
1:E:98:ALA:O	1:F:208:LYS:CE	2.34	0.54
3:J:17:THR:HG22	3:K:43:ARG:HG3	1.94	0.54
1:B:83:PHE:CD1	2:P:801:BEZ:H3	2.42	0.54
1:C:135:HIS:HB2	1:C:186:ASP:OD1	2.11	0.54
1:F:208:LYS:C	1:F:210:SER:H	2.11	0.54
3:M:101:GLU:C	3:M:101:GLU:OE1	2.58	0.54
3:H:119:ARG:HH11	3:I:142:GLN:HE21	1.56	0.54
1:D:165:GLU:OE1	1:D:180:ARG:NH1	5.11	0.54
1:F:135:HIS:HB2	1:F:186:ASP:OD1	2.09	0.54
1:B:135:HIS:HB2	1:B:186:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:PHE:HD1	3:L:126:LEU:O	6.88	0.53
1:E:165:GLU:OE1	1:E:180:ARG:NH1	5.11	0.53
1:G:142:VAL:HG22	3:N:130:THR:HG21	3.04	0.53
3:H:17:THR:CG2	3:I:43:ARG:HG3	2.54	0.53
1:E:135:HIS:HB2	1:E:186:ASP:OD1	2.08	0.53
1:G:48:VAL:HB	1:G:81:GLY:HA3	1.90	0.53
1:D:122:GLY:N	1:D:201:ASP:OD1	3.82	0.53
1:A:135:HIS:HB2	1:A:186:ASP:OD1	2.10	0.53
1:F:162:THR:HG22	1:F:180:ARG:NH1	2.20	0.53
1:A:86:LEU:HD11	1:A:114:VAL:HB	1.91	0.53
1:D:149:ASP:OD1	1:E:185:ARG:HD2	2.11	0.53
1:C:160:MET:HE3	2:Q:803:LEU:HD22	1.90	0.53
1:G:135:HIS:HB2	1:G:186:ASP:OD1	2.10	0.53
1:A:48:VAL:HB	1:A:81:GLY:HA3	1.91	0.53
1:C:91:ASP:HB3	1:D:127:LEU:HD13	1.99	0.53
1:C:142:VAL:HG22	3:J:130:THR:HG22	3.76	0.53
3:I:158:THR:HA	3:I:184:GLY:O	2.13	0.53
1:A:156:GLU:CD	1:B:188:ILE:CD1	4.08	0.52
1:B:48:VAL:HB	1:B:81:GLY:HA3	1.92	0.52
1:C:133:LEU:HD12	1:C:188:ILE:HD11	3.65	0.52
1:D:28:LYS:HZ1	1:D:38:GLU:CD	2.12	0.52
3:M:95:MET:HG3	3:M:96:ALA:N	2.22	0.52
1:A:106:GLY:CA	1:G:88:ALA:HB2	2.38	0.52
1:B:211:ALA:O	1:B:213:THR:N	3.01	0.52
1:B:86:LEU:HD11	1:B:114:VAL:HB	3.19	0.52
3:N:75:MET:HE1	3:N:102:PHE:CE1	2.44	0.52
3:N:98:SER:HB3	2:4:803:LEU:C	92.43	0.52
1:E:162:THR:HG22	1:E:180:ARG:NH1	4.52	0.52
3:M:119:ARG:NH2	3:N:142:GLN:OE1	5.13	0.52
1:B:57:MET:CE	1:C:105:LEU:HD13	2.43	0.52
1:G:107:GLN:HG3	1:G:131:ARG:NH1	5.07	0.52
3:J:98:SER:OG	3:J:123:HIS:NE2	2.41	0.52
3:K:158:THR:HA	3:K:184:GLY:O	2.09	0.52
1:F:146:GLN:OE1	1:G:185:ARG:NH2	3.47	0.52
1:F:165:GLU:OE1	1:F:180:ARG:NH1	2.43	0.51
3:H:158:THR:HA	3:H:184:GLY:O	2.09	0.51
1:A:105:LEU:HD13	1:G:57:MET:HE3	1.91	0.51
1:B:90:TYR:HA	1:B:93:MET:CE	2.34	0.51
3:H:119:ARG:HE	3:I:142:GLN:HE21	1.57	0.51
3:J:158:THR:HA	3:J:184:GLY:O	2.10	0.51
1:B:110:SER:C	2:P:801:BEZ:H5	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:95:MET:HG3	3:H:96:ALA:N	2.25	0.51
3:N:192:ARG:HH11	3:N:192:ARG:CG	2.24	0.51
1:A:207:ARG:NH1	1:G:64:GLU:OE2	2.59	0.51
1:A:185:ARG:HD2	1:G:149:ASP:OD1	2.13	0.51
1:A:97:ARG:HB3	1:B:209:LEU:HD12	1.92	0.51
1:C:159:ARG:NH1	1:D:190:THR:HG22	2.92	0.51
1:E:83:PHE:CD2	2:S:801:BEZ:H3	2.44	0.51
3:M:158:THR:HA	3:M:184:GLY:O	2.10	0.51
3:N:123:HIS:HE1	3:N:126:LEU:HD21	3.67	0.51
3:J:122:MET:CE	3:J:154:ASN:ND2	5.63	0.51
1:A:137:PRO:HB3	2:O:803:LEU:HD21	2.25	0.50
1:B:83:PHE:CE2	1:B:160:MET:CB	2.94	0.50
3:K:39:GLU:HA	3:K:39:GLU:OE1	4.65	0.50
3:M:98:SER:HB3	2:3:803:LEU:C	94.11	0.50
1:E:208:LYS:O	1:E:211:ALA:HB2	2.11	0.50
3:N:98:SER:HB3	2:2:803:LEU:C	2.31	0.50
1:B:163:LEU:O	1:B:167:THR:HG23	2.12	0.50
3:I:124:GLN:HB3	3:I:125:PRO:CD	3.84	0.50
1:B:107:GLN:HG3	1:B:131:ARG:NH1	2.26	0.50
1:D:82:GLY:HA2	2:R:802:LEU:O	3.02	0.50
1:B:83:PHE:CE2	1:B:160:MET:CG	2.94	0.50
1:B:162:THR:HG22	1:B:180:ARG:NH1	4.50	0.50
1:F:153:GLN:O	1:F:157:ILE:CG2	2.58	0.50
3:N:158:THR:HA	3:N:184:GLY:O	2.12	0.50
3:H:119:ARG:HH11	3:I:142:GLN:NE2	2.10	0.50
3:K:123:HIS:HE1	3:K:126:LEU:HD21	1.77	0.50
3:K:164:ARG:HH11	3:K:164:ARG:HG3	1.77	0.50
1:C:100:ILE:HG12	1:D:208:LYS:HZ1	1.76	0.50
3:K:98:SER:HB3	2:Y:803:LEU:OXT	2.32	0.50
1:E:79:PRO:HA	1:E:107:GLN:NE2	2.26	0.50
3:L:158:THR:HA	3:L:184:GLY:O	2.11	0.50
1:A:164:MET:HE2	2:O:801:BEZ:C5	2.42	0.49
3:K:98:SER:OG	3:K:123:HIS:NE2	2.40	0.49
1:G:164:MET:HE2	2:U:801:BEZ:C3	2.42	0.49
1:B:137:PRO:CD	1:B:164:MET:HE3	2.36	0.49
1:D:163:LEU:O	1:D:167:THR:HG23	2.13	0.49
1:G:156:GLU:OE2	1:G:159:ARG:NH1	4.81	0.49
1:G:159:ARG:HB3	1:G:159:ARG:HH11	4.35	0.49
3:L:98:SER:HB3	2:Z:803:LEU:OXT	2.13	0.49
3:L:117:HIS:HD2	3:M:149:GLU:OE2	2.61	0.49
3:L:123:HIS:HE1	3:L:126:LEU:HD21	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:O	1:B:208:LYS:NZ	2.37	0.49
1:E:163:LEU:O	1:E:167:THR:HG23	2.12	0.49
1:F:133:LEU:HD12	1:F:188:ILE:HD11	1.92	0.49
3:H:16:LEU:O	3:H:20:VAL:HG23	2.13	0.49
1:B:159:ARG:HB3	1:B:159:ARG:HH11	4.36	0.49
1:G:163:LEU:O	1:G:167:THR:HG23	2.12	0.49
4:M:303:HOH:O	2:3:803:LEU:CD1	97.39	0.49
1:F:149:ASP:OD1	1:G:185:ARG:HD2	2.13	0.49
1:E:149:ASP:OD1	1:F:185:ARG:HD2	2.13	0.49
1:D:153:GLN:O	1:D:157:ILE:CG2	2.61	0.49
1:C:163:LEU:O	1:C:167:THR:HG23	2.14	0.48
1:C:96:VAL:O	1:D:208:LYS:HB2	2.12	0.48
1:F:190:THR:HG22	1:F:193:GLU:CG	2.45	0.48
1:G:137:PRO:HD3	1:G:164:MET:CE	2.43	0.48
3:L:16:LEU:O	3:L:20:VAL:HG23	2.14	0.48
1:A:90:TYR:HA	1:A:93:MET:CE	2.34	0.48
1:F:163:LEU:O	1:F:167:THR:HG23	2.13	0.48
3:K:192:ARG:HD2	3:K:192:ARG:HA	1.75	0.48
3:L:164:ARG:HG3	3:L:164:ARG:HH11	1.78	0.48
3:M:16:LEU:O	3:M:20:VAL:HG23	2.13	0.48
1:B:91:ASP:HB3	1:C:127:LEU:HD13	2.02	0.48
3:L:17:THR:CG2	3:M:43:ARG:HG3	2.54	0.48
3:N:98:SER:HG	3:N:123:HIS:CD2	2.44	0.48
3:N:16:LEU:O	3:N:20:VAL:HG23	2.14	0.48
2:Q:803:LEU:HD23	2:Q:803:LEU:N	2.29	0.48
1:A:57:MET:HE3	1:B:105:LEU:HD13	2.07	0.48
1:B:98:ALA:O	1:C:208:LYS:HE2	3.61	0.48
1:G:111:ALA:CA	2:U:801:BEZ:H5	2.44	0.48
1:D:159:ARG:NH1	1:D:159:ARG:CG	2.70	0.48
1:F:64:GLU:OE2	1:G:207:ARG:NH1	2.46	0.48
3:I:16:LEU:O	3:I:20:VAL:HG23	2.15	0.48
3:J:16:LEU:O	3:J:20:VAL:HG23	2.15	0.48
2:P:802:LEU:C	2:P:803:LEU:HD23	2.50	0.48
1:B:73:THR:HB	1:B:101:GLN:HB3	4.18	0.47
1:D:133:LEU:HD12	1:D:188:ILE:HD11	3.68	0.47
1:G:164:MET:HE2	2:U:801:BEZ:C4	2.44	0.47
4:M:303:HOH:O	2:3:803:LEU:HD11	96.49	0.47
1:E:133:LEU:HD12	1:E:188:ILE:HD11	3.64	0.47
3:M:17:THR:CG2	3:N:43:ARG:HG3	2.43	0.47
1:B:209:LEU:C	1:B:211:ALA:N	3.62	0.47
1:B:160:MET:CE	2:P:803:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:PRO:HA	2:V:803:LEU:HD23	2.35	0.47
3:H:43:ARG:HG3	3:N:17:THR:CG2	2.57	0.47
3:M:98:SER:OG	3:M:123:HIS:NE2	2.43	0.47
3:N:192:ARG:NH1	3:N:192:ARG:HG2	2.29	0.47
1:E:57:MET:CE	1:F:105:LEU:HD13	3.64	0.47
1:F:42:ILE:HG23	1:F:59:GLN:NE2	2.29	0.47
3:H:98:SER:OG	3:H:123:HIS:NE2	2.41	0.47
3:J:98:SER:HB3	2:X:803:LEU:C	2.35	0.47
1:A:149:ASP:OD1	1:B:185:ARG:HD2	2.20	0.47
1:F:73:THR:HB	1:F:101:GLN:HB3	4.17	0.47
1:B:209:LEU:O	1:B:211:ALA:N	3.92	0.47
3:M:192:ARG:HA	3:M:192:ARG:HD2	1.63	0.47
3:N:98:SER:OG	3:N:123:HIS:NE2	2.41	0.47
1:A:110:SER:HB3	1:A:111:ALA:H	1.43	0.47
3:I:98:SER:OG	3:I:123:HIS:NE2	2.41	0.47
3:K:16:LEU:O	3:K:20:VAL:HG23	2.15	0.47
1:A:190:THR:HG22	1:A:193:GLU:CG	5.75	0.47
3:K:98:SER:HG	3:K:123:HIS:CD2	2.38	0.47
3:N:191:THR:HG23	3:N:192:ARG:NE	6.94	0.47
1:C:138:SER:HA	3:J:132:SER:HA	2.04	0.47
1:E:153:GLN:O	1:E:157:ILE:CG2	5.17	0.47
1:A:163:LEU:O	1:A:167:THR:HG23	2.14	0.46
3:N:192:ARG:HH11	3:N:192:ARG:HG2	1.80	0.46
1:E:157:ILE:CD1	3:L:136:ILE:HD13	3.21	0.46
1:A:73:THR:HB	1:A:101:GLN:HB3	4.17	0.46
1:G:73:THR:HB	1:G:101:GLN:HB3	1.97	0.46
3:L:55:ASP:OD1	3:L:58:LYS:HE2	2.16	0.46
1:B:82:GLY:HA2	2:P:802:LEU:O	2.16	0.46
1:C:73:THR:HB	1:C:101:GLN:HB3	1.97	0.46
1:B:160:MET:HE1	2:P:803:LEU:HD22	1.98	0.46
1:G:110:SER:HB3	1:G:111:ALA:H	1.44	0.46
3:I:17:THR:CG2	3:J:43:ARG:HD2	2.39	0.46
3:M:152:ARG:HD2	3:M:152:ARG:C	5.17	0.46
1:A:137:PRO:HA	2:O:801:BEZ:O1	2.15	0.46
1:B:149:ASP:OD1	1:C:185:ARG:HD2	2.17	0.46
3:I:192:ARG:C	3:I:192:ARG:HD3	3.82	0.46
3:L:98:SER:OG	3:L:123:HIS:NE2	2.42	0.46
1:B:133:LEU:HD12	1:B:188:ILE:HD11	1.97	0.46
1:C:149:ASP:OD1	1:D:185:ARG:HD2	2.15	0.46
3:M:98:SER:HB3	2:3:803:LEU:OXT	94.85	0.45
1:B:138:SER:O	2:P:803:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ARG:HG2	1:D:209:LEU:CD1	3.10	0.45
3:K:23:ARG:NH2	3:L:54:GLU:OE2	2.49	0.45
1:E:73:THR:HB	1:E:101:GLN:HB3	1.97	0.45
1:F:110:SER:HB3	1:F:111:ALA:H	1.43	0.45
3:L:37:ASN:HB2	3:L:39:GLU:H	1.81	0.45
3:M:37:ASN:HB2	3:M:39:GLU:H	1.82	0.45
1:G:133:LEU:HD12	1:G:188:ILE:HD11	6.68	0.45
3:H:129:VAL:HG13	3:H:136:ILE:HG12	1.99	0.45
3:H:148:LYS:HG3	3:H:152:ARG:NH1	3.34	0.45
3:N:191:THR:HG22	3:N:192:ARG:N	2.32	0.45
1:A:137:PRO:HD3	1:A:164:MET:CE	2.44	0.45
1:B:156:GLU:OE2	1:B:159:ARG:NH1	4.78	0.45
3:N:71:ILE:HG12	2:4:803:LEU:HB2	95.59	0.45
1:F:160:MET:CE	2:T:803:LEU:HD13	2.47	0.45
1:B:110:SER:HB3	1:B:111:ALA:H	1.44	0.45
1:E:208:LYS:HD3	1:E:208:LYS:HA	1.59	0.45
3:K:51:LEU:HD12	3:K:51:LEU:HA	1.45	0.45
1:C:147:PHE:CE2	3:J:125:PRO:HB2	2.52	0.45
3:K:149:GLU:OE2	3:K:153:LEU:HD12	2.17	0.45
1:C:142:VAL:HG22	3:J:130:THR:HG23	4.41	0.44
3:M:129:VAL:HG13	3:M:136:ILE:HG12	1.99	0.44
3:N:129:VAL:HG13	3:N:136:ILE:HG12	2.01	0.44
1:A:156:GLU:OE1	1:B:188:ILE:HD11	4.99	0.44
1:C:95:TYR:O	1:D:207:ARG:HG3	2.17	0.44
1:A:61:LEU:HD23	1:A:61:LEU:HA	4.37	0.44
1:B:81:GLY:O	2:P:801:BEZ:H6	4.25	0.44
1:D:28:LYS:HD2	1:E:20:ILE:HD12	1.99	0.44
3:L:129:VAL:HG13	3:L:136:ILE:HG12	1.99	0.44
1:C:28:LYS:NZ	1:C:38:GLU:CD	2.71	0.44
3:J:122:MET:HE3	3:J:154:ASN:ND2	5.93	0.44
3:N:24:LEU:HD23	3:N:24:LEU:HA	1.64	0.44
1:D:28:LYS:NZ	1:D:38:GLU:CD	2.71	0.44
1:E:98:ALA:N	1:F:208:LYS:HE2	2.32	0.44
1:C:72:ILE:HB	1:C:100:ILE:HD13	2.00	0.44
3:I:37:ASN:HB2	3:I:39:GLU:H	1.91	0.44
3:J:122:MET:HE2	3:J:154:ASN:ND2	6.15	0.44
3:N:192:ARG:HA	3:N:192:ARG:HD3	1.85	0.44
1:D:57:MET:HE3	1:E:105:LEU:HD13	2.00	0.44
3:K:191:THR:O	3:K:192:ARG:HG2	2.18	0.44
1:F:90:TYR:HA	1:F:93:MET:CE	2.36	0.44
3:I:116:PRO:HD2	3:J:79:ASP:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:129:VAL:HG13	3:K:136:ILE:HG12	1.98	0.44
1:B:57:MET:HE3	1:C:105:LEU:HD13	2.07	0.44
1:C:208:LYS:HA	1:C:208:LYS:HD3	4.41	0.44
1:D:64:GLU:OE2	1:E:207:ARG:NH1	2.51	0.44
3:I:129:VAL:HG13	3:I:136:ILE:HG12	2.00	0.44
3:J:55:ASP:OD1	3:J:58:LYS:HE2	2.42	0.44
1:D:122:GLY:CA	1:D:201:ASP:OD1	4.38	0.43
1:D:62:VAL:HG21	1:E:32:PRO:HA	2.01	0.43
1:F:57:MET:HE3	1:G:105:LEU:HD13	1.99	0.43
1:C:110:SER:HB3	1:C:111:ALA:H	1.41	0.43
1:F:190:THR:HG23	1:F:193:GLU:H	1.84	0.43
3:M:191:THR:O	3:M:192:ARG:NE	5.12	0.43
3:N:55:ASP:OD1	3:N:58:LYS:HE2	2.18	0.43
1:A:106:GLY:HA3	1:G:88:ALA:HB2	1.99	0.43
3:I:17:THR:HG22	3:J:43:ARG:HG3	2.00	0.43
3:J:98:SER:CB	2:X:803:LEU:OXT	3.17	0.43
1:B:83:PHE:HD2	1:B:160:MET:SD	2.41	0.43
1:D:96:VAL:O	1:E:208:LYS:HD3	2.19	0.43
1:E:62:VAL:HG21	1:F:32:PRO:HA	1.99	0.43
3:I:55:ASP:OD1	3:I:58:LYS:HE2	4.72	0.43
3:K:117:HIS:CE1	3:L:78:TYR:HE2	2.37	0.43
3:N:152:ARG:HD3	3:N:162:ILE:HD12	2.00	0.43
1:E:61:LEU:HD23	1:E:61:LEU:HA	1.80	0.43
1:F:156:GLU:HB2	1:G:188:ILE:HD13	2.01	0.43
3:N:37:ASN:HB2	3:N:39:GLU:H	1.88	0.43
1:B:83:PHE:CE2	1:B:160:MET:HB3	2.53	0.43
3:H:148:LYS:HD3	3:H:148:LYS:HA	1.90	0.43
1:D:97:ARG:HB3	1:E:209:LEU:HD12	1.99	0.43
1:E:110:SER:HB3	1:E:111:ALA:H	1.47	0.43
3:J:129:VAL:HG13	3:J:136:ILE:HG12	1.99	0.43
3:N:24:LEU:HD23	3:N:31:PHE:HE2	5.58	0.43
1:A:135:HIS:CB	1:A:186:ASP:OD1	2.69	0.43
1:C:125:MET:HE2	1:C:125:MET:HB2	1.80	0.43
1:C:31:ASN:HB2	1:C:34:ASN:H	1.88	0.43
3:I:24:LEU:HD23	3:I:31:PHE:HE2	1.87	0.43
3:L:98:SER:HB3	2:Z:803:LEU:O	2.55	0.43
1:C:135:HIS:CB	1:C:186:ASP:OD1	2.70	0.42
3:I:37:ASN:ND2	3:I:40:ILE:HG12	2.34	0.42
3:K:164:ARG:HH11	3:K:164:ARG:CG	2.31	0.42
3:L:24:LEU:HD23	3:L:31:PHE:HE2	1.86	0.42
1:A:52:SER:O	1:A:56:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLU:OE1	1:D:159:ARG:NH1	2.49	0.42
1:D:157:ILE:CD1	3:K:136:ILE:HD13	2.49	0.42
1:E:83:PHE:HB2	2:S:801:BEZ:H2	2.08	0.42
3:I:17:THR:HG23	3:J:43:ARG:NE	3.59	0.42
3:L:149:GLU:OE1	3:L:152:ARG:NH1	2.52	0.42
1:G:31:ASN:HB2	1:G:34:ASN:H	1.90	0.42
3:I:149:GLU:OE1	3:I:152:ARG:NH1	2.51	0.42
3:N:176:THR:OG1	3:N:179:GLU:HG3	2.20	0.42
2:Y:803:LEU:HA	2:Y:803:LEU:HD23	2.26	0.42
3:N:98:SER:HB3	2:2:803:LEU:O	2.18	0.42
1:B:135:HIS:CB	1:B:186:ASP:OD1	2.68	0.42
1:A:156:GLU:OE2	1:B:188:ILE:HD13	4.71	0.42
1:D:135:HIS:CB	1:D:186:ASP:OD1	2.69	0.42
1:D:157:ILE:HD12	2:R:803:LEU:HD23	2.01	0.42
3:J:134:ALA:O	3:J:138:ILE:HG13	2.20	0.42
1:G:142:VAL:HA	3:N:130:THR:HG22	4.82	0.42
1:B:137:PRO:HA	2:P:801:BEZ:H2	3.53	0.42
1:G:135:HIS:CB	1:G:186:ASP:OD1	2.69	0.42
3:I:95:MET:HE3	3:J:72:SER:HB2	4.50	0.42
3:K:24:LEU:HD23	3:K:31:PHE:HE2	1.84	0.42
3:K:51:LEU:N	3:K:51:LEU:HD13	2.34	0.42
1:A:62:VAL:HG21	1:B:32:PRO:HA	2.08	0.42
1:D:52:SER:O	1:D:56:ILE:HG12	2.20	0.42
3:J:191:THR:O	3:J:192:ARG:HD2	2.44	0.42
3:L:181:LEU:HD12	3:L:189:ILE:HG13	2.03	0.42
3:L:113:TYR:CD1	3:L:190:ILE:CD1	3.02	0.42
3:M:149:GLU:OE1	3:M:152:ARG:NH1	2.51	0.42
1:A:111:ALA:HA	2:O:801:BEZ:C4	2.50	0.42
1:A:190:THR:HG23	1:A:193:GLU:H	4.73	0.42
1:E:90:TYR:O	1:E:94:GLN:HG3	3.55	0.42
1:F:52:SER:O	1:F:56:ILE:HG12	2.22	0.42
1:A:64:GLU:OE2	1:B:207:ARG:NH1	2.53	0.42
1:D:138:SER:O	2:R:803:LEU:HD12	5.36	0.42
1:E:147:PHE:HB2	3:L:124:GLN:NE2	2.34	0.42
1:E:57:MET:HE3	1:F:105:LEU:HD13	3.15	0.42
1:B:141:GLY:O	3:I:130:THR:HG23	3.27	0.41
3:N:99:MET:HE3	3:N:102:PHE:CD1	2.55	0.41
3:L:164:ARG:HH11	3:L:164:ARG:CG	2.33	0.41
1:C:180:ARG:HH11	1:C:180:ARG:HD3	1.75	0.41
1:C:99:ASP:HA	1:D:208:LYS:NZ	2.34	0.41
3:H:46:ALA:HB1	3:N:24:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:181:LEU:HD12	3:H:189:ILE:HG13	2.07	0.41
1:B:162:THR:HG22	1:B:180:ARG:HH21	1.86	0.41
1:E:52:SER:O	1:E:56:ILE:HG12	2.20	0.41
3:M:116:PRO:HD2	3:N:79:ASP:CG	2.47	0.41
1:A:162:THR:HG22	1:A:180:ARG:HH21	1.85	0.41
1:G:52:SER:O	1:G:56:ILE:HG12	2.20	0.41
3:J:37:ASN:ND2	3:J:40:ILE:HG12	2.36	0.41
3:N:102:PHE:CE2	3:N:150:MET:HE1	2.55	0.41
3:N:92:ALA:HB2	3:N:104:LEU:HD22	2.03	0.41
1:B:31:ASN:HB2	1:B:34:ASN:H	1.86	0.41
1:F:135:HIS:CB	1:F:186:ASP:OD1	2.68	0.41
3:N:123:HIS:CE1	3:N:126:LEU:CD2	4.85	0.41
1:E:97:ARG:HA	1:F:207:ARG:O	2.67	0.41
3:J:24:LEU:HD23	3:J:31:PHE:HE2	1.86	0.41
1:E:110:SER:C	2:S:801:BEZ:H5	2.41	0.41
1:B:83:PHE:CD2	1:B:160:MET:CG	3.03	0.41
1:E:79:PRO:HA	1:E:107:GLN:HE21	1.86	0.41
3:I:124:GLN:CB	3:I:125:PRO:CD	3.20	0.41
3:L:113:TYR:CD1	3:L:190:ILE:HD13	2.55	0.41
1:C:162:THR:HG22	1:C:180:ARG:HH21	1.93	0.41
3:M:24:LEU:HD23	3:M:31:PHE:HE2	1.85	0.41
3:N:181:LEU:HD12	3:N:189:ILE:HG13	2.03	0.41
1:A:36:LEU:HD13	1:G:62:VAL:HG23	2.03	0.41
1:G:72:ILE:HB	1:G:100:ILE:HD13	2.03	0.41
3:L:98:SER:HG	3:L:123:HIS:CD2	2.42	0.41
3:M:165:ILE:O	3:M:169:SER:HB2	2.21	0.41
1:A:57:MET:HE1	1:B:105:LEU:CB	2.51	0.40
1:B:52:SER:O	1:B:56:ILE:HG12	2.21	0.40
1:C:71:ASP:OD2	1:C:99:ASP:HB2	2.25	0.40
1:D:137:PRO:HD2	1:D:161:ARG:HG3	2.02	0.40
3:K:95:MET:HE3	3:L:72:SER:HB2	2.04	0.40
3:H:148:LYS:CD	3:H:152:ARG:HH12	3.28	0.40
3:I:176:THR:OG1	3:I:179:GLU:HG3	2.23	0.40
3:J:176:THR:OG1	3:J:179:GLU:HG3	2.21	0.40
3:L:165:ILE:O	3:L:169:SER:HB2	2.24	0.40
3:M:92:ALA:HB2	3:M:104:LEU:HD22	2.04	0.40
1:C:64:GLU:CD	1:D:207:ARG:HH12	2.14	0.40
1:G:28:LYS:NZ	1:G:38:GLU:CD	2.75	0.40
3:I:164:ARG:HD2	3:I:168:ASP:OD2	2.21	0.40
1:D:160:MET:SD	2:R:803:LEU:HD11	2.62	0.40
1:E:135:HIS:CB	1:E:186:ASP:OD1	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:ASN:HB2	3:H:39:GLU:H	1.85	0.40
3:H:37:ASN:ND2	3:H:40:ILE:HG12	2.36	0.40
1:C:36:LEU:HD12	1:C:36:LEU:HA	1.95	0.40
3:K:181:LEU:HD12	3:K:189:ILE:HG13	2.04	0.40

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

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/214 (91%)	187 (96%)	6 (3%)	1 (0%)	34	72
1	B	198/214 (92%)	191 (96%)	5 (2%)	2 (1%)	19	58
1	C	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
1	D	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	34	72
1	E	198/214 (92%)	190 (96%)	6 (3%)	2 (1%)	19	58
1	F	194/214 (91%)	187 (96%)	5 (3%)	2 (1%)	19	58
1	G	193/214 (90%)	186 (96%)	6 (3%)	1 (0%)	34	72
1	a	195/214 (91%)	189 (97%)	5 (3%)	1 (0%)	34	72
1	b	198/214 (92%)	189 (96%)	6 (3%)	3 (2%)	13	47
1	c	195/214 (91%)	189 (97%)	4 (2%)	2 (1%)	19	58
1	d	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
1	e	198/214 (92%)	188 (95%)	8 (4%)	2 (1%)	19	58
1	f	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	194/214 (91%)	188 (97%)	4 (2%)	2 (1%)	19	58
2	1	1/3 (33%)	1 (100%)	0	0	100	100
2	2	1/3 (33%)	1 (100%)	0	0	100	100
2	3	1/3 (33%)	1 (100%)	0	0	100	100
2	4	1/3 (33%)	1 (100%)	0	0	100	100
2	O	1/3 (33%)	1 (100%)	0	0	100	100
2	P	1/3 (33%)	1 (100%)	0	0	100	100
2	Q	1/3 (33%)	1 (100%)	0	0	100	100
2	R	1/3 (33%)	1 (100%)	0	0	100	100
2	S	1/3 (33%)	1 (100%)	0	0	100	100
2	T	1/3 (33%)	1 (100%)	0	0	100	100
2	U	1/3 (33%)	1 (100%)	0	0	100	100
2	V	1/3 (33%)	1 (100%)	0	0	100	100
2	W	1/3 (33%)	1 (100%)	0	0	100	100
2	X	1/3 (33%)	1 (100%)	0	0	100	100
2	Y	1/3 (33%)	1 (100%)	0	0	100	100
2	Z	1/3 (33%)	1 (100%)	0	0	100	100
2	o	1/3 (33%)	1 (100%)	0	0	100	100
2	p	1/3 (33%)	1 (100%)	0	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	K	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	L	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	M	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	N	177/200 (88%)	170 (96%)	7 (4%)	0	100	100
3	h	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	i	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	j	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	k	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
3	l	176/200 (88%)	169 (96%)	7 (4%)	0	100	100
3	m	176/200 (88%)	171 (97%)	5 (3%)	0	100	100
3	n	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
All	All	5226/5880 (89%)	5047 (97%)	155 (3%)	24 (0%)	34	72

All (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
1	e	48	VAL
1	g	48	VAL
1	C	48	VAL
1	D	48	VAL
1	a	48	VAL
1	b	210	SER
1	c	48	VAL
1	d	48	VAL
1	f	48	VAL
1	F	48	VAL
1	A	48	VAL
1	B	106	GLY
1	E	106	GLY
1	e	106	GLY
1	g	106	GLY
1	C	106	GLY

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Mol	Chain	Res	Type
1	b	106	GLY
1	c	106	GLY
1	d	106	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
2	v	2/2 (100%)	1 (50%)	1 (50%)	0 0
2	w	2/2 (100%)	2 (100%)	0	100 100
2	x	2/2 (100%)	1 (50%)	1 (50%)	0 0
2	y	2/2 (100%)	2 (100%)	0	100 100
2	z	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	H	139/157 (88%)	117 (84%)	22 (16%)	3 13
3	I	139/157 (88%)	121 (87%)	18 (13%)	5 21
3	J	139/157 (88%)	119 (86%)	20 (14%)	4 17
3	K	139/157 (88%)	114 (82%)	25 (18%)	2 9
3	L	139/157 (88%)	120 (86%)	19 (14%)	4 19
3	M	139/157 (88%)	117 (84%)	22 (16%)	3 13
3	N	139/157 (88%)	121 (87%)	18 (13%)	5 21
3	h	139/157 (88%)	115 (83%)	24 (17%)	2 11
3	i	139/157 (88%)	116 (84%)	23 (16%)	3 12
3	j	139/157 (88%)	121 (87%)	18 (13%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	k	139/157 (88%)	117 (84%)	22 (16%)	3 13
3	l	139/157 (88%)	116 (84%)	23 (16%)	3 12
3	m	139/157 (88%)	115 (83%)	24 (17%)	2 11
3	n	139/157 (88%)	118 (85%)	21 (15%)	3 15
All	All	4291/4746 (90%)	3663 (85%)	628 (15%)	4 16

All (628) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	22	HIS
1	A	27	VAL
1	A	36	LEU
1	A	50	ASP
1	A	61	LEU
1	A	86	LEU
1	A	87	MET
1	A	110	SER
1	A	131	ARG
1	A	135	HIS
1	A	136	GLN
1	A	142	VAL
1	A	144	GLN
1	A	151	GLU
1	A	152	ILE
1	A	158	GLU
1	A	184	ASP
1	A	185	ARG
1	A	207	ARG
1	A	209	LEU
1	B	15	ILE
1	B	22	HIS
1	B	27	VAL
1	B	36	LEU
1	B	50	ASP
1	B	61	LEU
1	B	86	LEU
1	B	87	MET
1	B	97	ARG
1	B	110	SER
1	B	135	HIS

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	140	SER
1	B	144	GLN
1	B	152	ILE
1	B	158	GLU
1	B	163	LEU
1	B	184	ASP
1	B	185	ARG
1	B	207	ARG
1	B	209	LEU
1	B	210	SER
1	B	212	GLN
2	P	802	LEU
2	P	803	LEU
1	C	15	ILE
1	C	27	VAL
1	C	36	LEU
1	C	43	PHE
1	C	50	ASP
1	C	61	LEU
1	C	73	THR
1	C	86	LEU
1	C	87	MET
1	C	97	ARG
1	C	107	GLN
1	C	110	SER
1	C	131	ARG
1	C	135	HIS
1	C	136	GLN
1	C	144	GLN
1	C	152	ILE
1	C	158	GLU
1	C	164	MET
1	C	168	LEU
1	C	185	ARG
1	C	207	ARG
1	C	209	LEU
1	D	15	ILE
1	D	22	HIS
1	D	27	VAL
1	D	36	LEU
1	D	61	LEU

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Mol	Chain	Res	Type
1	D	86	LEU
1	D	87	MET
1	D	97	ARG
1	D	110	SER
1	D	131	ARG
1	D	135	HIS
1	D	136	GLN
1	D	144	GLN
1	D	152	ILE
1	D	157	ILE
1	D	158	GLU
1	D	159	ARG
1	D	164	MET
1	D	184	ASP
1	D	185	ARG
1	D	207	ARG
1	D	210	SER
2	R	802	LEU
1	E	15	ILE
1	E	22	HIS
1	E	27	VAL
1	E	36	LEU
1	E	50	ASP
1	E	73	THR
1	E	86	LEU
1	E	87	MET
1	E	110	SER
1	E	131	ARG
1	E	135	HIS
1	E	144	GLN
1	E	152	ILE
1	E	164	MET
1	E	185	ARG
1	E	207	ARG
1	E	208	LYS
1	E	209	LEU
1	E	210	SER
1	E	212	GLN
2	S	802	LEU
2	S	803	LEU
1	F	15	ILE
1	F	22	HIS

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Mol	Chain	Res	Type
1	F	27	VAL
1	F	36	LEU
1	F	43	PHE
1	F	50	ASP
1	F	61	LEU
1	F	71	ASP
1	F	84	THR
1	F	86	LEU
1	F	87	MET
1	F	110	SER
1	F	131	ARG
1	F	135	HIS
1	F	136	GLN
1	F	144	GLN
1	F	152	ILE
1	F	157	ILE
1	F	158	GLU
1	F	159	ARG
1	F	164	MET
1	F	170	ARG
1	F	185	ARG
1	F	207	ARG
1	F	208	LYS
1	F	209	LEU
2	T	802	LEU
2	T	803	LEU
1	G	15	ILE
1	G	22	HIS
1	G	24	SER
1	G	27	VAL
1	G	36	LEU
1	G	73	THR
1	G	86	LEU
1	G	87	MET
1	G	110	SER
1	G	131	ARG
1	G	135	HIS
1	G	136	GLN
1	G	144	GLN
1	G	152	ILE
1	G	158	GLU
1	G	184	ASP

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Mol	Chain	Res	Type
1	G	185	ARG
1	G	188	ILE
1	G	207	ARG
3	H	17	THR
3	H	19	SER
3	H	22	GLU
3	H	24	LEU
3	H	25	LEU
3	H	35	GLU
3	H	37	ASN
3	H	44	LEU
3	H	49	LEU
3	H	50	LEU
3	H	62	LEU
3	H	72	SER
3	H	95	MET
3	H	101	GLU
3	H	121	LEU
3	H	123	HIS
3	H	129	VAL
3	H	147	LYS
3	H	173	ARG
3	H	186	VAL
3	H	191	THR
3	H	192	ARG
2	V	803	LEU
3	I	17	THR
3	I	19	SER
3	I	22	GLU
3	I	24	LEU
3	I	35	GLU
3	I	37	ASN
3	I	44	LEU
3	I	49	LEU
3	I	50	LEU
3	I	62	LEU
3	I	72	SER
3	I	101	GLU
3	I	121	LEU
3	I	123	HIS
3	I	129	VAL
3	I	173	ARG

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Mol	Chain	Res	Type
3	I	186	VAL
3	I	192	ARG
3	J	17	THR
3	J	19	SER
3	J	22	GLU
3	J	24	LEU
3	J	25	LEU
3	J	35	GLU
3	J	37	ASN
3	J	44	LEU
3	J	49	LEU
3	J	50	LEU
3	J	62	LEU
3	J	67	PRO
3	J	72	SER
3	J	101	GLU
3	J	121	LEU
3	J	123	HIS
3	J	129	VAL
3	J	173	ARG
3	J	186	VAL
3	J	192	ARG
2	X	802	LEU
3	K	17	THR
3	K	19	SER
3	K	22	GLU
3	K	24	LEU
3	K	25	LEU
3	K	35	GLU
3	K	37	ASN
3	K	40	ILE
3	K	44	LEU
3	K	49	LEU
3	K	50	LEU
3	K	51	LEU
3	K	62	LEU
3	K	72	SER
3	K	95	MET
3	K	101	GLU
3	K	121	LEU
3	K	123	HIS
3	K	126	LEU

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Mol	Chain	Res	Type
3	K	129	VAL
3	K	149	GLU
3	K	173	ARG
3	K	186	VAL
3	K	191	THR
3	K	192	ARG
3	L	17	THR
3	L	19	SER
3	L	22	GLU
3	L	25	LEU
3	L	35	GLU
3	L	37	ASN
3	L	44	LEU
3	L	49	LEU
3	L	50	LEU
3	L	62	LEU
3	L	67	PRO
3	L	72	SER
3	L	95	MET
3	L	101	GLU
3	L	121	LEU
3	L	123	HIS
3	L	126	LEU
3	L	129	VAL
3	L	173	ARG
2	Z	803	LEU
3	M	17	THR
3	M	19	SER
3	M	22	GLU
3	M	24	LEU
3	M	25	LEU
3	M	35	GLU
3	M	37	ASN
3	M	44	LEU
3	M	49	LEU
3	M	50	LEU
3	M	59	ASP
3	M	62	LEU
3	M	72	SER
3	M	101	GLU
3	M	121	LEU
3	M	123	HIS

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Mol	Chain	Res	Type
3	M	129	VAL
3	M	173	ARG
3	M	182	GLU
3	M	186	VAL
3	M	191	THR
3	M	192	ARG
2	1	802	LEU
3	N	17	THR
3	N	19	SER
3	N	22	GLU
3	N	35	GLU
3	N	37	ASN
3	N	44	LEU
3	N	49	LEU
3	N	50	LEU
3	N	62	LEU
3	N	72	SER
3	N	95	MET
3	N	101	GLU
3	N	121	LEU
3	N	123	HIS
3	N	129	VAL
3	N	173	ARG
3	N	186	VAL
3	N	192	ARG
2	2	803	LEU
1	a	15	ILE
1	a	22	HIS
1	a	27	VAL
1	a	36	LEU
1	a	50	ASP
1	a	73	THR
1	a	86	LEU
1	a	87	MET
1	a	110	SER
1	a	131	ARG
1	a	135	HIS
1	a	136	GLN
1	a	144	GLN
1	a	152	ILE
1	a	158	GLU
1	a	164	MET

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Mol	Chain	Res	Type
1	a	185	ARG
1	a	207	ARG
1	a	209	LEU
1	a	210	SER
2	o	802	LEU
1	b	15	ILE
1	b	22	HIS
1	b	27	VAL
1	b	36	LEU
1	b	50	ASP
1	b	61	LEU
1	b	73	THR
1	b	84	THR
1	b	86	LEU
1	b	87	MET
1	b	110	SER
1	b	135	HIS
1	b	136	GLN
1	b	144	GLN
1	b	152	ILE
1	b	158	GLU
1	b	159	ARG
1	b	164	MET
1	b	180	ARG
1	b	185	ARG
1	b	188	ILE
1	b	207	ARG
1	b	209	LEU
1	b	210	SER
1	b	212	GLN
2	p	802	LEU
2	p	803	LEU
1	c	15	ILE
1	c	22	HIS
1	c	27	VAL
1	c	36	LEU
1	c	50	ASP
1	c	86	LEU
1	c	87	MET
1	c	110	SER
1	c	131	ARG
1	c	135	HIS

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Mol	Chain	Res	Type
1	c	136	GLN
1	c	144	GLN
1	c	152	ILE
1	c	158	GLU
1	c	163	LEU
1	c	164	MET
1	c	185	ARG
1	c	207	ARG
1	c	208	LYS
1	c	209	LEU
1	c	210	SER
2	q	802	LEU
2	q	803	LEU
1	d	15	ILE
1	d	22	HIS
1	d	27	VAL
1	d	36	LEU
1	d	50	ASP
1	d	61	LEU
1	d	86	LEU
1	d	87	MET
1	d	97	ARG
1	d	110	SER
1	d	131	ARG
1	d	135	HIS
1	d	136	GLN
1	d	144	GLN
1	d	152	ILE
1	d	157	ILE
1	d	158	GLU
1	d	159	ARG
1	d	164	MET
1	d	185	ARG
1	d	207	ARG
2	r	803	LEU
1	e	15	ILE
1	e	22	HIS
1	e	27	VAL
1	e	36	LEU
1	e	86	LEU
1	e	87	MET
1	e	100	ILE

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Mol	Chain	Res	Type
1	e	110	SER
1	e	135	HIS
1	e	144	GLN
1	e	152	ILE
1	e	157	ILE
1	e	158	GLU
1	e	164	MET
1	e	184	ASP
1	e	185	ARG
1	e	207	ARG
1	e	209	LEU
1	e	210	SER
1	e	212	GLN
2	s	802	LEU
2	s	803	LEU
1	f	15	ILE
1	f	22	HIS
1	f	27	VAL
1	f	36	LEU
1	f	50	ASP
1	f	61	LEU
1	f	73	THR
1	f	86	LEU
1	f	87	MET
1	f	110	SER
1	f	131	ARG
1	f	135	HIS
1	f	144	GLN
1	f	152	ILE
1	f	164	MET
1	f	175	ASP
1	f	185	ARG
1	f	207	ARG
1	f	209	LEU
1	f	210	SER
1	g	15	ILE
1	g	22	HIS
1	g	27	VAL
1	g	36	LEU
1	g	50	ASP
1	g	61	LEU
1	g	73	THR

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Mol	Chain	Res	Type
1	g	86	LEU
1	g	87	MET
1	g	110	SER
1	g	135	HIS
1	g	136	GLN
1	g	144	GLN
1	g	152	ILE
1	g	158	GLU
1	g	159	ARG
1	g	164	MET
1	g	184	ASP
1	g	185	ARG
1	g	207	ARG
1	g	209	LEU
2	u	802	LEU
2	u	803	LEU
3	h	17	THR
3	h	19	SER
3	h	22	GLU
3	h	24	LEU
3	h	25	LEU
3	h	35	GLU
3	h	37	ASN
3	h	39	GLU
3	h	44	LEU
3	h	49	LEU
3	h	50	LEU
3	h	62	LEU
3	h	72	SER
3	h	95	MET
3	h	101	GLU
3	h	121	LEU
3	h	123	HIS
3	h	129	VAL
3	h	148	LYS
3	h	152	ARG
3	h	173	ARG
3	h	186	VAL
3	h	191	THR
3	h	192	ARG
2	v	802	LEU
3	i	17	THR

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Mol	Chain	Res	Type
3	i	19	SER
3	i	22	GLU
3	i	24	LEU
3	i	25	LEU
3	i	35	GLU
3	i	37	ASN
3	i	44	LEU
3	i	49	LEU
3	i	50	LEU
3	i	62	LEU
3	i	72	SER
3	i	95	MET
3	i	101	GLU
3	i	121	LEU
3	i	123	HIS
3	i	126	LEU
3	i	129	VAL
3	i	130	THR
3	i	173	ARG
3	i	186	VAL
3	i	191	THR
3	i	192	ARG
3	j	17	THR
3	j	19	SER
3	j	22	GLU
3	j	24	LEU
3	j	35	GLU
3	j	37	ASN
3	j	44	LEU
3	j	49	LEU
3	j	50	LEU
3	j	62	LEU
3	j	72	SER
3	j	101	GLU
3	j	121	LEU
3	j	123	HIS
3	j	129	VAL
3	j	173	ARG
3	j	186	VAL
3	j	191	THR
2	x	803	LEU
3	k	17	THR

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Mol	Chain	Res	Type
3	k	19	SER
3	k	22	GLU
3	k	24	LEU
3	k	35	GLU
3	k	37	ASN
3	k	39	GLU
3	k	43	ARG
3	k	44	LEU
3	k	49	LEU
3	k	50	LEU
3	k	62	LEU
3	k	72	SER
3	k	95	MET
3	k	101	GLU
3	k	121	LEU
3	k	123	HIS
3	k	129	VAL
3	k	148	LYS
3	k	171	ARG
3	k	173	ARG
3	k	182	GLU
3	l	17	THR
3	l	19	SER
3	l	22	GLU
3	l	24	LEU
3	l	25	LEU
3	l	35	GLU
3	l	37	ASN
3	l	40	ILE
3	l	44	LEU
3	l	49	LEU
3	l	50	LEU
3	l	62	LEU
3	l	72	SER
3	l	83	LEU
3	l	101	GLU
3	l	121	LEU
3	l	123	HIS
3	l	129	VAL
3	l	148	LYS
3	l	173	ARG
3	l	186	VAL

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Mol	Chain	Res	Type
3	l	191	THR
3	l	192	ARG
2	z	803	LEU
3	m	17	THR
3	m	19	SER
3	m	22	GLU
3	m	24	LEU
3	m	25	LEU
3	m	35	GLU
3	m	37	ASN
3	m	44	LEU
3	m	49	LEU
3	m	50	LEU
3	m	62	LEU
3	m	72	SER
3	m	95	MET
3	m	101	GLU
3	m	121	LEU
3	m	123	HIS
3	m	129	VAL
3	m	149	GLU
3	m	152	ARG
3	m	156	GLU
3	m	173	ARG
3	m	186	VAL
3	m	191	THR
3	m	192	ARG
2	3	803	LEU
3	n	17	THR
3	n	19	SER
3	n	22	GLU
3	n	24	LEU
3	n	25	LEU
3	n	35	GLU
3	n	37	ASN
3	n	44	LEU
3	n	49	LEU
3	n	50	LEU
3	n	62	LEU
3	n	67	PRO
3	n	72	SER
3	n	101	GLU

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Mol	Chain	Res	Type
3	n	121	LEU
3	n	123	HIS
3	n	126	LEU
3	n	129	VAL
3	n	173	ARG
3	n	186	VAL
3	n	192	ARG
2	4	803	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	B	94	GLN
1	B	107	GLN
1	C	94	GLN
1	C	144	GLN
1	E	212	GLN
1	F	59	GLN
1	F	94	GLN
1	F	107	GLN
1	F	171	HIS
1	G	94	GLN
1	G	107	GLN
3	H	37	ASN
3	I	37	ASN
3	I	65	ASN
3	I	142	GLN
3	J	37	ASN
3	J	65	ASN
3	K	37	ASN
3	L	37	ASN
3	L	124	GLN
3	M	37	ASN
3	M	65	ASN
3	N	37	ASN
3	N	117	HIS
3	N	124	GLN
1	a	94	GLN
1	a	144	GLN
1	b	94	GLN
1	b	146	GLN

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Mol	Chain	Res	Type
1	c	94	GLN
1	e	212	GLN
1	f	94	GLN
1	g	94	GLN
3	h	37	ASN
3	i	37	ASN
3	i	65	ASN
3	j	37	ASN
3	j	154	ASN
3	k	37	ASN
3	k	124	GLN
3	l	37	ASN
3	m	37	ASN
3	m	124	GLN
3	n	37	ASN
3	n	124	GLN

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

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

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

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.