Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID	:	2ZL2 / pdb_00002zl2
Title	:	Crystal structure of H.pylori ClpP in complex with the peptide NVLGFTQ
Authors	:	Kim, D.Y.; Kim, K.K.
Deposited on	:	2008-04-02
Resolution	:	2.50 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

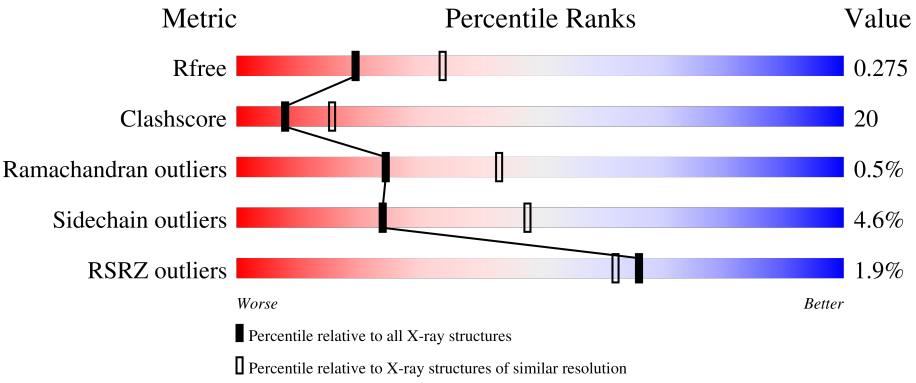
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	196	2% 62% 24% • 11%
1	B	196	% 59% 27% • 12%
1	C	196	% 47% 39% • 11%
1	D	196	% 54% 31% • • 12%
1	E	196	3% 47% 35% 6% 12%

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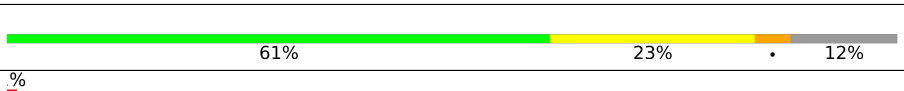
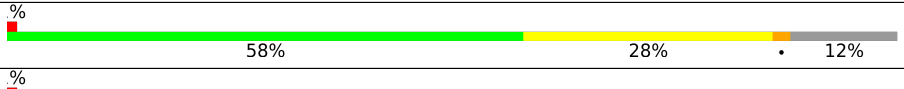
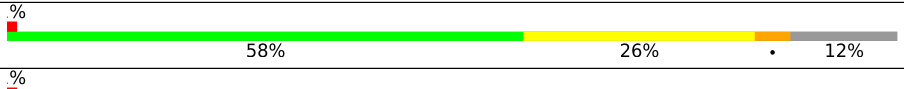
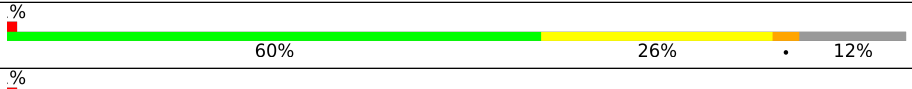
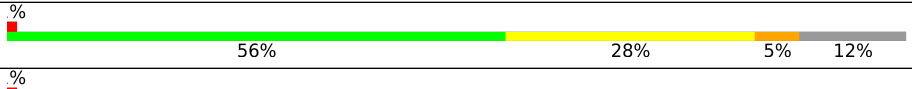
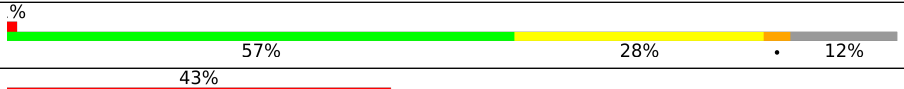
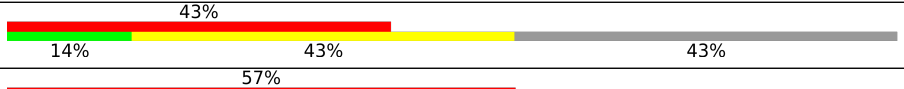
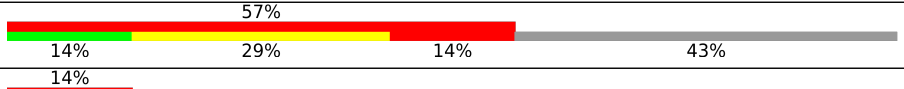
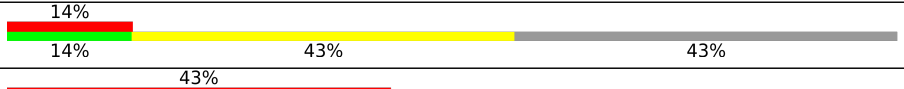
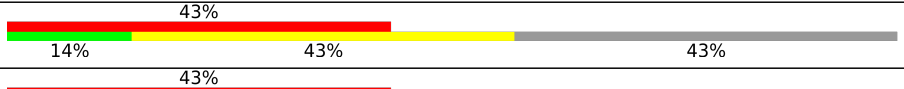
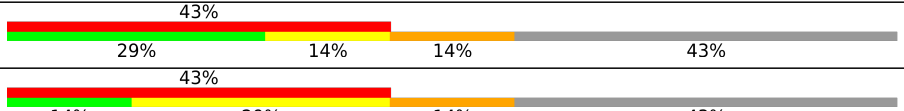
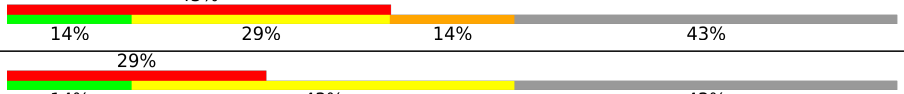
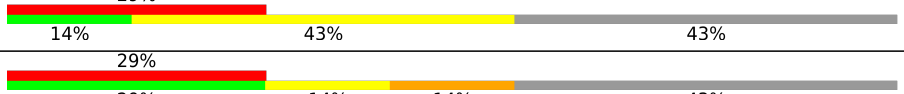
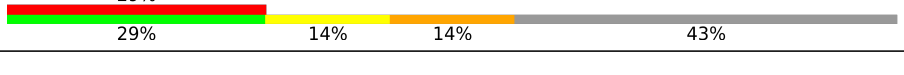
Mol	Chain	Length	Quality of chain
1	F	196	
1	G	196	
1	H	196	
1	I	196	
1	J	196	
1	K	196	
1	L	196	
1	M	196	
1	N	196	
2	O	7	
2	P	7	
2	Q	7	
2	T	7	
2	U	7	
2	V	7	
2	W	7	
2	X	7	
3	R	7	
3	S	7	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18687 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1324	834	224	259	7			
1	B	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	C	174	Total	C	N	O	S	0	0	0
			1324	834	224	259	7			
1	D	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	E	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	F	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	G	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	H	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	I	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	J	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	K	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	L	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	M	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			
1	N	173	Total	C	N	O	S	0	0	0
			1315	828	222	258	7			

- Molecule 2 is a protein called A peptide substrate-NVLGFTQ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	P	4	Total	C	N	O	0	0	0
			32	20	5	7			
2	Q	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	T	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	U	4	Total	C	N	O	0	0	0
			30	22	4	4			
2	V	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	W	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	X	4	Total	C	N	O	0	0	0
			27	17	5	5			

- Molecule 3 is a protein called A peptide substrate-NVLGFTQ for Chain R and S.

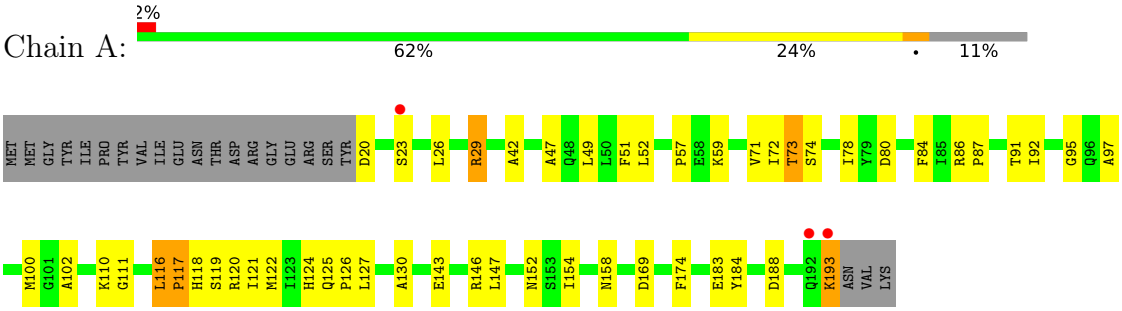
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	3	Total	C	N	O	0	0	0
			15	9	3	3			
3	S	4	Total	C	N	O	0	0	0
			20	12	4	4			

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.

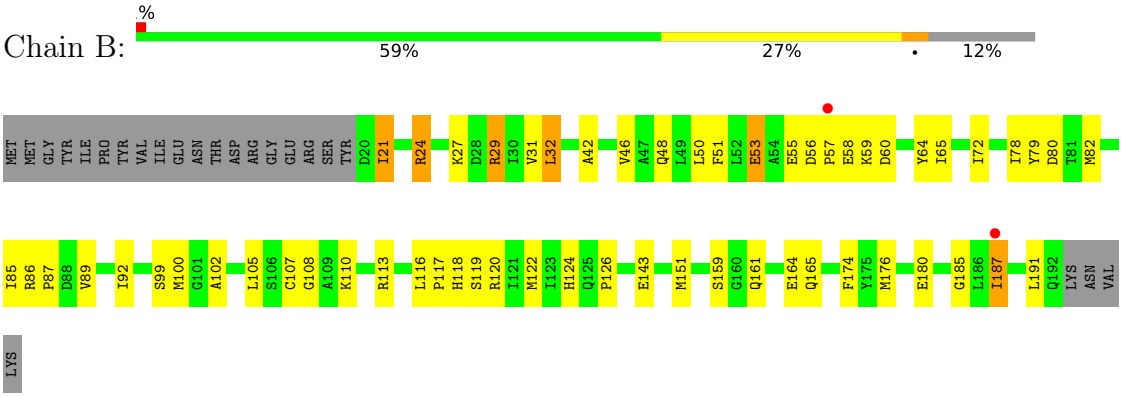
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



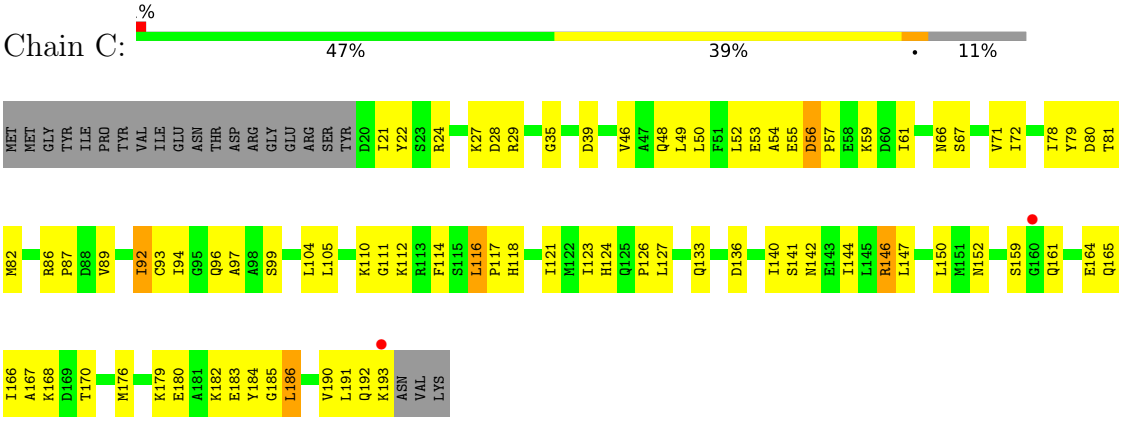
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



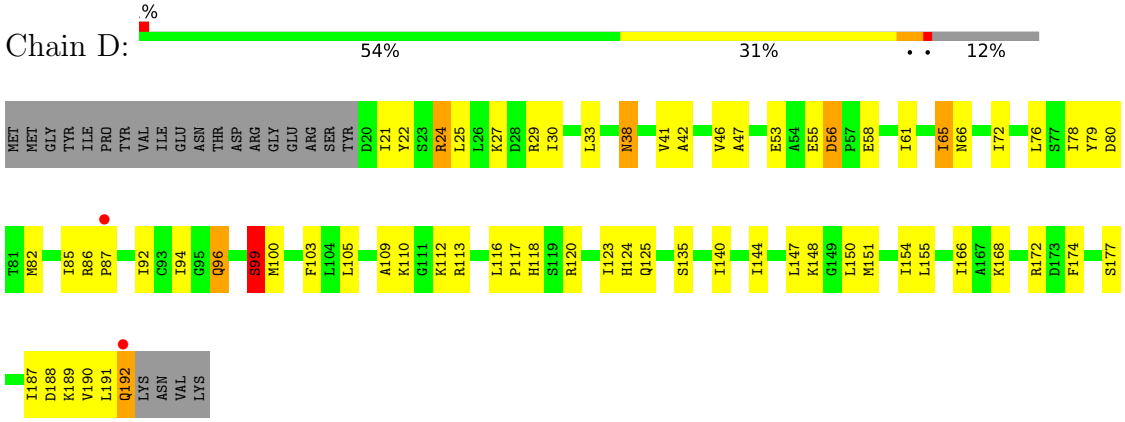
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



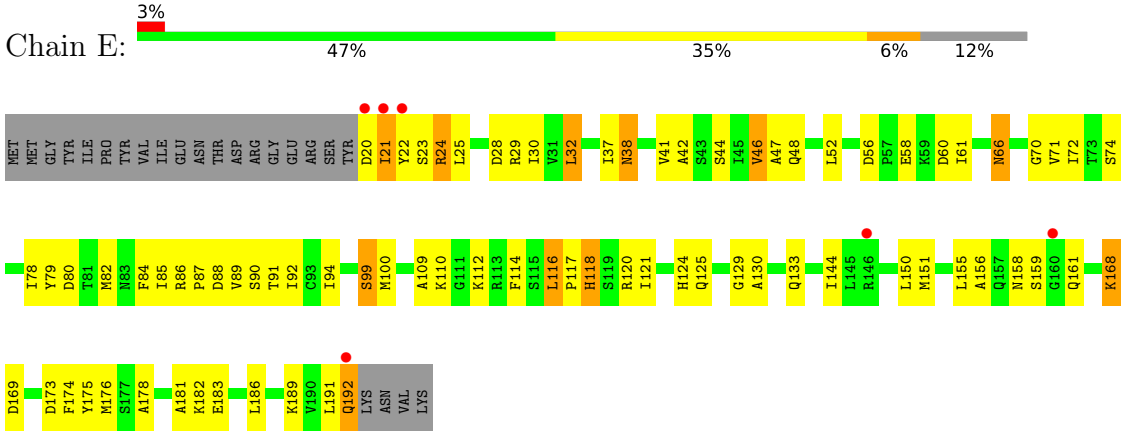
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



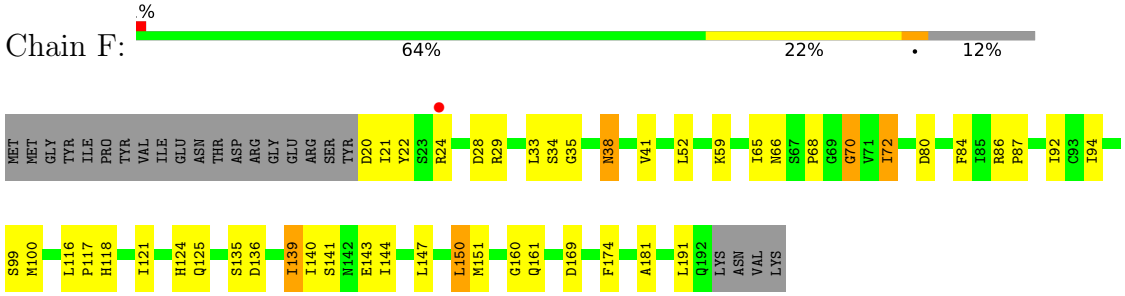
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



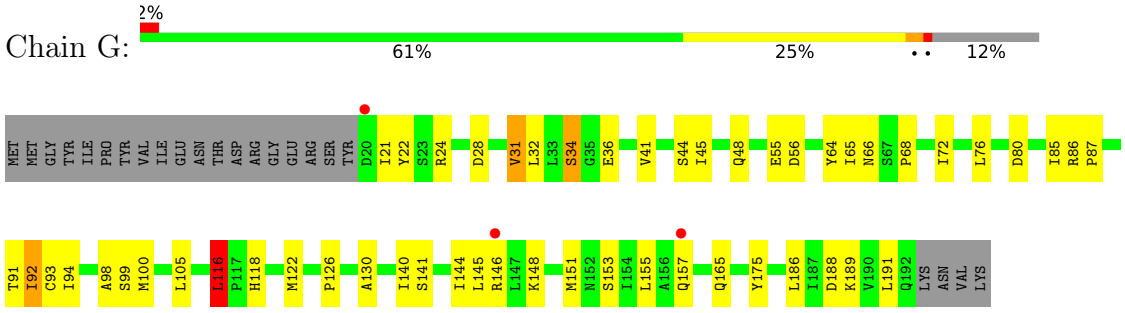
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



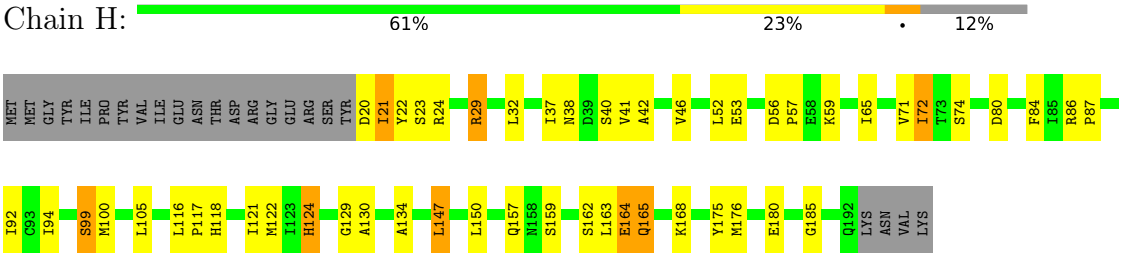
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



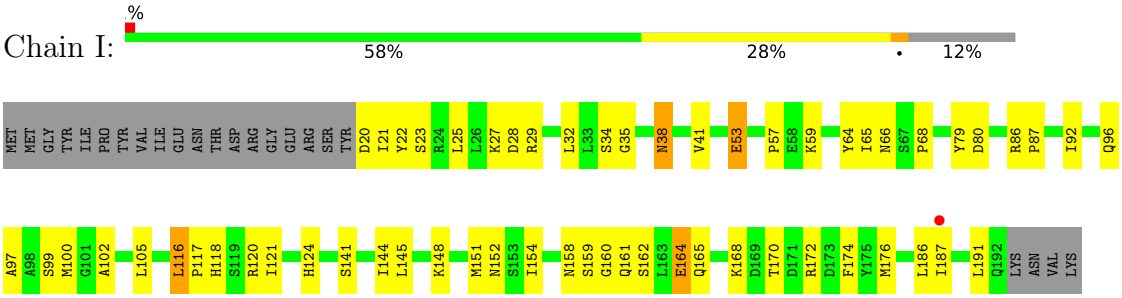
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



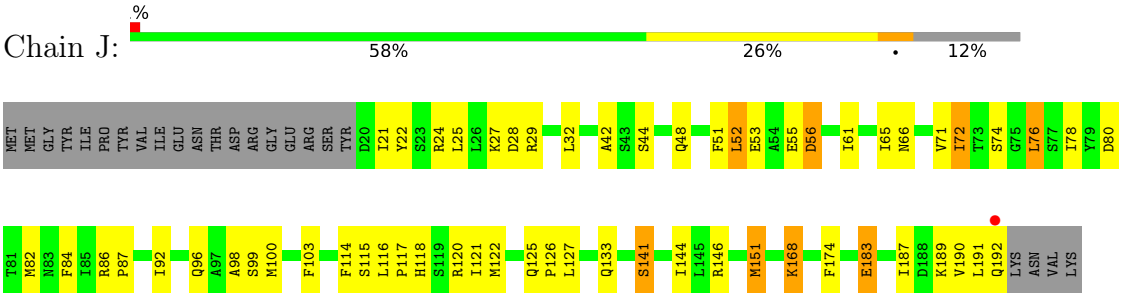
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



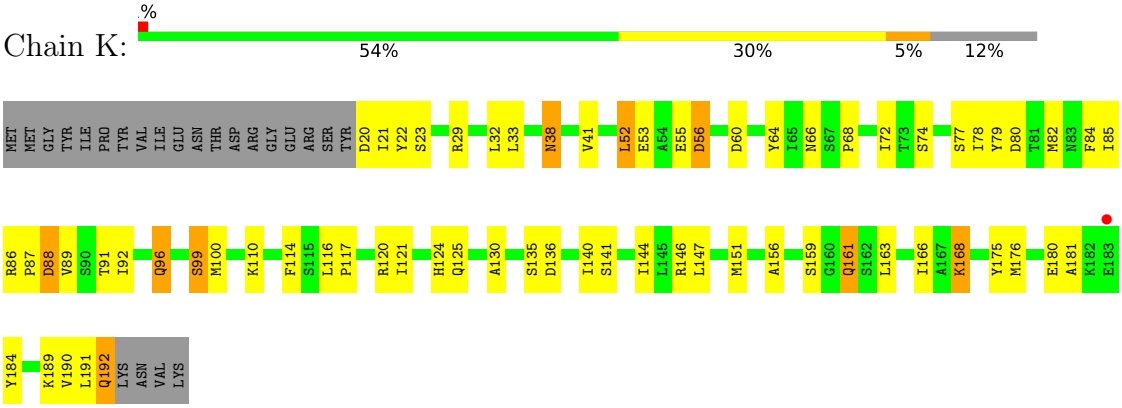
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



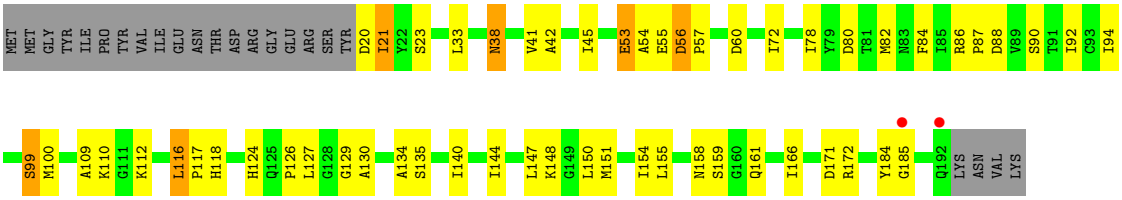
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



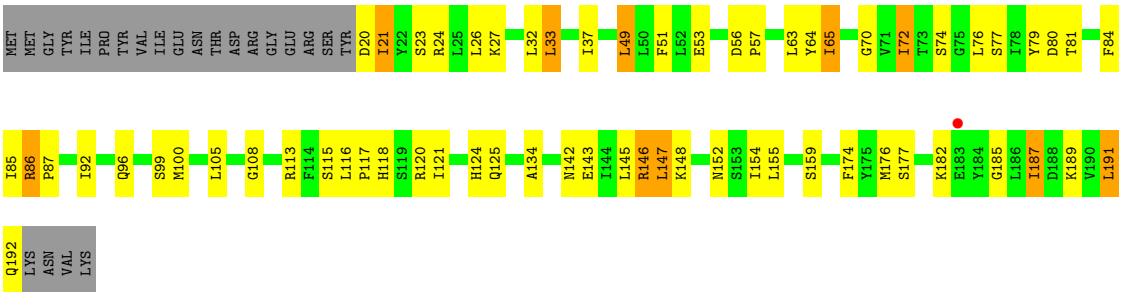
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



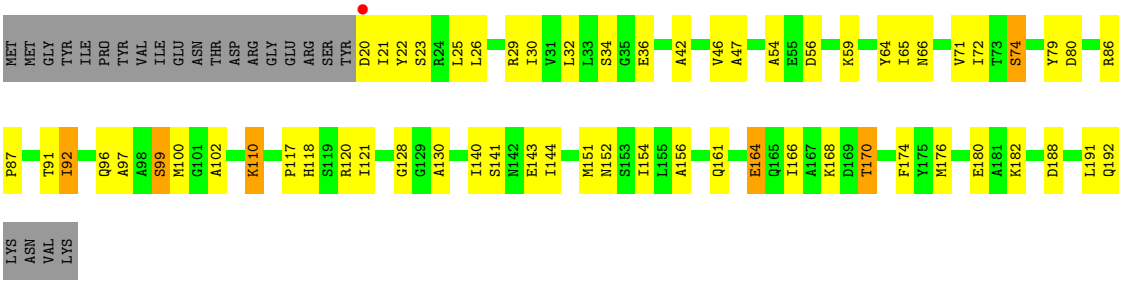
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



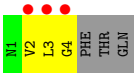
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



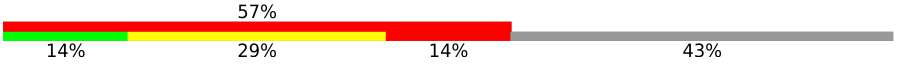
• Molecule 2: A peptide substrate-NVLGFTQ

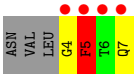
Chain O:



• Molecule 2: A peptide substrate-NVLGFTQ

Chain P:



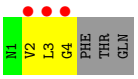


• Molecule 2: A peptide substrate-NVLGFTQ

Chain Q:

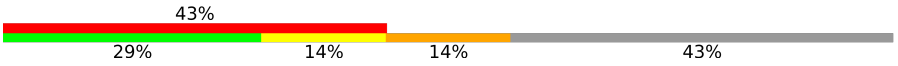
• Molecule 2: A peptide substrate-NVLGFTQ

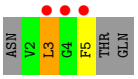
Chain T:



• Molecule 2: A peptide substrate-NVLGFTQ

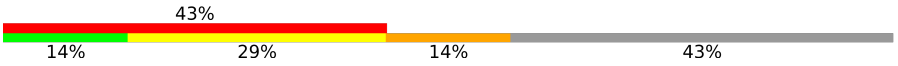
Chain U:

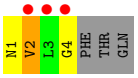




• Molecule 2: A peptide substrate-NVLGFTQ

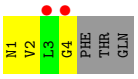
Chain V:





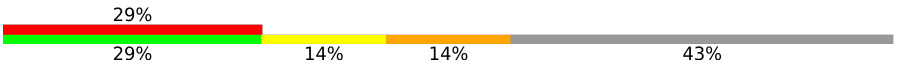
• Molecule 2: A peptide substrate-NVLGFTQ

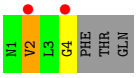
Chain W:



• Molecule 2: A peptide substrate-NVLGFTQ

Chain X:



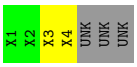


• Molecule 3: A peptide substrate-NVLGFTQ for Chain R and S

Chain R:

• Molecule 3: A peptide substrate-NVLGFTQ for Chain R and S

Chain S:


X1
X2
X3
X4
UNK
UNK
UNK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.74Å 166.43Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.50) 99.4 (19.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.50Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.274 0.231 , 0.275	Depositor DCC
R_{free} test set	10067 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18687	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.47	0/1340	0.95	3/1803 (0.2%)
1	B	0.44	0/1331	0.94	3/1792 (0.2%)
1	C	0.40	0/1340	0.94	7/1803 (0.4%)
1	D	0.42	0/1331	0.93	3/1792 (0.2%)
1	E	0.44	0/1331	0.88	3/1792 (0.2%)
1	F	0.44	0/1331	0.95	5/1792 (0.3%)
1	G	0.50	0/1331	0.98	5/1792 (0.3%)
1	H	0.46	0/1331	0.97	5/1792 (0.3%)
1	I	0.44	0/1331	0.98	6/1792 (0.3%)
1	J	0.45	0/1331	0.90	2/1792 (0.1%)
1	K	0.42	0/1331	0.94	3/1792 (0.2%)
1	L	0.43	0/1331	0.96	5/1792 (0.3%)
1	M	0.46	0/1331	0.96	7/1792 (0.4%)
1	N	0.48	0/1331	0.97	5/1792 (0.3%)
2	O	0.53	0/26	0.60	0/34
2	P	0.74	0/32	0.66	0/40
2	Q	0.47	0/26	0.61	0/34
2	T	0.52	0/26	0.67	0/34
2	U	0.59	0/30	1.12	0/39
2	V	0.59	0/26	1.25	1/34 (2.9%)
2	W	0.56	0/26	0.72	0/34
2	X	0.66	0/26	0.79	0/34
All	All	0.45	0/18870	0.95	63/25393 (0.2%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	171	ASP	N-CA-C	-8.21	96.71	109.76
1	L	116	LEU	CA-C-N	8.16	127.73	119.24
1	L	116	LEU	C-N-CA	8.16	127.73	119.24
1	F	65	ILE	N-CA-C	7.11	118.29	107.77
1	G	31	VAL	N-CA-C	6.98	118.30	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	PRO	N-CA-C	6.84	122.73	113.84
1	I	160	GLY	N-CA-C	-6.77	105.12	114.67
1	I	116	LEU	CA-C-N	6.76	126.27	119.24
1	I	116	LEU	C-N-CA	6.76	126.27	119.24
1	I	65	ILE	N-CA-C	6.75	117.61	107.75
1	C	72	ILE	N-CA-C	6.75	117.25	110.23
1	B	102	ALA	N-CA-C	-6.60	104.16	111.36
1	D	99	SER	CB-CA-C	-6.41	109.17	116.54
1	M	72	ILE	N-CA-C	6.24	116.36	110.30
1	L	54	ALA	N-CA-C	-6.23	105.95	112.93
1	N	54	ALA	N-CA-C	-6.06	104.59	111.07
1	J	72	ILE	N-CA-C	6.04	116.16	110.30
1	B	53	GLU	N-CA-C	-5.97	104.69	111.14
1	D	65	ILE	N-CA-C	5.95	116.43	107.75
1	G	116	LEU	CA-C-N	5.94	127.27	119.84
1	G	116	LEU	C-N-CA	5.94	127.27	119.84
1	N	99	SER	CB-CA-C	-5.83	109.84	116.54
1	H	117	PRO	N-CA-C	5.81	121.61	113.53
1	C	39	ASP	N-CA-C	5.78	117.58	111.28
1	H	21	ILE	N-CA-C	5.70	116.34	110.36
1	F	99	SER	CB-CA-C	-5.70	110.02	116.63
1	H	65	ILE	N-CA-C	5.70	116.07	107.75
1	A	116	LEU	N-CA-C	-5.63	102.08	110.20
1	M	26	LEU	N-CA-C	-5.61	105.16	111.28
1	N	65	ILE	N-CA-C	5.61	115.94	107.75
1	K	68	PRO	N-CA-C	-5.59	106.86	114.80
1	B	65	ILE	N-CA-C	5.56	115.87	107.75
1	F	72	ILE	N-CA-C	5.53	115.73	110.42
1	I	152	ASN	N-CA-C	-5.45	105.42	111.36
1	L	99	SER	CB-CA-C	-5.45	110.28	116.54
1	M	65	ILE	N-CA-C	5.44	115.70	107.75
1	C	28	ASP	N-CA-C	-5.43	106.24	112.92
1	C	116	LEU	CA-C-N	5.43	125.07	119.05
1	C	116	LEU	C-N-CA	5.43	125.07	119.05
1	J	65	ILE	N-CA-C	5.42	115.70	108.11
1	H	72	ILE	N-CA-C	5.38	115.52	110.30
1	A	152	ASN	N-CA-C	-5.38	106.22	112.89
1	C	50	LEU	N-CA-C	-5.37	105.47	112.23
1	C	99	SER	CB-CA-C	-5.36	110.42	116.63
1	F	160	GLY	N-CA-C	-5.35	108.25	115.21
2	V	2	VAL	N-CA-C	5.35	115.90	108.84
1	G	116	LEU	N-CA-C	-5.33	103.21	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	70	GLY	N-CA-C	5.31	117.09	110.29
1	K	99	SER	CB-CA-C	-5.25	110.50	116.54
1	E	78	ILE	N-CA-C	-5.25	105.60	110.53
1	G	65	ILE	N-CA-C	5.24	115.40	107.75
1	E	99	SER	CB-CA-C	-5.21	110.55	116.54
1	M	177	SER	N-CA-C	-5.18	103.08	110.59
1	H	99	SER	CB-CA-C	-5.16	110.64	116.63
1	N	74	SER	N-CA-C	-5.16	105.66	111.28
1	M	152	ASN	N-CA-C	-5.15	105.75	111.36
1	D	177	SER	N-CA-C	-5.10	102.45	110.36
1	E	118	HIS	N-CA-C	5.10	119.14	113.02
1	N	152	ASN	N-CA-C	-5.09	105.85	111.71
1	K	184	TYR	N-CA-C	-5.06	107.14	113.72
1	I	99	SER	CB-CA-C	-5.05	110.74	116.54
1	M	56	ASP	CA-C-N	5.02	124.74	119.82
1	M	56	ASP	C-N-CA	5.02	124.74	119.82

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	1324	0	1351	53	0
1	B	1315	0	1338	74	0
1	C	1324	0	1351	76	0
1	D	1315	0	1338	65	0
1	E	1315	0	1338	85	0
1	F	1315	0	1338	48	0
1	G	1315	0	1338	43	0
1	H	1315	0	1338	43	0
1	I	1315	0	1338	44	0
1	J	1315	0	1338	52	0
1	K	1315	0	1338	67	0
1	L	1315	0	1338	52	0
1	M	1315	0	1338	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1315	0	1338	52	0
2	O	27	0	31	7	0
2	P	32	0	26	13	0
2	Q	27	0	31	6	0
2	T	27	0	31	3	0
2	U	30	0	31	10	0
2	V	27	0	31	2	0
2	W	27	0	31	8	0
2	X	27	0	31	7	0
3	R	15	0	5	3	0
3	S	20	0	6	3	0
All	All	18687	0	19012	739	0

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 20.

All (739) 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)
1:B:110:LYS:H	1:B:110:LYS:HD2	1.12	1.03
1:A:193:LYS:H	1:A:193:LYS:HD3	1.19	1.03
1:K:116:LEU:HD23	1:L:80:ASP:HB3	1.49	0.94
1:B:80:ASP:HB3	1:C:116:LEU:HD23	1.48	0.93
1:E:182:LYS:HE2	1:E:189:LYS:HA	1.51	0.93
2:U:3:LEU:HD23	2:U:3:LEU:H	1.34	0.92
1:G:94:ILE:HG22	1:G:116:LEU:HD22	1.51	0.91
1:G:32:LEU:HD23	1:G:64:TYR:HB2	1.53	0.91
1:E:82:MET:HG2	1:E:89:VAL:HG11	1.51	0.90
1:N:72:ILE:HA	1:N:100:MET:HE3	1.54	0.90
1:C:192:GLN:O	1:C:193:LYS:HD2	1.71	0.90
1:K:146:ARG:HE	1:K:146:ARG:HA	1.36	0.89
1:K:72:ILE:HD12	2:V:2:VAL:HB	1.53	0.88
1:D:80:ASP:HB3	1:E:116:LEU:HD23	1.55	0.87
1:C:79:TYR:HA	1:C:82:MET:HE3	1.56	0.86
1:B:72:ILE:HG12	2:P:7:GLN:HB2	1.55	0.86
1:A:193:LYS:HD3	1:A:193:LYS:N	1.90	0.85
1:I:32:LEU:HD13	1:I:64:TYR:HB2	1.57	0.84
1:F:100:MET:HE2	3:S:4:UNK:CB	2.08	0.83
1:L:38:ASN:ND2	1:L:41:VAL:H	1.77	0.82
1:D:125:GLN:HE22	1:K:135:SER:H	1.28	0.82
1:B:32:LEU:HD12	1:B:64:TYR:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:LYS:HA	1:E:168:LYS:HE3	1.61	0.81
1:B:110:LYS:HD2	1:B:110:LYS:N	1.93	0.81
1:E:94:ILE:HG22	1:E:116:LEU:HD22	1.64	0.80
1:K:32:LEU:HD12	1:K:64:TYR:HB2	1.64	0.79
1:A:125:GLN:HE21	1:H:134:ALA:HB3	1.48	0.79
1:E:72:ILE:HA	1:E:100:MET:HE3	1.66	0.78
1:A:47:ALA:HB1	1:B:21:ILE:HD12	1.62	0.78
1:I:25:LEU:HD11	1:J:51:PHE:HB2	1.64	0.78
1:I:38:ASN:ND2	1:I:41:VAL:H	1.81	0.78
1:N:110:LYS:O	1:N:110:LYS:HD3	1.83	0.78
1:C:110:LYS:HD3	1:C:111:GLY:N	2.00	0.77
1:K:168:LYS:HE3	1:K:168:LYS:HA	1.67	0.77
1:C:133:GLN:HE22	1:D:172:ARG:HH22	1.32	0.76
1:C:166:ILE:HD12	1:C:167:ALA:N	2.00	0.76
1:E:25:LEU:HD13	1:E:30:ILE:HD11	1.67	0.76
1:B:51:PHE:HB2	1:C:21:ILE:HD11	1.68	0.76
1:A:146:ARG:HD2	1:B:120:ARG:HH22	1.49	0.76
1:F:135:SER:O	1:F:139:ILE:HG22	1.86	0.75
1:N:164:GLU:O	1:N:168:LYS:HG2	1.86	0.74
1:K:20:ASP:HB3	1:K:23:SER:OG	1.87	0.74
1:E:99:SER:HB3	3:R:3:UNK:C	2.18	0.74
1:K:146:ARG:HA	1:K:146:ARG:NE	2.03	0.74
1:E:38:ASN:ND2	1:E:41:VAL:H	1.87	0.73
1:N:96:GLN:HE22	1:N:120:ARG:HH21	1.35	0.73
1:G:34:SER:HA	1:G:66:ASN:O	1.88	0.73
1:M:105:LEU:HD21	1:M:187:ILE:HD12	1.70	0.72
1:B:105:LEU:HD11	1:B:187:ILE:HD11	1.71	0.72
1:N:166:ILE:O	1:N:170:THR:HB	1.90	0.72
1:H:29:ARG:NH2	1:H:52:LEU:O	2.23	0.72
1:H:100:MET:HB2	2:U:5:PHE:HB3	1.71	0.72
1:A:146:ARG:CD	1:B:120:ARG:HH22	2.03	0.72
1:K:38:ASN:C	1:K:38:ASN:HD22	1.98	0.72
2:T:3:LEU:H	2:T:3:LEU:HD23	1.54	0.71
2:U:3:LEU:HD23	2:U:3:LEU:N	2.06	0.71
1:I:164:GLU:CD	1:I:164:GLU:H	1.99	0.71
1:K:60:ASP:OD2	1:K:88:ASP:HB2	1.90	0.71
1:M:115:SER:HB2	1:M:187:ILE:HD13	1.73	0.71
1:A:146:ARG:HD2	1:B:120:ARG:NH2	2.06	0.71
1:C:110:LYS:HD3	1:C:111:GLY:H	1.54	0.71
1:E:38:ASN:C	1:E:38:ASN:HD22	1.99	0.71
1:C:79:TYR:HA	1:C:82:MET:CE	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:GLN:NE2	1:K:135:SER:H	1.88	0.70
1:J:141:SER:O	1:J:144:ILE:HG22	1.90	0.70
1:H:118:HIS:HD2	1:I:80:ASP:OD1	1.75	0.70
1:D:66:ASN:HB2	1:D:94:ILE:HG13	1.73	0.70
1:F:139:ILE:HD13	1:F:139:ILE:C	2.16	0.70
1:N:32:LEU:HD23	1:N:64:TYR:HB2	1.74	0.69
1:L:21:ILE:HD11	1:M:51:PHE:HB2	1.72	0.69
1:D:72:ILE:HA	1:D:100:MET:HE3	1.72	0.69
1:I:38:ASN:C	1:I:38:ASN:HD22	2.00	0.69
1:D:38:ASN:ND2	1:D:41:VAL:H	1.90	0.69
1:M:20:ASP:HB3	1:M:23:SER:HB2	1.74	0.69
1:C:24:ARG:O	1:C:27:LYS:HG2	1.93	0.69
1:B:110:LYS:H	1:B:110:LYS:CD	1.96	0.69
1:K:191:LEU:HD13	1:L:84:PHE:CE1	2.28	0.69
1:A:29:ARG:NH2	1:A:52:LEU:O	2.26	0.68
1:C:35:GLY:O	1:C:67:SER:HB2	1.94	0.68
1:M:24:ARG:O	1:M:27:LYS:HB3	1.92	0.68
1:D:33:LEU:HD23	1:D:65:ILE:HG12	1.75	0.68
1:B:80:ASP:OD2	1:C:118:HIS:HD2	1.77	0.67
1:K:72:ILE:HA	1:K:100:MET:HE3	1.76	0.67
1:L:42:ALA:HA	1:L:78:ILE:HD11	1.75	0.67
1:B:99:SER:HB3	2:P:7:GLN:OXT	1.94	0.67
1:E:114:PHE:HE1	1:E:189:LYS:HE3	1.59	0.67
1:F:80:ASP:OD1	1:G:118:HIS:HD2	1.76	0.67
1:I:105:LEU:HD21	1:I:187:ILE:HD11	1.76	0.67
1:M:117:PRO:HD3	1:M:191:LEU:O	1.95	0.67
1:A:126:PRO:HA	2:O:4:GLY:HA3	1.75	0.67
1:B:164:GLU:CD	1:B:164:GLU:H	2.01	0.67
1:F:72:ILE:HA	1:F:100:MET:HE3	1.75	0.67
1:H:24:ARG:O	1:H:24:ARG:HD3	1.95	0.67
1:J:117:PRO:HG2	1:K:80:ASP:OD1	1.95	0.67
1:N:92:ILE:N	1:N:92:ILE:HD12	2.09	0.67
1:M:72:ILE:HA	1:M:100:MET:HE3	1.77	0.66
1:I:38:ASN:HD21	1:I:41:VAL:H	1.43	0.66
1:M:99:SER:HB3	2:W:4:GLY:O	1.94	0.66
1:A:125:GLN:NE2	1:H:134:ALA:HB3	2.10	0.66
1:B:151:MET:HG2	2:P:7:GLN:CD	2.20	0.66
1:I:116:LEU:HB3	1:I:117:PRO:HD2	1.78	0.66
1:N:96:GLN:NE2	1:N:120:ARG:HE	1.94	0.66
1:E:37:ILE:HB	1:E:70:GLY:HA3	1.77	0.65
1:I:120:ARG:HB3	1:J:146:ARG:HH22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:MET:HE1	1:E:186:LEU:HD11	1.79	0.65
1:C:182:LYS:HD3	1:C:182:LYS:C	2.21	0.65
1:M:21:ILE:HD13	1:M:21:ILE:O	1.95	0.65
1:E:72:ILE:HD12	3:R:1:UNK:H	1.62	0.65
1:K:189:LYS:HG2	1:K:190:VAL:N	2.12	0.65
1:M:96:GLN:HE22	1:M:120:ARG:HH21	1.43	0.65
1:L:38:ASN:C	1:L:38:ASN:HD22	2.05	0.64
1:F:34:SER:HA	1:F:66:ASN:O	1.98	0.64
1:A:84:PHE:CE1	1:B:191:LEU:HD13	2.33	0.64
1:H:21:ILE:HG23	1:H:22:TYR:N	2.12	0.64
1:I:162:SER:HB2	1:I:164:GLU:OE1	1.97	0.64
1:N:91:THR:C	1:N:92:ILE:HD12	2.22	0.64
1:C:127:LEU:HD23	1:J:133:GLN:HA	1.78	0.64
1:K:141:SER:O	1:K:144:ILE:HG22	1.97	0.64
1:B:72:ILE:CG2	1:B:151:MET:HE1	2.28	0.64
1:C:92:ILE:HD12	1:C:92:ILE:N	2.13	0.64
1:C:46:VAL:HG13	1:C:81:THR:HG21	1.80	0.63
1:E:80:ASP:OD2	1:F:118:HIS:HD2	1.80	0.63
1:L:42:ALA:CA	1:L:78:ILE:HD11	2.28	0.63
1:A:143:GLU:O	1:A:147:LEU:HD13	1.99	0.63
1:B:99:SER:HB3	2:P:7:GLN:C	2.23	0.63
1:I:118:HIS:HD2	1:J:80:ASP:OD1	1.82	0.63
1:F:86:ARG:HB2	1:F:87:PRO:HD3	1.80	0.63
1:L:118:HIS:HD2	1:M:80:ASP:OD1	1.82	0.63
1:A:80:ASP:OD2	1:B:118:HIS:HB2	2.00	0.62
1:A:124:HIS:NE2	2:O:4:GLY:HA2	2.15	0.62
1:G:24:ARG:O	1:G:24:ARG:HD3	1.98	0.62
1:K:92:ILE:N	1:K:92:ILE:HD12	2.15	0.62
1:A:72:ILE:HD12	2:O:2:VAL:HG12	1.80	0.62
1:A:20:ASP:HB3	1:A:23:SER:HB2	1.82	0.62
1:J:116:LEU:HD13	1:K:80:ASP:HB3	1.82	0.62
1:H:116:LEU:HD23	1:I:80:ASP:HB3	1.81	0.62
1:K:21:ILE:HG23	1:K:22:TYR:N	2.15	0.62
1:D:80:ASP:CB	1:E:116:LEU:HD23	2.27	0.62
1:C:78:ILE:HG22	1:C:82:MET:HE2	1.81	0.61
1:G:92:ILE:N	1:G:92:ILE:HD12	2.15	0.61
1:N:96:GLN:HE21	1:N:120:ARG:HE	1.48	0.61
1:L:38:ASN:HD21	1:L:41:VAL:H	1.47	0.61
1:H:86:ARG:HG3	1:H:86:ARG:HH11	1.66	0.61
1:E:21:ILE:O	1:E:22:TYR:HB2	1.99	0.61
1:G:99:SER:OG	1:G:100:MET:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:HB3	1:C:89:VAL:HG11	1.82	0.61
1:D:135:SER:H	1:K:125:GLN:HE22	1.48	0.61
1:M:32:LEU:HD23	1:M:64:TYR:HB2	1.83	0.61
1:M:85:ILE:HD12	1:M:87:PRO:HG2	1.81	0.61
1:N:128:GLY:HA3	2:X:2:VAL:HG12	1.83	0.61
1:J:114:PHE:HE1	1:J:189:LYS:HD3	1.65	0.61
1:K:99:SER:OG	1:K:100:MET:N	2.32	0.60
1:M:96:GLN:NE2	1:M:120:ARG:HH21	1.98	0.60
1:E:150:LEU:C	1:E:150:LEU:HD23	2.26	0.60
1:G:94:ILE:HG22	1:G:116:LEU:CD2	2.27	0.60
1:C:164:GLU:H	1:C:164:GLU:CD	2.09	0.60
1:D:47:ALA:HB1	1:E:21:ILE:HD12	1.84	0.60
1:G:188:ASP:O	1:G:189:LYS:HD3	2.01	0.60
1:B:100:MET:HE2	2:P:7:GLN:HE21	1.66	0.60
1:F:84:PHE:CE1	1:G:191:LEU:HD13	2.37	0.60
1:K:55:GLU:O	1:K:56:ASP:HB2	2.00	0.60
1:E:48:GLN:HA	1:F:21:ILE:HD11	1.83	0.60
1:J:21:ILE:O	1:J:25:LEU:HD13	2.01	0.60
1:F:20:ASP:O	1:F:24:ARG:HG3	2.02	0.60
1:D:140:ILE:O	1:D:144:ILE:HG13	2.02	0.60
1:M:53:GLU:O	1:M:57:PRO:HG3	2.02	0.59
1:C:150:LEU:C	1:C:150:LEU:HD23	2.27	0.59
1:E:21:ILE:HD13	1:E:22:TYR:H	1.65	0.59
1:E:168:LYS:HA	1:E:168:LYS:CE	2.31	0.59
1:E:28:ASP:O	1:E:29:ARG:HB2	2.01	0.59
1:M:108:GLY:HA3	1:M:113:ARG:HG2	1.83	0.59
1:G:130:ALA:HB2	1:G:140:ILE:HG21	1.84	0.59
1:C:136:ASP:O	1:C:140:ILE:HG12	2.02	0.59
1:M:105:LEU:HD21	1:M:187:ILE:CD1	2.31	0.59
1:M:72:ILE:HG12	2:W:4:GLY:CA	2.33	0.59
1:A:80:ASP:OD1	1:B:118:HIS:HD2	1.86	0.59
1:D:92:ILE:N	1:D:92:ILE:HD12	2.17	0.59
1:E:124:HIS:CD2	1:E:124:HIS:C	2.80	0.59
1:H:72:ILE:HA	1:H:100:MET:HE3	1.83	0.59
1:B:124:HIS:NE2	2:P:7:GLN:OXT	2.35	0.58
1:C:166:ILE:HD12	1:C:166:ILE:C	2.28	0.58
1:E:86:ARG:N	1:E:87:PRO:HD2	2.18	0.58
1:E:44:SER:O	1:E:48:GLN:HG3	2.03	0.58
1:H:94:ILE:HG22	1:H:116:LEU:HD22	1.84	0.58
1:N:120:ARG:HH22	2:U:3:LEU:HD21	1.68	0.58
1:B:116:LEU:HB3	1:B:117:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:HE21	1:C:165:GLN:HG2	1.68	0.58
1:B:85:ILE:HB	1:B:87:PRO:HD2	1.86	0.58
1:C:21:ILE:HG23	1:C:22:TYR:N	2.19	0.58
1:C:93:CYS:HB2	1:C:105:LEU:HD22	1.86	0.58
1:C:192:GLN:C	1:C:193:LYS:HD2	2.27	0.58
1:F:121:ILE:HD12	1:F:181:ALA:CB	2.33	0.58
1:J:120:ARG:C	1:J:121:ILE:HD12	2.29	0.58
1:F:29:ARG:NH2	1:F:52:LEU:O	2.37	0.58
1:B:57:PRO:HA	1:B:87:PRO:HG3	1.86	0.58
1:C:53:GLU:C	1:C:55:GLU:H	2.12	0.58
1:C:71:VAL:HG13	2:Q:1:ASN:HB3	1.85	0.57
1:F:139:ILE:HD13	1:F:140:ILE:N	2.18	0.57
1:K:78:ILE:O	1:K:82:MET:HG3	2.04	0.57
1:E:151:MET:O	1:E:155:LEU:HB2	2.04	0.57
1:K:130:ALA:HB1	1:K:140:ILE:HD12	1.86	0.57
1:D:96:GLN:HE22	2:Q:1:ASN:ND2	2.02	0.57
1:E:21:ILE:C	1:E:23:SER:H	2.13	0.57
1:D:105:LEU:HD21	1:D:187:ILE:HD11	1.85	0.57
1:I:20:ASP:HB3	1:I:23:SER:OG	2.04	0.57
1:I:100:MET:HE1	1:I:151:MET:SD	2.45	0.57
1:C:159:SER:HA	1:C:185:GLY:O	2.04	0.57
1:D:187:ILE:HG22	1:D:188:ASP:N	2.18	0.57
1:E:38:ASN:HD21	1:E:41:VAL:HG23	1.69	0.57
1:E:92:ILE:HD12	1:E:92:ILE:N	2.19	0.57
1:G:21:ILE:HG23	1:G:22:TYR:N	2.19	0.57
1:J:22:TYR:CE1	1:J:32:LEU:HD22	2.40	0.57
1:H:72:ILE:HG12	2:U:5:PHE:HB2	1.86	0.57
1:C:152:ASN:HB3	1:C:166:ILE:HD11	1.87	0.56
1:L:78:ILE:O	1:L:82:MET:HG3	2.04	0.56
1:M:72:ILE:HG12	2:W:4:GLY:N	2.19	0.56
1:C:57:PRO:HA	1:C:87:PRO:HG3	1.86	0.56
1:E:85:ILE:HD12	1:E:87:PRO:HG2	1.88	0.56
1:B:72:ILE:HG23	1:B:151:MET:HE1	1.88	0.56
1:B:122:MET:HA	1:B:174:PHE:O	2.06	0.56
1:F:139:ILE:HD11	1:G:175:TYR:HE1	1.70	0.56
1:H:124:HIS:C	1:H:124:HIS:CD2	2.82	0.56
1:M:182:LYS:HE3	1:M:189:LYS:HA	1.86	0.56
1:F:21:ILE:HG23	1:F:22:TYR:N	2.21	0.56
1:L:72:ILE:HA	1:L:100:MET:HE3	1.86	0.56
1:M:121:ILE:HD12	1:M:121:ILE:N	2.20	0.56
1:B:80:ASP:CB	1:C:116:LEU:HD23	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:TYR:CE1	1:I:154:ILE:HD13	2.40	0.56
1:C:94:ILE:HG22	1:C:116:LEU:HD13	1.88	0.56
1:C:182:LYS:HD3	1:C:183:GLU:N	2.20	0.56
1:K:161:GLN:HB2	1:K:166:ILE:HD11	1.87	0.56
1:H:38:ASN:H	1:H:41:VAL:HG22	1.71	0.56
1:L:45:ILE:HB	1:L:78:ILE:HD12	1.87	0.56
1:M:92:ILE:HD12	1:M:92:ILE:N	2.20	0.56
1:L:147:LEU:O	1:L:151:MET:HG2	2.05	0.55
1:A:92:ILE:N	1:A:92:ILE:HD12	2.21	0.55
1:B:51:PHE:HB2	1:C:21:ILE:CD1	2.37	0.55
1:K:147:LEU:O	1:K:151:MET:HG2	2.07	0.55
1:F:141:SER:O	1:F:144:ILE:HG22	2.06	0.55
1:L:116:LEU:HD13	1:M:80:ASP:HB3	1.89	0.55
1:K:38:ASN:ND2	1:K:41:VAL:H	2.05	0.55
1:M:63:LEU:HD22	1:M:65:ILE:HG13	1.87	0.55
1:M:105:LEU:HD11	1:M:187:ILE:HD11	1.89	0.55
1:E:125:GLN:HE22	1:L:135:SER:H	1.55	0.55
1:M:143:GLU:O	1:M:147:LEU:HD13	2.07	0.55
1:N:23:SER:O	1:N:26:LEU:HB3	2.07	0.55
1:K:38:ASN:C	1:K:38:ASN:ND2	2.65	0.54
1:M:86:ARG:N	1:M:87:PRO:HD2	2.22	0.54
1:F:86:ARG:HG3	1:F:86:ARG:HH11	1.70	0.54
1:C:164:GLU:O	1:C:168:LYS:HG3	2.08	0.54
1:G:86:ARG:N	1:G:87:PRO:HD2	2.23	0.54
1:H:176:MET:HB2	1:H:180:GLU:HB2	1.89	0.54
1:J:168:LYS:HA	1:J:168:LYS:HZ3	1.72	0.54
1:B:57:PRO:HG2	1:B:58:GLU:OE2	2.07	0.54
1:G:31:VAL:O	1:G:32:LEU:HB2	2.07	0.54
1:J:55:GLU:O	1:J:56:ASP:HB2	2.07	0.54
1:K:189:LYS:HG2	1:K:190:VAL:H	1.70	0.54
1:M:79:TYR:CE1	1:M:154:ILE:HD13	2.43	0.54
1:B:72:ILE:HD11	1:B:126:PRO:HB3	1.87	0.54
1:B:151:MET:HG2	2:P:7:GLN:OE1	2.08	0.54
1:H:37:ILE:HA	1:H:41:VAL:HG21	1.90	0.54
2:P:4:GLY:O	2:P:5:PHE:C	2.51	0.54
1:C:116:LEU:HB3	1:C:117:PRO:HD2	1.90	0.54
1:E:48:GLN:HA	1:F:21:ILE:CD1	2.38	0.54
1:E:60:ASP:OD2	1:E:88:ASP:HB2	2.07	0.54
1:K:91:THR:C	1:K:92:ILE:HD12	2.32	0.54
1:M:32:LEU:CD2	1:M:64:TYR:HB2	2.38	0.54
1:M:74:SER:O	1:M:77:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:PHE:HB3	1:J:191:LEU:CD2	2.37	0.54
1:J:116:LEU:HB3	1:J:117:PRO:HD2	1.89	0.53
1:D:24:ARG:HH21	1:D:27:LYS:NZ	2.06	0.53
1:I:53:GLU:OE1	1:I:87:PRO:HD3	2.08	0.53
1:N:97:ALA:O	1:N:102:ALA:HB2	2.06	0.53
1:C:146:ARG:HB3	1:D:120:ARG:NH2	2.24	0.53
1:E:42:ALA:O	1:E:46:VAL:HG13	2.08	0.53
1:I:29:ARG:NH1	1:I:59:LYS:O	2.41	0.53
1:M:115:SER:HB2	1:M:187:ILE:CD1	2.38	0.53
1:B:78:ILE:O	1:B:82:MET:HG3	2.08	0.53
1:F:29:ARG:NH1	1:F:59:LYS:O	2.41	0.53
1:C:94:ILE:HG22	1:C:116:LEU:HD22	1.90	0.53
1:F:86:ARG:HG3	1:F:86:ARG:NH1	2.24	0.53
2:W:1:ASN:N	2:W:1:ASN:HD22	2.05	0.53
1:H:99:SER:HB3	2:U:5:PHE:C	2.33	0.53
1:K:124:HIS:NE2	2:V:4:GLY:HA2	2.24	0.53
1:H:164:GLU:OE1	1:H:168:LYS:HE2	2.09	0.53
1:B:176:MET:HB2	1:B:180:GLU:HB2	1.91	0.53
1:G:165:GLN:HA	1:G:165:GLN:NE2	2.24	0.53
1:H:165:GLN:OE1	1:H:165:GLN:HA	2.07	0.53
1:J:122:MET:HA	1:J:174:PHE:O	2.09	0.53
1:N:130:ALA:HB2	1:N:140:ILE:HG21	1.90	0.53
1:B:92:ILE:N	1:B:92:ILE:HD12	2.23	0.53
1:C:133:GLN:HE22	1:D:172:ARG:NH2	2.05	0.53
1:E:156:ALA:O	1:E:159:SER:O	2.27	0.53
1:K:32:LEU:CD1	1:K:64:TYR:HB2	2.35	0.53
1:M:86:ARG:HG3	1:M:86:ARG:HH11	1.74	0.53
1:A:42:ALA:HA	1:A:78:ILE:HD11	1.91	0.52
1:C:127:LEU:HD21	1:J:133:GLN:HG2	1.90	0.52
1:E:173:ASP:HB3	1:E:175:TYR:CE1	2.44	0.52
1:F:136:ASP:O	1:F:139:ILE:HG23	2.10	0.52
1:F:92:ILE:N	1:F:92:ILE:HD12	2.24	0.52
1:C:161:GLN:NE2	1:C:165:GLN:HG2	2.24	0.52
1:E:29:ARG:HH21	1:E:56:ASP:HB3	1.73	0.52
1:H:100:MET:HE2	2:U:5:PHE:CB	2.40	0.52
1:I:165:GLN:HE21	1:I:165:GLN:HA	1.75	0.52
1:M:120:ARG:C	1:M:121:ILE:HD12	2.35	0.52
1:B:29:ARG:HD3	1:B:60:ASP:O	2.09	0.52
1:H:80:ASP:OD2	1:N:117:PRO:O	2.27	0.52
2:P:5:PHE:CD1	2:P:5:PHE:N	2.76	0.52
1:B:99:SER:HB3	2:P:7:GLN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ARG:HH21	1:D:27:LYS:CE	2.22	0.52
1:B:21:ILE:HD13	1:B:21:ILE:O	2.09	0.52
1:D:24:ARG:HH21	1:D:27:LYS:HE3	1.74	0.52
1:J:22:TYR:HE1	1:J:32:LEU:HD22	1.75	0.52
1:A:73:THR:HG22	1:A:74:SER:N	2.25	0.52
1:B:100:MET:CE	2:P:7:GLN:HE21	2.22	0.52
1:D:38:ASN:HD21	1:D:41:VAL:H	1.56	0.52
1:K:120:ARG:NH2	1:K:175:TYR:HE2	2.08	0.52
1:J:53:GLU:HG3	1:J:87:PRO:HD3	1.91	0.52
1:M:174:PHE:CD2	1:M:176:MET:HE2	2.45	0.52
1:A:116:LEU:HB3	1:A:117:PRO:HD2	1.92	0.52
1:I:172:ARG:NH2	1:J:133:GLN:OE1	2.37	0.52
1:C:48:GLN:O	1:C:52:LEU:HG	2.09	0.51
1:C:66:ASN:HA	1:C:96:GLN:O	2.10	0.51
1:E:80:ASP:OD2	1:F:118:HIS:CD2	2.61	0.51
1:F:117:PRO:HD3	1:F:191:LEU:O	2.09	0.51
1:A:80:ASP:HB3	1:B:116:LEU:HD13	1.92	0.51
1:D:21:ILE:HG23	1:D:22:TYR:N	2.26	0.51
1:M:118:HIS:HD2	1:N:80:ASP:OD1	1.92	0.51
1:B:72:ILE:HG21	1:B:151:MET:HE1	1.93	0.51
1:E:38:ASN:HD22	1:E:41:VAL:H	1.57	0.51
1:M:124:HIS:C	1:M:124:HIS:CD2	2.87	0.51
1:A:124:HIS:C	1:A:124:HIS:CD2	2.89	0.51
1:E:32:LEU:HD12	1:E:32:LEU:N	2.24	0.51
1:G:31:VAL:HG13	1:G:48:GLN:OE1	2.11	0.51
1:M:86:ARG:HH11	1:M:86:ARG:CG	2.24	0.51
1:A:120:ARG:HH22	1:G:146:ARG:HD2	1.75	0.51
1:B:143:GLU:HA	1:B:143:GLU:OE2	2.10	0.51
1:N:99:SER:HB3	2:X:4:GLY:O	2.11	0.51
1:B:50:LEU:O	1:B:53:GLU:HB3	2.10	0.51
1:H:86:ARG:HG3	1:H:86:ARG:NH1	2.25	0.51
1:K:121:ILE:HG13	1:K:181:ALA:CB	2.41	0.51
1:N:182:LYS:HE2	1:N:188:ASP:O	2.11	0.51
1:A:193:LYS:H	1:A:193:LYS:CD	2.05	0.51
1:L:21:ILE:HD13	1:L:21:ILE:O	2.11	0.51
1:M:120:ARG:HD2	1:N:143:GLU:OE2	2.10	0.51
1:F:94:ILE:HG22	1:F:116:LEU:CD1	2.40	0.51
1:I:124:HIS:C	1:I:124:HIS:CD2	2.88	0.51
1:B:86:ARG:N	1:B:87:PRO:CD	2.74	0.50
1:I:21:ILE:O	1:I:25:LEU:HD13	2.11	0.50
1:M:20:ASP:HB3	1:M:23:SER:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ALA:O	1:H:46:VAL:HG23	2.11	0.50
1:J:183:GLU:OE1	1:J:183:GLU:HA	2.09	0.50
1:J:191:LEU:HG	1:K:84:PHE:CE1	2.46	0.50
1:K:136:ASP:O	1:K:140:ILE:HG13	2.11	0.50
1:N:141:SER:O	1:N:144:ILE:HG22	2.12	0.50
1:J:66:ASN:HA	1:J:96:GLN:O	2.12	0.50
1:E:86:ARG:H	1:E:87:PRO:HD2	1.74	0.50
1:G:126:PRO:HD2	1:G:148:LYS:HG3	1.93	0.50
1:K:191:LEU:HD13	1:L:84:PHE:CZ	2.46	0.50
1:D:80:ASP:HB3	1:E:116:LEU:CD2	2.34	0.50
1:N:71:VAL:HB	1:N:74:SER:OG	2.12	0.50
1:L:33:LEU:C	1:L:33:LEU:HD23	2.36	0.50
1:D:99:SER:HB3	1:D:124:HIS:NE2	2.26	0.50
1:J:120:ARG:HH22	1:K:146:ARG:HG2	1.76	0.50
1:A:118:HIS:HD2	1:G:80:ASP:OD1	1.95	0.50
1:K:168:LYS:HE3	1:K:168:LYS:CA	2.41	0.50
1:D:86:ARG:N	1:D:87:PRO:HD2	2.27	0.50
1:L:86:ARG:H	1:L:87:PRO:HD2	1.77	0.50
1:B:105:LEU:CD1	1:B:187:ILE:HD11	2.40	0.49
1:E:66:ASN:C	1:E:66:ASN:HD22	2.18	0.49
1:H:92:ILE:HD12	1:H:92:ILE:N	2.27	0.49
1:M:53:GLU:HG3	1:M:87:PRO:HD2	1.92	0.49
1:E:25:LEU:HB3	1:E:30:ILE:CG1	2.42	0.49
1:I:97:ALA:O	1:I:102:ALA:HB2	2.12	0.49
1:N:20:ASP:HB3	1:N:23:SER:HB2	1.93	0.49
1:B:31:VAL:HG13	1:B:48:GLN:OE1	2.11	0.49
1:E:178:ALA:O	1:E:181:ALA:HB3	2.13	0.49
1:H:162:SER:OG	1:H:165:GLN:HB2	2.11	0.49
1:I:34:SER:HA	1:I:66:ASN:O	2.12	0.49
1:N:110:LYS:HD3	1:N:110:LYS:C	2.38	0.49
1:D:105:LEU:CG	1:D:187:ILE:HD11	2.42	0.49
1:A:57:PRO:HA	1:A:87:PRO:HG3	1.94	0.49
1:H:20:ASP:HB3	1:H:23:SER:HB2	1.94	0.49
1:H:122:MET:HG3	1:H:175:TYR:CE2	2.48	0.49
1:J:44:SER:O	1:J:48:GLN:HG3	2.13	0.49
1:D:24:ARG:NH2	1:D:27:LYS:NZ	2.61	0.49
1:E:25:LEU:HB3	1:E:30:ILE:HD11	1.95	0.49
1:E:129:GLY:HA2	1:L:130:ALA:O	2.13	0.49
1:I:164:GLU:O	1:I:168:LYS:HG3	2.12	0.49
1:B:29:ARG:HD2	1:B:59:LYS:HB3	1.95	0.49
1:F:28:ASP:O	1:F:29:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:3:LEU:N	2:U:3:LEU:CD2	2.75	0.49
1:C:124:HIS:NE2	2:Q:4:GLY:HA2	2.28	0.48
1:F:169:ASP:HB3	1:F:174:PHE:CD1	2.48	0.48
2:T:2:VAL:HG23	2:T:2:VAL:O	2.13	0.48
1:D:78:ILE:O	1:D:82:MET:HG3	2.13	0.48
1:G:141:SER:O	1:G:144:ILE:HG22	2.12	0.48
1:H:100:MET:HE2	2:U:5:PHE:CD2	2.48	0.48
1:I:57:PRO:HB2	1:I:86:ARG:HE	1.76	0.48
1:J:118:HIS:HD2	1:K:80:ASP:OD1	1.96	0.48
1:B:32:LEU:CD1	1:B:64:TYR:HB2	2.38	0.48
1:C:71:VAL:HA	2:Q:2:VAL:O	2.12	0.48
1:C:176:MET:HA	1:C:180:GLU:OE2	2.13	0.48
1:E:80:ASP:HB3	1:F:116:LEU:HD13	1.95	0.48
1:F:136:ASP:HA	1:F:139:ILE:CG2	2.43	0.48
1:G:36:GLU:HG2	1:G:68:PRO:HG2	1.94	0.48
1:L:38:ASN:HD22	1:L:41:VAL:H	1.61	0.48
1:D:125:GLN:HE22	1:K:135:SER:N	2.04	0.48
1:H:56:ASP:OD1	1:H:59:LYS:HG3	2.13	0.48
1:K:33:LEU:C	1:K:33:LEU:HD23	2.38	0.48
1:A:121:ILE:N	1:A:121:ILE:HD12	2.28	0.48
1:D:103:PHE:CD1	1:D:151:MET:HE3	2.49	0.48
1:L:53:GLU:C	1:L:55:GLU:H	2.22	0.48
1:A:95:GLY:O	1:A:119:SER:HA	2.14	0.48
1:B:72:ILE:HD13	1:B:151:MET:HE1	1.96	0.48
1:B:99:SER:HG	1:B:124:HIS:CE1	2.31	0.48
1:D:29:ARG:O	1:D:61:ILE:O	2.31	0.48
1:J:121:ILE:HD12	1:J:121:ILE:N	2.28	0.48
1:K:21:ILE:CG2	1:K:22:TYR:N	2.77	0.48
1:K:85:ILE:HB	1:K:87:PRO:HD2	1.96	0.48
1:D:189:LYS:HG2	1:D:190:VAL:N	2.29	0.48
1:M:72:ILE:HG13	2:W:2:VAL:O	2.14	0.48
1:C:82:MET:HE1	1:C:104:LEU:HD22	1.96	0.48
1:E:90:SER:HB2	1:E:112:LYS:O	2.14	0.48
1:E:100:MET:HE1	1:E:151:MET:SD	2.54	0.48
1:H:150:LEU:HD12	1:H:150:LEU:O	2.14	0.48
1:A:91:THR:C	1:A:92:ILE:HD12	2.38	0.47
1:A:130:ALA:O	1:H:129:GLY:HA2	2.14	0.47
1:D:116:LEU:HB3	1:D:117:PRO:HD2	1.96	0.47
1:G:165:GLN:HA	1:G:165:GLN:HE21	1.77	0.47
1:L:92:ILE:HD12	1:L:92:ILE:N	2.29	0.47
1:M:125:GLN:NE2	1:M:148:LYS:NZ	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:SER:O	1:C:144:ILE:HG22	2.14	0.47
1:D:105:LEU:CD2	1:D:187:ILE:HD11	2.44	0.47
1:E:38:ASN:ND2	1:E:41:VAL:HG23	2.28	0.47
1:I:159:SER:C	1:I:161:GLN:H	2.22	0.47
1:I:191:LEU:HD13	1:J:84:PHE:CE1	2.49	0.47
1:K:20:ASP:OD2	1:K:21:ILE:N	2.48	0.47
1:J:21:ILE:CG2	1:J:22:TYR:N	2.77	0.47
1:A:154:ILE:HG22	1:A:158:ASN:ND2	2.29	0.47
1:E:29:ARG:NH1	1:E:61:ILE:HG12	2.29	0.47
1:J:92:ILE:HG12	1:J:114:PHE:HB2	1.97	0.47
1:N:56:ASP:OD1	1:N:59:LYS:HG3	2.15	0.47
1:N:120:ARG:HH12	2:U:3:LEU:HD11	1.79	0.47
1:A:154:ILE:HG22	1:A:158:ASN:HD21	1.78	0.47
1:M:159:SER:HA	1:M:185:GLY:O	2.14	0.47
1:N:96:GLN:NE2	1:N:120:ARG:HH21	2.09	0.47
1:E:24:ARG:NH1	1:E:24:ARG:HB3	2.30	0.47
1:C:93:CYS:SG	1:C:97:ALA:HB2	2.54	0.47
1:D:113:ARG:O	1:D:187:ILE:HG23	2.14	0.47
1:G:36:GLU:HG2	1:G:68:PRO:CG	2.45	0.47
1:E:191:LEU:O	1:E:192:GLN:HG3	2.14	0.47
1:N:100:MET:HE1	1:N:151:MET:SD	2.55	0.47
1:E:20:ASP:O	1:E:23:SER:HB2	2.15	0.47
1:E:21:ILE:CD1	1:E:22:TYR:H	2.26	0.47
1:K:156:ALA:O	1:K:159:SER:O	2.32	0.47
1:M:63:LEU:HD23	1:M:63:LEU:C	2.40	0.47
1:B:159:SER:HA	1:B:185:GLY:O	2.15	0.47
1:F:125:GLN:HE21	1:M:134:ALA:HB3	1.80	0.47
1:G:44:SER:O	1:G:48:GLN:HG3	2.15	0.47
1:K:29:ARG:NH1	1:K:52:LEU:O	2.44	0.47
1:F:38:ASN:ND2	1:F:41:VAL:H	2.13	0.46
1:A:72:ILE:HA	1:A:100:MET:HE3	1.97	0.46
1:B:80:ASP:OD2	1:C:118:HIS:CD2	2.65	0.46
1:F:124:HIS:C	1:F:124:HIS:CD2	2.92	0.46
1:M:142:ASN:O	1:M:146:ARG:HD2	2.15	0.46
2:O:2:VAL:C	2:O:3:LEU:HD23	2.39	0.46
1:A:80:ASP:OD1	1:B:118:HIS:CD2	2.68	0.46
1:G:93:CYS:HB2	1:G:105:LEU:HD22	1.97	0.46
1:J:21:ILE:HG23	1:J:22:TYR:N	2.30	0.46
1:M:33:LEU:HD12	1:M:33:LEU:C	2.40	0.46
1:N:29:ARG:HG2	1:N:29:ARG:HH11	1.80	0.46
1:B:24:ARG:O	1:B:27:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:SER:HB2	1:L:112:LYS:O	2.16	0.46
1:L:21:ILE:HD11	1:M:51:PHE:CB	2.41	0.46
1:L:86:ARG:N	1:L:87:PRO:HD2	2.30	0.46
1:M:116:LEU:HB3	1:M:117:PRO:HD2	1.97	0.46
1:N:120:ARG:C	1:N:121:ILE:HD12	2.40	0.46
1:A:71:VAL:HA	2:O:2:VAL:O	2.15	0.46
1:H:21:ILE:CG2	1:H:22:TYR:N	2.77	0.46
1:A:97:ALA:O	1:A:102:ALA:HB2	2.16	0.46
1:D:109:ALA:O	1:D:112:LYS:HB2	2.15	0.46
1:E:121:ILE:HG22	1:E:176:MET:HE3	1.98	0.46
1:F:35:GLY:O	1:F:68:PRO:HD2	2.16	0.46
1:I:27:LYS:HE3	1:I:28:ASP:OD1	2.16	0.46
1:I:158:ASN:N	1:I:158:ASN:HD22	2.12	0.46
1:N:72:ILE:HG13	2:X:4:GLY:N	2.31	0.46
1:D:25:LEU:HD22	1:D:30:ILE:HD12	1.97	0.46
1:F:121:ILE:HD12	1:F:181:ALA:HB2	1.98	0.46
1:F:143:GLU:O	1:F:147:LEU:CD2	2.64	0.46
1:D:96:GLN:HE22	2:Q:1:ASN:HD21	1.64	0.46
1:F:124:HIS:HE2	3:S:4:UNK:C	2.28	0.46
1:F:139:ILE:HD11	1:G:175:TYR:CE1	2.49	0.46
1:H:121:ILE:HD12	1:H:121:ILE:N	2.31	0.46
1:N:72:ILE:HG12	2:X:4:GLY:CA	2.46	0.46
1:A:47:ALA:O	1:B:21:ILE:HD11	2.16	0.45
1:C:82:MET:CE	1:C:104:LEU:HD22	2.46	0.45
1:C:127:LEU:CD2	1:J:133:GLN:HG2	2.46	0.45
1:M:72:ILE:HG12	2:W:4:GLY:HA3	1.98	0.45
1:N:117:PRO:O	1:N:118:HIS:HB2	2.17	0.45
1:J:24:ARG:O	1:J:24:ARG:HD3	2.16	0.45
1:K:176:MET:HB2	1:K:180:GLU:HB3	1.98	0.45
1:L:60:ASP:OD1	1:L:88:ASP:HB2	2.16	0.45
1:A:23:SER:O	1:A:26:LEU:HB3	2.17	0.45
1:B:56:ASP:HB3	1:B:59:LYS:HB2	1.98	0.45
1:I:164:GLU:CD	1:I:164:GLU:N	2.73	0.45
1:C:123:ILE:HG13	1:C:170:THR:HG22	1.99	0.45
1:D:42:ALA:O	1:D:46:VAL:HG23	2.17	0.45
1:E:79:TYR:O	1:E:82:MET:HB2	2.15	0.45
1:J:190:VAL:O	1:J:192:GLN:NE2	2.50	0.45
1:I:159:SER:OG	1:I:161:GLN:HB2	2.17	0.45
1:A:122:MET:HA	1:A:174:PHE:O	2.17	0.45
1:D:79:TYR:CE2	1:E:118:HIS:CD2	3.05	0.45
1:H:24:ARG:HD3	1:H:24:ARG:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:ILE:HG22	1:L:116:LEU:CD1	2.47	0.45
2:W:1:ASN:N	2:W:1:ASN:ND2	2.64	0.45
1:M:192:GLN:HE21	1:M:192:GLN:HA	1.82	0.45
1:C:29:ARG:NH1	1:C:59:LYS:O	2.50	0.45
1:D:53:GLU:OE2	1:D:85:ILE:HA	2.16	0.45
1:D:85:ILE:HD12	1:D:87:PRO:HG2	1.98	0.45
1:D:166:ILE:C	1:D:168:LYS:N	2.75	0.45
1:D:187:ILE:CG2	1:D:188:ASP:N	2.79	0.45
1:H:164:GLU:O	1:H:168:LYS:HG3	2.17	0.45
1:K:38:ASN:HD21	1:K:41:VAL:H	1.64	0.45
1:K:86:ARG:N	1:K:87:PRO:CD	2.80	0.45
1:A:72:ILE:HD12	2:O:2:VAL:CG1	2.46	0.45
1:B:105:LEU:HD21	1:B:187:ILE:HD11	1.99	0.45
1:B:108:GLY:HA3	1:B:113:ARG:HG2	1.98	0.45
1:E:114:PHE:CE1	1:E:189:LYS:HE3	2.46	0.45
1:J:191:LEU:H	1:J:191:LEU:HD22	1.82	0.45
1:N:72:ILE:HG12	2:X:4:GLY:HA3	1.98	0.45
1:N:99:SER:HB3	2:X:4:GLY:C	2.41	0.45
1:D:116:LEU:HB3	1:D:117:PRO:CD	2.47	0.45
1:E:29:ARG:HH12	1:E:61:ILE:HG12	1.82	0.45
1:E:56:ASP:C	1:E:58:GLU:H	2.25	0.45
1:A:29:ARG:HD2	1:A:59:LYS:CG	2.47	0.44
1:D:124:HIS:C	1:D:124:HIS:CD2	2.93	0.44
1:E:80:ASP:O	1:E:84:PHE:HB2	2.17	0.44
1:H:53:GLU:HG3	1:H:87:PRO:HD3	1.99	0.44
1:C:79:TYR:CE2	1:D:118:HIS:CD2	3.05	0.44
1:C:80:ASP:OD1	1:D:118:HIS:HD2	2.00	0.44
1:E:176:MET:HE1	1:E:186:LEU:CD1	2.46	0.44
1:K:79:TYR:O	1:K:82:MET:HB2	2.18	0.44
1:K:82:MET:HE3	1:K:89:VAL:HG11	1.98	0.44
1:C:97:ALA:O	1:C:121:ILE:HA	2.18	0.44
1:D:38:ASN:HD22	1:D:38:ASN:H	1.66	0.44
1:D:56:ASP:OD1	1:D:58:GLU:HB2	2.18	0.44
1:D:150:LEU:O	1:D:154:ILE:HG13	2.17	0.44
1:G:21:ILE:CG2	1:G:22:TYR:N	2.81	0.44
1:C:86:ARG:N	1:C:87:PRO:CD	2.79	0.44
1:J:115:SER:HB3	1:J:187:ILE:HD13	1.99	0.44
1:L:117:PRO:HB2	1:L:118:HIS:CD2	2.53	0.44
1:M:192:GLN:HA	1:M:192:GLN:NE2	2.32	0.44
1:C:79:TYR:HE2	1:D:118:HIS:CD2	2.35	0.44
1:F:70:GLY:O	3:S:3:UNK:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:42:ALA:O	1:N:46:VAL:HG23	2.17	0.44
1:K:176:MET:HB2	1:K:180:GLU:CB	2.48	0.44
1:L:159:SER:HA	1:L:185:GLY:O	2.18	0.44
1:B:161:GLN:OE1	1:B:165:GLN:HG2	2.17	0.44
1:E:66:ASN:C	1:E:66:ASN:ND2	2.75	0.44
1:E:71:VAL:HB	1:E:74:SER:OG	2.18	0.44
1:I:145:LEU:O	1:I:148:LYS:HB3	2.17	0.44
1:C:94:ILE:O	1:C:94:ILE:HG13	2.18	0.44
1:E:84:PHE:HE1	1:F:191:LEU:HD13	1.83	0.44
1:N:174:PHE:CD2	1:N:176:MET:HE2	2.52	0.44
1:J:72:ILE:HA	1:J:100:MET:HE3	2.00	0.43
1:M:147:LEU:N	1:M:147:LEU:CD1	2.81	0.43
1:B:79:TYR:CD1	1:B:107:CYS:SG	3.11	0.43
1:H:71:VAL:HB	1:H:74:SER:OG	2.19	0.43
1:N:29:ARG:HG2	1:N:29:ARG:NH1	2.33	0.43
1:B:124:HIS:C	1:B:124:HIS:CD2	2.95	0.43
1:C:59:LYS:O	1:C:87:PRO:HB3	2.18	0.43
1:E:38:ASN:ND2	1:E:38:ASN:C	2.71	0.43
1:G:151:MET:O	1:G:155:LEU:HB2	2.19	0.43
1:L:38:ASN:ND2	1:L:38:ASN:C	2.75	0.43
1:L:140:ILE:O	1:L:144:ILE:HG13	2.18	0.43
1:M:49:LEU:HD12	1:M:49:LEU:HA	1.86	0.43
1:C:112:LYS:HA	1:C:114:PHE:CE1	2.54	0.43
1:K:52:LEU:HD12	1:K:52:LEU:HA	1.81	0.43
1:K:110:LYS:HA	1:K:110:LYS:HD2	1.84	0.43
1:K:192:GLN:OE1	1:K:192:GLN:HA	2.18	0.43
1:L:55:GLU:O	1:L:56:ASP:HB2	2.18	0.43
1:B:72:ILE:HD13	1:B:151:MET:CE	2.48	0.43
1:E:169:ASP:O	1:E:174:PHE:HB2	2.19	0.43
1:J:78:ILE:O	1:J:82:MET:HG3	2.18	0.43
1:J:103:PHE:CE1	1:J:151:MET:HG3	2.54	0.43
1:A:29:ARG:HD2	1:A:59:LYS:HG3	2.00	0.43
1:A:80:ASP:HB3	1:B:116:LEU:CD1	2.49	0.43
1:I:124:HIS:C	1:I:170:THR:HB	2.43	0.43
1:J:191:LEU:HG	1:K:84:PHE:HE1	1.83	0.43
1:L:53:GLU:O	1:L:57:PRO:HG3	2.18	0.43
1:L:158:ASN:N	1:L:158:ASN:HD22	2.17	0.43
1:D:38:ASN:HD21	1:D:41:VAL:HG23	1.83	0.43
1:E:117:PRO:HG3	1:E:192:GLN:HG3	2.01	0.43
1:E:158:ASN:N	1:E:158:ASN:HD22	2.16	0.43
1:J:52:LEU:HD23	1:J:61:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:LEU:O	1:L:151:MET:CG	2.66	0.43
1:C:184:TYR:HD2	1:C:186:LEU:HD13	1.83	0.43
1:E:29:ARG:HG2	1:E:52:LEU:HD22	2.00	0.43
1:K:74:SER:O	1:K:77:SER:HB2	2.17	0.43
1:L:20:ASP:OD2	1:L:23:SER:N	2.43	0.43
1:L:109:ALA:O	1:L:110:LYS:C	2.62	0.43
1:L:124:HIS:CD2	1:L:124:HIS:C	2.96	0.43
1:C:21:ILE:HG23	1:C:22:TYR:H	1.82	0.43
1:L:126:PRO:HD2	1:L:148:LYS:HG3	2.00	0.43
1:D:166:ILE:C	1:D:168:LYS:H	2.25	0.42
1:I:38:ASN:ND2	1:I:38:ASN:C	2.70	0.42
1:J:28:ASP:O	1:J:29:ARG:HB2	2.19	0.42
1:D:66:ASN:HA	1:D:96:GLN:O	2.19	0.42
1:E:91:THR:C	1:E:92:ILE:HD12	2.43	0.42
1:F:72:ILE:HD13	1:F:151:MET:HE1	2.01	0.42
1:G:153:SER:O	1:G:157:GLN:HB2	2.20	0.42
1:I:105:LEU:CD2	1:I:121:ILE:HD12	2.49	0.42
1:J:168:LYS:HA	1:J:168:LYS:NZ	2.35	0.42
1:D:110:LYS:C	1:D:112:LYS:H	2.26	0.42
1:G:91:THR:C	1:G:92:ILE:HD12	2.44	0.42
1:I:92:ILE:N	1:I:92:ILE:HD12	2.34	0.42
1:B:55:GLU:O	1:B:56:ASP:C	2.62	0.42
1:B:82:MET:HE3	1:B:89:VAL:HG11	2.01	0.42
1:F:35:GLY:C	1:F:68:PRO:HD2	2.44	0.42
1:G:41:VAL:O	1:G:45:ILE:HG12	2.19	0.42
1:G:72:ILE:HG13	2:T:4:GLY:N	2.34	0.42
1:I:21:ILE:HG23	1:I:22:TYR:N	2.34	0.42
1:K:117:PRO:HB3	1:K:192:GLN:OE1	2.19	0.42
1:E:99:SER:HB3	3:R:3:UNK:O	2.19	0.42
1:F:84:PHE:HE1	1:G:191:LEU:HD13	1.82	0.42
1:F:143:GLU:O	1:F:147:LEU:HD22	2.19	0.42
1:B:100:MET:CE	2:P:7:GLN:NE2	2.82	0.42
1:I:174:PHE:HD2	1:I:176:MET:HE2	1.85	0.42
1:J:42:ALA:HA	1:J:78:ILE:HD11	2.01	0.42
1:N:176:MET:HB2	1:N:180:GLU:HB2	2.02	0.42
1:A:130:ALA:N	1:H:130:ALA:O	2.53	0.42
1:C:55:GLU:O	1:C:56:ASP:HB2	2.20	0.42
1:E:21:ILE:C	1:E:23:SER:N	2.76	0.42
1:J:24:ARG:HD3	1:J:24:ARG:C	2.44	0.42
1:J:99:SER:OG	1:J:100:MET:N	2.52	0.42
1:K:53:GLU:HG3	1:K:87:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:76:LEU:HA	1:M:79:TYR:HB3	2.01	0.42
1:B:21:ILE:HD13	1:B:21:ILE:C	2.45	0.42
1:B:105:LEU:CG	1:B:187:ILE:HD11	2.50	0.42
1:C:53:GLU:C	1:C:55:GLU:N	2.78	0.42
1:C:179:LYS:O	1:C:182:LYS:HB3	2.20	0.42
1:G:85:ILE:HD12	1:G:87:PRO:HG2	2.00	0.42
1:H:147:LEU:HD12	1:H:147:LEU:HA	1.85	0.42
1:I:158:ASN:N	1:I:158:ASN:ND2	2.68	0.42
1:M:53:GLU:HG3	1:M:87:PRO:CD	2.50	0.42
1:N:25:LEU:O	1:N:30:ILE:HB	2.20	0.42
1:A:116:LEU:HD13	1:G:80:ASP:HB3	2.02	0.42
1:D:38:ASN:HD22	1:D:38:ASN:C	2.26	0.42
1:D:123:ILE:HD11	1:D:174:PHE:HD2	1.84	0.42
1:D:125:GLN:HB2	1:D:148:LYS:HE3	2.01	0.42
1:G:24:ARG:HD3	1:G:24:ARG:C	2.45	0.42
1:J:76:LEU:HA	1:J:76:LEU:HD12	1.77	0.42
1:L:130:ALA:HB1	1:L:140:ILE:HD12	2.00	0.42
1:L:150:LEU:O	1:L:154:ILE:HG13	2.20	0.42
1:D:105:LEU:HG	1:D:187:ILE:HD11	2.02	0.41
1:E:109:ALA:O	1:E:110:LYS:C	2.61	0.41
1:H:159:SER:HA	1:H:185:GLY:O	2.20	0.41
1:M:118:HIS:CE1	1:N:154:ILE:HD11	2.55	0.41
1:E:47:ALA:C	1:F:21:ILE:HD11	2.46	0.41
1:E:144:ILE:HG22	1:L:134:ALA:HB2	2.01	0.41
1:M:63:LEU:HD22	1:M:65:ILE:CG1	2.50	0.41
1:N:121:ILE:HD12	1:N:121:ILE:N	2.35	0.41
1:C:190:VAL:O	1:C:191:LEU:C	2.63	0.41
1:G:55:GLU:O	1:G:56:ASP:HB2	2.20	0.41
1:I:141:SER:O	1:I:144:ILE:HG22	2.21	0.41
1:N:156:ALA:HB1	1:N:161:GLN:O	2.20	0.41
1:A:71:VAL:HG22	2:O:3:LEU:CD2	2.50	0.41
1:F:116:LEU:HB3	1:F:117:PRO:HD2	2.02	0.41
1:H:38:ASN:OD1	1:H:40:SER:HB3	2.20	0.41
1:K:124:HIS:CD2	1:K:124:HIS:C	2.97	0.41
1:M:81:THR:HA	1:M:84:PHE:HB3	2.02	0.41
1:G:24:ARG:NH1	1:G:28:ASP:OD2	2.54	0.41
1:K:116:LEU:HB3	1:K:117:PRO:HD2	2.02	0.41
1:L:99:SER:OG	1:L:124:HIS:CE1	2.73	0.41
1:L:166:ILE:HD13	1:L:184:TYR:OH	2.19	0.41
1:C:82:MET:CB	1:C:89:VAL:HG11	2.48	0.41
1:I:165:GLN:HA	1:I:165:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:VAL:HB	1:J:74:SER:OG	2.21	0.41
1:J:98:ALA:HB1	1:J:122:MET:HE3	2.02	0.41
1:J:125:GLN:HB2	1:J:126:PRO:HD2	2.02	0.41
1:M:21:ILE:HD12	1:N:47:ALA:HB1	2.02	0.41
1:M:72:ILE:CG1	2:W:4:GLY:N	2.83	0.41
1:C:29:ARG:NH2	1:C:52:LEU:O	2.53	0.41
1:F:21:ILE:HG23	1:F:22:TYR:H	1.83	0.41
1:G:141:SER:O	1:G:145:LEU:HG	2.21	0.41
1:G:165:GLN:HE21	1:G:165:GLN:CA	2.33	0.41
1:L:161:GLN:HG3	1:L:184:TYR:CZ	2.56	0.41
1:A:86:ARG:N	1:A:87:PRO:CD	2.84	0.41
1:E:130:ALA:O	1:L:129:GLY:HA2	2.20	0.41
1:I:35:GLY:C	1:I:68:PRO:HD2	2.46	0.41
1:J:114:PHE:HB3	1:J:191:LEU:HD21	2.02	0.41
1:M:145:LEU:HD23	1:M:145:LEU:HA	1.87	0.41
1:N:34:SER:HA	1:N:66:ASN:O	2.20	0.41
1:A:169:ASP:OD2	1:A:184:TYR:OH	2.39	0.41
1:B:24:ARG:O	1:B:24:ARG:HD2	2.21	0.41
1:C:116:LEU:CB	1:C:117:PRO:HD2	2.51	0.41
1:C:126:PRO:HA	2:Q:4:GLY:HA3	2.03	0.41
1:D:55:GLU:O	1:D:56:ASP:HB2	2.21	0.41
1:E:90:SER:CB	1:E:112:LYS:HB3	2.51	0.41
1:G:32:LEU:HD23	1:G:64:TYR:CB	2.38	0.41
1:G:98:ALA:HA	1:G:122:MET:O	2.20	0.41
1:H:84:PHE:CE1	1:N:191:LEU:HD13	2.55	0.41
1:I:105:LEU:CD2	1:I:187:ILE:HD11	2.48	0.41
1:K:66:ASN:HA	1:K:96:GLN:O	2.20	0.41
1:K:121:ILE:HG13	1:K:181:ALA:HB2	2.01	0.41
1:M:63:LEU:C	1:M:63:LEU:CD2	2.94	0.41
1:N:79:TYR:CE1	1:N:154:ILE:HD13	2.55	0.41
1:A:51:PHE:HE1	1:B:24:ARG:HE	1.68	0.41
1:A:120:ARG:C	1:A:121:ILE:HD12	2.46	0.41
1:E:25:LEU:HB3	1:E:30:ILE:HG12	2.02	0.41
1:E:133:GLN:HA	1:L:127:LEU:HD23	2.03	0.41
1:H:57:PRO:HA	1:H:87:PRO:HG3	2.03	0.41
1:K:114:PHE:N	1:K:114:PHE:CD1	2.88	0.41
1:N:21:ILE:HG23	1:N:22:TYR:N	2.36	0.41
1:L:100:MET:HE1	1:L:151:MET:SD	2.61	0.40
1:A:111:GLY:H	1:A:188:ASP:CG	2.29	0.40
1:B:72:ILE:HA	1:B:100:MET:CE	2.51	0.40
1:C:133:GLN:HA	1:J:127:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ASN:HD22	1:D:38:ASN:N	2.18	0.40
1:F:150:LEU:O	1:F:150:LEU:HD12	2.21	0.40
1:K:116:LEU:HD23	1:L:80:ASP:CB	2.34	0.40
1:B:72:ILE:HG12	2:P:7:GLN:CB	2.39	0.40
1:C:52:LEU:HD13	1:C:61:ILE:HG23	2.04	0.40
1:C:142:ASN:O	1:C:146:ARG:HD2	2.22	0.40
1:E:159:SER:C	1:E:161:GLN:H	2.28	0.40
1:L:42:ALA:CB	1:L:78:ILE:HD11	2.51	0.40
1:M:37:ILE:HB	1:M:70:GLY:HA3	2.03	0.40
1:N:56:ASP:OD1	1:N:59:LYS:NZ	2.48	0.40
1:N:86:ARG:HB2	1:N:87:PRO:HD3	2.03	0.40
1:B:42:ALA:O	1:B:46:VAL:HG23	2.21	0.40
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.95	0.40
1:D:190:VAL:O	1:D:192:GLN:N	2.54	0.40
1:E:24:ARG:HB3	1:E:24:ARG:HH11	1.86	0.40
1:K:147:LEU:O	1:K:151:MET:CG	2.69	0.40
1:L:155:LEU:HD12	1:L:155:LEU:HA	1.89	0.40
1:N:72:ILE:CG1	2:X:4:GLY:N	2.84	0.40
1:N:86:ARG:N	1:N:87:PRO:CD	2.84	0.40
1:A:86:ARG:HB2	1:A:87:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

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	172/196 (88%)	165 (96%)	7 (4%)	0	100	100
1	B	171/196 (87%)	161 (94%)	9 (5%)	1 (1%)	21	38
1	C	172/196 (88%)	160 (93%)	10 (6%)	2 (1%)	10	20
1	D	171/196 (87%)	155 (91%)	14 (8%)	2 (1%)	10	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	171/196 (87%)	156 (91%)	15 (9%)	0	100	100
1	F	171/196 (87%)	164 (96%)	7 (4%)	0	100	100
1	G	171/196 (87%)	163 (95%)	7 (4%)	1 (1%)	21	38
1	H	171/196 (87%)	165 (96%)	6 (4%)	0	100	100
1	I	171/196 (87%)	166 (97%)	5 (3%)	0	100	100
1	J	171/196 (87%)	161 (94%)	8 (5%)	2 (1%)	10	20
1	K	171/196 (87%)	162 (95%)	7 (4%)	2 (1%)	10	20
1	L	171/196 (87%)	162 (95%)	7 (4%)	2 (1%)	10	20
1	M	171/196 (87%)	168 (98%)	3 (2%)	0	100	100
1	N	171/196 (87%)	166 (97%)	5 (3%)	0	100	100
2	O	2/7 (29%)	2 (100%)	0	0	100	100
2	P	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
2	Q	2/7 (29%)	2 (100%)	0	0	100	100
2	T	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
2	U	2/7 (29%)	2 (100%)	0	0	100	100
2	V	2/7 (29%)	2 (100%)	0	0	100	100
2	W	2/7 (29%)	2 (100%)	0	0	100	100
2	X	2/7 (29%)	2 (100%)	0	0	100	100
All	All	2412/2800 (86%)	2288 (95%)	111 (5%)	13 (0%)	24	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	34	SER
1	K	161	GLN
1	D	191	LEU
1	C	56	ASP
1	K	56	ASP
1	L	172	ARG
2	P	5	PHE
1	C	54	ALA
1	J	56	ASP
1	B	119	SER
1	J	141	SER
1	L	56	ASP
1	D	56	ASP

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	146/166 (88%)	139 (95%)	7 (5%)	23 46
1	B	145/166 (87%)	140 (97%)	5 (3%)	32 60
1	C	146/166 (88%)	141 (97%)	5 (3%)	32 60
1	D	145/166 (87%)	138 (95%)	7 (5%)	23 46
1	E	145/166 (87%)	134 (92%)	11 (8%)	12 26
1	F	145/166 (87%)	140 (97%)	5 (3%)	32 60
1	G	145/166 (87%)	141 (97%)	4 (3%)	38 66
1	H	145/166 (87%)	136 (94%)	9 (6%)	16 34
1	I	145/166 (87%)	140 (97%)	5 (3%)	32 60
1	J	145/166 (87%)	138 (95%)	7 (5%)	23 46
1	K	145/166 (87%)	138 (95%)	7 (5%)	23 46
1	L	145/166 (87%)	142 (98%)	3 (2%)	47 74
1	M	145/166 (87%)	136 (94%)	9 (6%)	16 34
1	N	145/166 (87%)	139 (96%)	6 (4%)	27 53
2	O	3/6 (50%)	3 (100%)	0	100 100
2	P	3/6 (50%)	2 (67%)	1 (33%)	0 0
2	Q	3/6 (50%)	3 (100%)	0	100 100
2	T	3/6 (50%)	3 (100%)	0	100 100
2	U	3/6 (50%)	2 (67%)	1 (33%)	0 0
2	V	3/6 (50%)	2 (67%)	1 (33%)	0 0
2	W	3/6 (50%)	3 (100%)	0	100 100
2	X	3/6 (50%)	2 (67%)	1 (33%)	0 0
All	All	2056/2372 (87%)	1962 (95%)	94 (5%)	24 48

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	49	LEU
1	A	73	THR
1	A	110	LYS
1	A	127	LEU
1	A	183	GLU
1	A	193	LYS
1	B	21	ILE
1	B	24	ARG
1	B	29	ARG
1	B	32	LEU
1	B	187	ILE
1	C	49	LEU
1	C	92	ILE
1	C	146	ARG
1	C	147	LEU
1	C	186	LEU
1	D	24	ARG
1	D	38	ASN
1	D	76	LEU
1	D	96	GLN
1	D	99	SER
1	D	147	LEU
1	D	192	GLN
1	E	21	ILE
1	E	24	ARG
1	E	32	LEU
1	E	38	ASN
1	E	46	VAL
1	E	66	ASN
1	E	116	LEU
1	E	120	ARG
1	E	168	LYS
1	E	183	GLU
1	E	192	GLN
1	F	33	LEU
1	F	38	ASN
1	F	139	ILE
1	F	150	LEU
1	F	161	GLN
1	G	76	LEU
1	G	92	ILE
1	G	116	LEU

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Mol	Chain	Res	Type
1	G	186	LEU
1	H	29	ARG
1	H	32	LEU
1	H	105	LEU
1	H	124	HIS
1	H	147	LEU
1	H	157	GLN
1	H	163	LEU
1	H	164	GLU
1	H	165	GLN
1	I	38	ASN
1	I	53	GLU
1	I	96	GLN
1	I	164	GLU
1	I	186	LEU
1	J	27	LYS
1	J	52	LEU
1	J	76	LEU
1	J	86	ARG
1	J	151	MET
1	J	168	LYS
1	J	183	GLU
1	K	38	ASN
1	K	52	LEU
1	K	88	ASP
1	K	96	GLN
1	K	163	LEU
1	K	168	LYS
1	K	192	GLN
1	L	21	ILE
1	L	38	ASN
1	L	53	GLU
1	M	21	ILE
1	M	33	LEU
1	M	49	LEU
1	M	86	ARG
1	M	146	ARG
1	M	147	LEU
1	M	155	LEU
1	M	187	ILE
1	M	191	LEU
1	N	36	GLU

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Mol	Chain	Res	Type
1	N	92	ILE
1	N	110	LYS
1	N	164	GLU
1	N	170	THR
1	N	192	GLN
2	P	5	PHE
2	U	3	LEU
2	V	1	ASN
2	X	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	125	GLN
1	A	158	ASN
1	A	161	GLN
1	B	48	GLN
1	B	66	ASN
1	B	118	HIS
1	B	125	GLN
1	B	158	ASN
1	B	165	GLN
1	B	192	GLN
1	C	96	GLN
1	C	118	HIS
1	C	133	GLN
1	C	142	ASN
1	C	161	GLN
1	C	165	GLN
1	D	38	ASN
1	D	96	GLN
1	D	118	HIS
1	D	125	GLN
1	D	158	ASN
1	D	192	GLN
1	E	38	ASN
1	E	66	ASN
1	E	83	ASN
1	E	118	HIS
1	E	124	HIS
1	E	125	GLN

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Mol	Chain	Res	Type
1	E	142	ASN
1	E	158	ASN
1	F	38	ASN
1	F	83	ASN
1	F	118	HIS
1	F	125	GLN
1	F	142	ASN
1	F	152	ASN
1	F	157	GLN
1	F	161	GLN
1	F	165	GLN
1	F	192	GLN
1	G	83	ASN
1	G	118	HIS
1	G	131	GLN
1	G	142	ASN
1	G	165	GLN
1	H	83	ASN
1	H	118	HIS
1	H	124	HIS
1	H	131	GLN
1	I	38	ASN
1	I	66	ASN
1	I	96	GLN
1	I	118	HIS
1	I	124	HIS
1	I	152	ASN
1	I	158	ASN
1	I	165	GLN
1	J	96	GLN
1	J	118	HIS
1	J	125	GLN
1	J	152	ASN
1	J	157	GLN
1	J	158	ASN
1	J	165	GLN
1	K	38	ASN
1	K	48	GLN
1	K	96	GLN
1	K	118	HIS
1	K	125	GLN
1	K	158	ASN

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Mol	Chain	Res	Type
1	K	165	GLN
1	L	38	ASN
1	L	48	GLN
1	L	118	HIS
1	L	157	GLN
1	L	158	ASN
1	L	165	GLN
1	M	96	GLN
1	M	118	HIS
1	M	125	GLN
1	M	165	GLN
1	M	192	GLN
1	N	96	GLN
1	N	125	GLN
1	N	165	GLN
2	P	7	GLN
2	W	1	ASN

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 oligosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	174/196 (88%)	-0.02	3 (1%) 69 65	28, 42, 63, 73	0
1	B	173/196 (88%)	0.00	2 (1%) 76 73	33, 42, 66, 77	0
1	C	174/196 (88%)	0.27	2 (1%) 78 75	38, 52, 70, 77	0
1	D	173/196 (88%)	0.25	2 (1%) 76 73	36, 50, 66, 76	0
1	E	173/196 (88%)	0.21	6 (3%) 47 42	34, 48, 67, 85	0
1	F	173/196 (88%)	-0.11	1 (0%) 85 83	29, 42, 60, 72	0
1	G	173/196 (88%)	-0.21	3 (1%) 69 65	27, 37, 55, 63	0
1	H	173/196 (88%)	-0.14	0 100 100	26, 39, 57, 64	0
1	I	173/196 (88%)	-0.04	1 (0%) 85 83	31, 43, 59, 73	0
1	J	173/196 (88%)	0.05	1 (0%) 85 83	37, 46, 59, 67	0
1	K	173/196 (88%)	0.09	1 (0%) 85 83	38, 48, 63, 75	0
1	L	173/196 (88%)	0.05	2 (1%) 76 73	34, 46, 68, 75	0
1	M	173/196 (88%)	-0.25	1 (0%) 85 83	27, 39, 56, 61	0
1	N	173/196 (88%)	-0.14	1 (0%) 85 83	26, 39, 55, 67	0
2	O	4/7 (57%)	3.17	3 (75%) 0 0	80, 83, 85, 88	0
2	P	4/7 (57%)	2.81	4 (100%) 0 0	80, 82, 88, 88	0
2	Q	4/7 (57%)	1.96	1 (25%) 2 1	76, 80, 83, 86	0
2	T	4/7 (57%)	2.77	3 (75%) 0 0	68, 73, 80, 84	0
2	U	4/7 (57%)	3.36	3 (75%) 0 0	76, 79, 80, 88	0
2	V	4/7 (57%)	3.07	3 (75%) 0 0	85, 87, 87, 88	0
2	W	4/7 (57%)	2.69	2 (50%) 0 0	75, 77, 77, 79	0
2	X	4/7 (57%)	2.42	2 (50%) 0 0	67, 70, 70, 74	0
3	R	0/7	-	-	-	-
3	S	0/7	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	2456/2814 (87%)	0.04	47 (1%) 66 62	26, 44, 65, 88	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	5	PHE	6.0
2	W	4	GLY	5.0
2	V	4	GLY	4.6
2	T	4	GLY	4.4
2	O	4	GLY	4.2
1	E	160	GLY	4.1
2	X	4	GLY	4.1
2	O	3	LEU	4.0
2	T	2	VAL	3.7
2	O	2	VAL	3.6
2	V	2	VAL	3.6
2	W	3	LEU	3.3
2	P	4	GLY	3.3
2	P	5	PHE	3.2
2	U	3	LEU	2.9
2	U	4	GLY	2.9
1	E	22	TYR	2.9
1	G	20	ASP	2.9
1	E	20	ASP	2.8
2	V	3	LEU	2.7
1	E	21	ILE	2.6
1	F	24	ARG	2.6
2	Q	1	ASN	2.5
1	K	183	GLU	2.5
1	L	192	GLN	2.5
1	E	192	GLN	2.4
2	X	2	VAL	2.4
2	P	7	GLN	2.4
2	P	6	THR	2.3
1	D	192	GLN	2.3
2	T	3	LEU	2.3
1	J	192	GLN	2.3
1	A	192	GLN	2.2
1	M	183	GLU	2.2
1	A	23	SER	2.2
1	L	185	GLY	2.1
1	E	146	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	146	ARG	2.1
1	N	20	ASP	2.1
1	B	187	ILE	2.1
1	I	187	ILE	2.1
1	A	193	LYS	2.1
1	C	193	LYS	2.1
1	G	157	GLN	2.0
1	B	57	PRO	2.0
1	D	87	PRO	2.0
1	C	160	GLY	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 oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.