



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:02 PM UTC

PDB ID : 2ZL3 / pdb_00002zl3
Title : Crystal structure of H.pylori ClpP S99A
Authors : Kim, D.Y.; Kim, K.K.
Deposited on : 2008-04-02
Resolution : 2.81 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

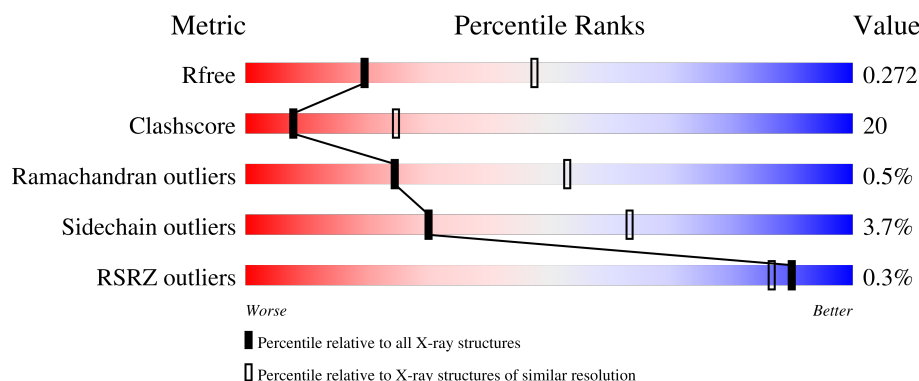
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	57% 28% • 12%
1	B	196	51% 33% • 12%
1	C	196	47% 37% • 12%
1	D	196	53% 32% • 12%
1	E	196	50% 37% • 12%

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Mol	Chain	Length	Quality of chain
1	F	196	% 54% 30% • • 12%
1	G	196	57% 30% • 12%
1	H	196	58% 27% • 12%
1	I	196	56% 30% • 12%
1	J	196	62% 24% • 12%
1	K	196	48% 39% • 12%
1	L	196	56% 29% • 12%
1	M	196	55% 32% • 12%
1	N	196	% 62% 26% • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18396 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	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	B	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	C	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	D	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	E	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	F	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	G	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	H	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	I	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	J	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	K	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	L	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	M	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			
1	N	173	Total	C	N	O	S	0	0	0
			1314	828	222	257	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ALA	SER	engineered mutation	UNP P56156

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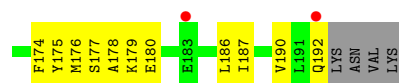
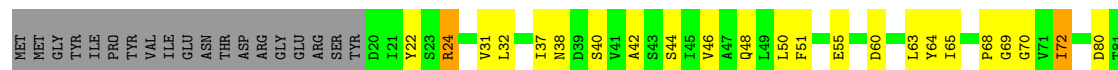
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	ALA	SER	engineered mutation	UNP P56156
C	99	ALA	SER	engineered mutation	UNP P56156
D	99	ALA	SER	engineered mutation	UNP P56156
E	99	ALA	SER	engineered mutation	UNP P56156
F	99	ALA	SER	engineered mutation	UNP P56156
G	99	ALA	SER	engineered mutation	UNP P56156
H	99	ALA	SER	engineered mutation	UNP P56156
I	99	ALA	SER	engineered mutation	UNP P56156
J	99	ALA	SER	engineered mutation	UNP P56156
K	99	ALA	SER	engineered mutation	UNP P56156
L	99	ALA	SER	engineered mutation	UNP P56156
M	99	ALA	SER	engineered mutation	UNP P56156
N	99	ALA	SER	engineered mutation	UNP P56156



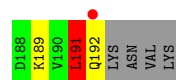
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



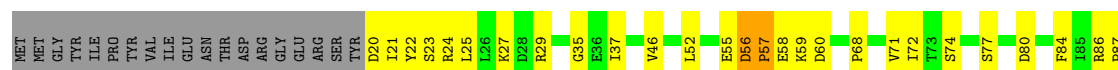
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

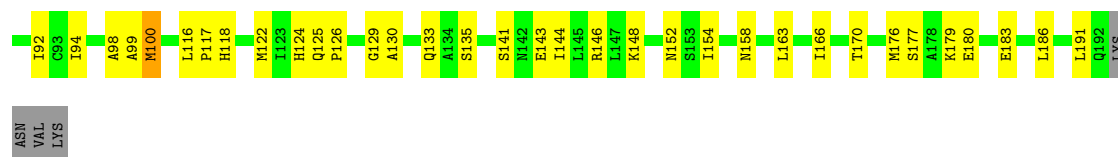


- Molecule 1: ATP-dependent Clp protease proteolytic subunit



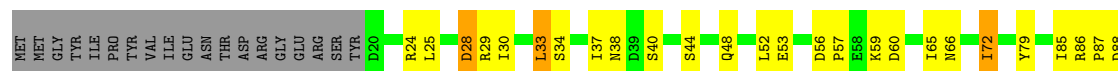
- Molecule 1: ATP-dependent Clp protease proteolytic subunit





- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H: 58% 27% 12%



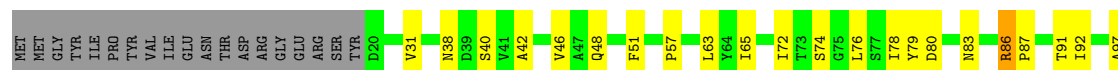
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I: 56% 30% 12%



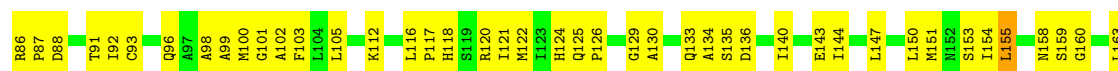
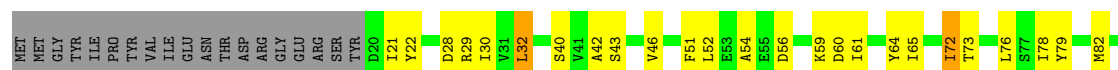
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 62% 24% 12%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

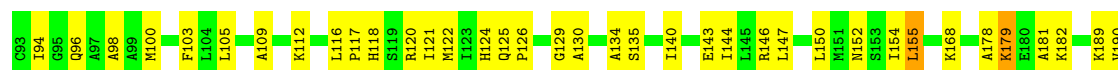
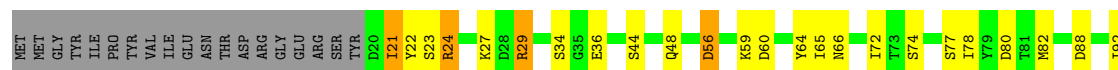
Chain K: 48% 39% 12%





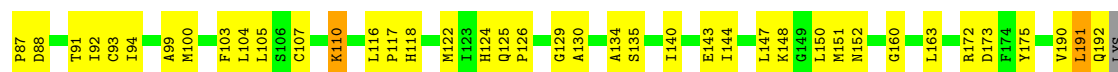
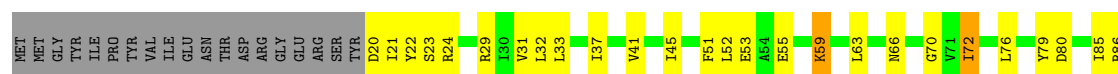
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 56% 29% 12%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 55% 32% 12%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 62% 26% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 166.41Å 186.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.81 19.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.99-2.81) 97.4 (19.99-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.272 0.212 , 0.272	Depositor DCC
R_{free} test set	6960 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18396	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.44	0/1330	0.95	2/1791 (0.1%)
1	B	0.46	0/1330	0.94	3/1791 (0.2%)
1	C	0.42	0/1330	0.95	5/1791 (0.3%)
1	D	0.43	0/1330	0.94	7/1791 (0.4%)
1	E	0.42	0/1330	0.95	4/1791 (0.2%)
1	F	0.45	0/1330	0.96	4/1791 (0.2%)
1	G	0.46	0/1330	0.93	1/1791 (0.1%)
1	H	0.47	0/1330	0.93	3/1791 (0.2%)
1	I	0.47	0/1330	0.97	3/1791 (0.2%)
1	J	0.46	0/1330	0.90	5/1791 (0.3%)
1	K	0.43	0/1330	0.96	5/1791 (0.3%)
1	L	0.43	0/1330	0.95	6/1791 (0.3%)
1	M	0.42	0/1330	0.98	5/1791 (0.3%)
1	N	0.46	0/1330	0.99	4/1791 (0.2%)
All	All	0.44	0/18620	0.95	57/25074 (0.2%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ILE	N-CA-C	8.00	118.78	110.62
1	I	72	ILE	N-CA-C	7.63	117.70	110.30
1	C	84	PHE	N-CA-C	-7.60	103.61	113.12
1	J	65	ILE	N-CA-C	6.98	118.11	107.77
1	M	160	GLY	N-CA-C	-6.96	105.72	115.32
1	A	72	ILE	N-CA-C	6.87	117.38	110.23
1	D	156	ALA	N-CA-C	-6.71	104.26	113.18
1	M	152	ASN	N-CA-C	-6.69	103.92	111.14
1	L	65	ILE	N-CA-C	6.63	117.43	107.75
1	J	72	ILE	N-CA-C	6.59	117.08	110.23
1	B	65	ILE	N-CA-C	6.57	117.31	108.11
1	K	158	ASN	N-CA-C	6.54	118.40	111.28
1	E	72	ILE	N-CA-C	6.42	116.45	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	56	ASP	CA-C-N	6.27	125.97	119.82
1	N	56	ASP	C-N-CA	6.27	125.97	119.82
1	K	65	ILE	N-CA-C	6.23	116.83	107.80
1	I	59	LYS	N-CA-C	6.22	118.74	110.53
1	D	72	ILE	N-CA-C	6.19	116.24	110.42
1	E	65	ILE	N-CA-C	6.16	116.73	108.11
1	J	118	HIS	N-CA-C	5.82	119.14	112.97
1	B	132	GLY	N-CA-C	5.82	118.29	110.43
1	H	72	ILE	N-CA-C	5.81	116.28	110.23
1	D	96	GLN	N-CA-C	5.74	117.57	108.79
1	C	72	ILE	N-CA-C	5.71	116.36	110.36
1	K	118	HIS	N-CA-C	5.67	119.90	112.92
1	N	70	GLY	N-CA-C	5.67	117.55	110.29
1	C	65	ILE	N-CA-C	5.65	116.08	108.17
1	D	65	ILE	N-CA-C	5.64	115.99	107.75
1	E	169	ASP	N-CA-C	5.64	117.23	111.14
1	F	182	LYS	N-CA-C	-5.64	105.21	111.36
1	C	21	ILE	N-CA-C	5.58	115.78	110.53
1	K	72	ILE	N-CA-C	5.57	116.35	110.72
1	M	72	ILE	N-CA-C	5.57	115.70	110.30
1	F	99	ALA	CB-CA-C	-5.54	110.20	116.63
1	H	65	ILE	N-CA-C	5.52	115.84	108.11
1	H	28	ASP	N-CA-C	-5.51	106.41	113.02
1	K	102	ALA	N-CA-C	-5.46	104.98	111.69
1	C	99	ALA	CB-CA-C	-5.43	110.30	116.54
1	G	99	ALA	CB-CA-C	-5.37	110.40	116.63
1	L	56	ASP	CA-C-N	5.36	126.54	119.84
1	L	56	ASP	C-N-CA	5.36	126.54	119.84
1	I	65	ILE	N-CA-C	5.32	116.14	108.48
1	M	59	LYS	N-CA-C	5.28	118.09	110.28
1	D	68	PRO	N-CA-C	-5.25	107.34	114.80
1	N	182	LYS	N-CA-C	-5.25	105.00	111.40
1	D	116	LEU	CA-C-N	5.24	124.69	119.24
1	D	116	LEU	C-N-CA	5.24	124.69	119.24
1	L	152	ASN	N-CA-C	-5.20	105.79	111.82
1	A	99	ALA	CB-CA-C	-5.12	110.69	116.63
1	F	125	GLN	CA-C-N	5.12	125.11	119.89
1	F	125	GLN	C-N-CA	5.12	125.11	119.89
1	L	21	ILE	N-CA-C	5.06	115.49	110.23
1	J	114	PHE	N-CA-C	5.03	117.20	109.95
1	J	160	GLY	N-CA-C	-5.03	108.67	115.21
1	L	118	HIS	N-CA-C	5.03	119.11	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	99	ALA	CB-CA-C	-5.01	110.81	116.63
1	E	99	ALA	CB-CA-C	-5.01	110.78	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1314	0	1338	71	0
1	B	1314	0	1338	83	0
1	C	1314	0	1338	70	0
1	D	1314	0	1338	63	0
1	E	1314	0	1338	71	0
1	F	1314	0	1338	63	0
1	G	1314	0	1338	57	0
1	H	1314	0	1338	46	0
1	I	1314	0	1338	54	0
1	J	1314	0	1338	39	0
1	K	1314	0	1338	70	0
1	L	1314	0	1338	57	0
1	M	1314	0	1338	67	0
1	N	1314	0	1338	40	0
All	All	18396	0	18732	735	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 (735) 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:E:117:PRO:HG3	1:E:192:GLN:HA	1.43	1.00
1:L:24:ARG:HD2	1:L:27:LYS:HD3	1.45	0.98
1:A:146:ARG:HG2	1:B:120:ARG:NH2	1.88	0.88
1:B:24:ARG:HD2	1:B:27:LYS:HD2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASN:C	1:B:38:ASN:HD22	1.83	0.86
1:L:182:LYS:HE2	1:L:189:LYS:HA	1.56	0.86
1:N:72:ILE:HD12	1:N:72:ILE:H	1.40	0.84
1:E:179:LYS:HZ1	1:E:192:GLN:NE2	1.74	0.84
1:A:120:ARG:HH12	1:G:146:ARG:HD2	1.40	0.83
1:K:116:LEU:HD13	1:L:80:ASP:HB3	1.60	0.82
1:K:98:ALA:HB1	1:K:122:MET:HE3	1.62	0.81
1:B:24:ARG:HH11	1:B:27:LYS:HD2	1.45	0.80
1:C:98:ALA:HB1	1:C:122:MET:HE3	1.62	0.80
1:E:72:ILE:HA	1:E:100:MET:HE3	1.63	0.79
1:B:134:ALA:HB3	1:I:125:GLN:HE21	1.48	0.79
1:L:182:LYS:HE3	1:L:190:VAL:HG23	1.64	0.77
1:K:32:LEU:HD12	1:K:64:TYR:HB2	1.67	0.76
1:G:117:PRO:HD3	1:G:191:LEU:O	1.84	0.76
1:K:72:ILE:HD11	1:K:126:PRO:HB3	1.66	0.74
1:C:146:ARG:HD2	1:D:120:ARG:HH22	1.51	0.74
1:C:24:ARG:O	1:C:27:LYS:HG2	1.88	0.74
1:K:126:PRO:HB2	1:K:144:ILE:HD11	1.68	0.74
1:L:72:ILE:HD11	1:L:126:PRO:HB3	1.69	0.74
1:F:125:GLN:HE21	1:M:134:ALA:HB3	1.54	0.73
1:I:72:ILE:HD11	1:I:126:PRO:HB3	1.69	0.73
1:A:146:ARG:HG2	1:B:120:ARG:HH22	1.52	0.72
1:C:29:ARG:NH1	1:C:61:ILE:HG12	2.05	0.72
1:J:142:ASN:HB3	1:J:146:ARG:NH1	2.05	0.72
1:E:179:LYS:NZ	1:E:192:GLN:NE2	2.37	0.72
1:C:72:ILE:HD11	1:C:126:PRO:HB3	1.72	0.71
1:M:72:ILE:HD11	1:M:126:PRO:HB3	1.71	0.71
1:D:141:SER:O	1:D:144:ILE:HG22	1.89	0.71
1:L:116:LEU:HD13	1:M:80:ASP:HB3	1.71	0.71
1:K:91:THR:C	1:K:92:ILE:HD12	2.16	0.71
1:B:72:ILE:HD11	1:B:126:PRO:HB3	1.71	0.70
1:K:29:ARG:HH12	1:K:52:LEU:HB3	1.55	0.70
1:H:48:GLN:HA	1:N:21:ILE:HD11	1.72	0.70
1:C:60:ASP:OD1	1:C:88:ASP:HB2	1.91	0.70
1:K:29:ARG:NH1	1:K:61:ILE:HG12	2.07	0.70
1:F:141:SER:O	1:F:144:ILE:HG22	1.92	0.69
1:J:147:LEU:O	1:J:151:MET:HG2	1.92	0.69
1:B:134:ALA:HB3	1:I:125:GLN:NE2	2.07	0.69
1:M:94:ILE:HG22	1:M:116:LEU:CD1	2.22	0.69
1:E:80:ASP:HB3	1:F:116:LEU:HD13	1.74	0.69
1:D:29:ARG:NH1	1:D:59:LYS:HB2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:GLN:NE2	1:M:134:ALA:HB3	2.08	0.69
1:I:21:ILE:HD11	1:J:51:PHE:HB2	1.74	0.69
1:C:180:GLU:O	1:C:183:GLU:HG2	1.93	0.69
1:G:177:SER:OG	1:G:180:GLU:HG3	1.92	0.68
1:I:117:PRO:HD3	1:I:192:GLN:HA	1.74	0.68
1:F:84:PHE:CE1	1:G:191:LEU:HD13	2.29	0.68
1:H:38:ASN:OD1	1:H:40:SER:HB3	1.94	0.68
1:C:24:ARG:O	1:C:24:ARG:HD3	1.93	0.67
1:C:56:ASP:OD2	1:C:59:LYS:HG3	1.94	0.67
1:G:94:ILE:HG22	1:G:116:LEU:HD12	1.76	0.67
1:J:182:LYS:HD3	1:J:182:LYS:C	2.20	0.67
1:K:176:MET:HE1	1:K:186:LEU:CD1	2.25	0.67
1:M:94:ILE:HG22	1:M:116:LEU:HD12	1.77	0.67
1:B:85:ILE:HD11	1:B:89:VAL:CG2	2.25	0.67
1:B:24:ARG:HH11	1:B:27:LYS:CD	2.07	0.66
1:L:98:ALA:HB1	1:L:122:MET:HE3	1.76	0.66
1:A:92:ILE:N	1:A:92:ILE:HD12	2.10	0.66
1:B:38:ASN:HD21	1:B:40:SER:HB2	1.59	0.66
1:B:59:LYS:O	1:B:87:PRO:HB3	1.96	0.66
1:I:20:ASP:HB3	1:I:23:SER:OG	1.95	0.66
1:N:32:LEU:HD23	1:N:64:TYR:HB2	1.77	0.66
1:A:80:ASP:OD1	1:B:118:HIS:HD2	1.79	0.66
1:C:78:ILE:O	1:C:82:MET:HG3	1.96	0.66
1:K:120:ARG:HH22	1:L:146:ARG:HG2	1.60	0.66
1:D:177:SER:OG	1:D:180:GLU:HG3	1.95	0.65
1:H:125:GLN:NE2	1:H:148:LYS:NZ	2.44	0.65
1:L:72:ILE:HA	1:L:100:MET:HE3	1.76	0.65
1:F:38:ASN:OD1	1:F:41:VAL:HG23	1.95	0.65
1:N:141:SER:O	1:N:144:ILE:HG22	1.96	0.65
1:C:135:SER:H	1:J:125:GLN:HE22	1.45	0.65
1:M:66:ASN:HD22	1:M:94:ILE:HG13	1.62	0.65
1:C:164:GLU:O	1:C:168:LYS:HG3	1.96	0.65
1:C:42:ALA:O	1:C:46:VAL:HG23	1.97	0.65
1:D:184:TYR:HD2	1:D:186:LEU:HD13	1.62	0.65
1:H:116:LEU:HD13	1:I:80:ASP:HB3	1.78	0.64
1:N:74:SER:O	1:N:77:SER:HB3	1.98	0.64
1:G:24:ARG:HD3	1:G:24:ARG:C	2.22	0.64
1:L:74:SER:O	1:L:77:SER:HB3	1.97	0.64
1:C:32:LEU:N	1:C:32:LEU:HD22	2.12	0.64
1:B:164:GLU:CD	1:B:164:GLU:H	2.06	0.64
1:B:190:VAL:O	1:B:192:GLN:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:HH11	1:D:59:LYS:HB2	1.62	0.64
1:F:29:ARG:HD3	1:F:60:ASP:O	1.98	0.64
1:C:24:ARG:NH1	1:C:27:LYS:HD2	2.13	0.64
1:F:29:ARG:HA	1:F:52:LEU:HD21	1.80	0.64
1:G:29:ARG:NH1	1:G:59:LYS:O	2.31	0.64
1:G:24:ARG:HD3	1:G:24:ARG:O	1.97	0.63
1:F:125:GLN:HE22	1:M:135:SER:H	1.44	0.63
1:C:80:ASP:HB3	1:D:116:LEU:HD13	1.80	0.63
1:K:176:MET:HE1	1:K:186:LEU:HD12	1.79	0.63
1:B:38:ASN:C	1:B:38:ASN:ND2	2.56	0.63
1:E:38:ASN:OD1	1:E:40:SER:HB3	1.98	0.63
1:L:24:ARG:HA	1:L:27:LYS:HD3	1.80	0.63
1:B:150:LEU:HD11	1:C:118:HIS:HD2	1.62	0.63
1:A:60:ASP:OD1	1:A:88:ASP:HB2	1.99	0.63
1:L:120:ARG:HD3	1:M:147:LEU:HD21	1.81	0.62
1:N:29:ARG:NH2	1:N:52:LEU:HB3	2.15	0.62
1:C:164:GLU:H	1:C:164:GLU:CD	2.08	0.62
1:D:94:ILE:HG22	1:D:116:LEU:CD1	2.29	0.62
1:G:20:ASP:HB3	1:G:23:SER:HB2	1.82	0.62
1:E:69:GLY:HA3	1:E:99:ALA:HB3	1.82	0.61
1:C:24:ARG:HD3	1:C:24:ARG:C	2.26	0.61
1:A:72:ILE:HD11	1:A:126:PRO:HB3	1.80	0.61
1:I:156:ALA:HB2	1:I:166:ILE:HG13	1.83	0.61
1:J:191:LEU:O	1:J:192:GLN:HB3	2.00	0.61
1:E:60:ASP:OD1	1:E:88:ASP:HB2	2.00	0.61
1:H:92:ILE:HD12	1:H:92:ILE:N	2.16	0.61
1:K:21:ILE:HG23	1:K:22:TYR:N	2.15	0.61
1:M:100:MET:HE3	1:M:104:LEU:HG	1.82	0.61
1:N:82:MET:HE3	1:N:89:VAL:HG11	1.82	0.61
1:A:120:ARG:HH22	1:G:146:ARG:HG2	1.65	0.61
1:A:172:ARG:NH2	1:G:133:GLN:OE1	2.34	0.61
1:B:56:ASP:OD1	1:B:59:LYS:HG3	2.00	0.61
1:F:80:ASP:OD1	1:G:118:HIS:HD2	1.84	0.61
1:C:135:SER:H	1:J:125:GLN:NE2	1.99	0.61
1:A:29:ARG:NH1	1:A:59:LYS:HB2	2.16	0.61
1:A:120:ARG:NH2	1:G:146:ARG:HG2	2.15	0.61
1:D:144:ILE:HD12	1:K:134:ALA:HB2	1.83	0.60
1:A:141:SER:O	1:A:144:ILE:HG22	2.01	0.60
1:D:125:GLN:HE21	1:K:134:ALA:HB3	1.66	0.60
1:H:34:SER:HA	1:H:66:ASN:O	2.00	0.60
1:G:125:GLN:HE22	1:G:148:LYS:NZ	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ILE:HD11	1:J:51:PHE:CB	2.32	0.60
1:G:125:GLN:NE2	1:G:148:LYS:NZ	2.49	0.60
1:G:129:GLY:HA2	1:N:130:ALA:O	2.02	0.60
1:C:136:ASP:OD1	1:D:172:ARG:NH1	2.33	0.60
1:E:190:VAL:HG12	1:E:192:GLN:HG3	1.83	0.60
1:A:116:LEU:HB3	1:A:117:PRO:HD2	1.84	0.60
1:D:130:ALA:HB1	1:D:140:ILE:HD12	1.83	0.60
1:F:92:ILE:N	1:F:92:ILE:HD12	2.16	0.60
1:G:141:SER:O	1:G:144:ILE:HG22	2.01	0.60
1:H:72:ILE:HD12	1:H:151:MET:HE1	1.83	0.60
1:B:24:ARG:NH1	1:B:27:LYS:HD2	2.14	0.60
1:G:94:ILE:HG22	1:G:116:LEU:CD1	2.31	0.60
1:F:125:GLN:NE2	1:M:135:SER:H	1.99	0.60
1:M:85:ILE:HB	1:M:87:PRO:HD2	1.82	0.60
1:E:133:GLN:OE1	1:F:172:ARG:NH2	2.35	0.59
1:G:154:ILE:HG22	1:G:158:ASN:ND2	2.18	0.59
1:A:146:ARG:NE	1:B:120:ARG:HH22	2.01	0.59
1:C:29:ARG:HH12	1:C:61:ILE:HG12	1.66	0.59
1:E:85:ILE:HD12	1:E:87:PRO:HG2	1.84	0.59
1:C:59:LYS:HZ2	1:C:59:LYS:HB3	1.67	0.59
1:M:41:VAL:O	1:M:45:ILE:HG12	2.02	0.59
1:G:57:PRO:HA	1:G:87:PRO:HG3	1.84	0.59
1:B:84:PHE:CE1	1:C:191:LEU:HD13	2.37	0.59
1:H:189:LYS:HE2	1:H:191:LEU:HD23	1.83	0.59
1:B:21:ILE:HG23	1:B:22:TYR:N	2.16	0.58
1:B:57:PRO:HA	1:B:87:PRO:HG3	1.83	0.58
1:C:134:ALA:HB3	1:J:125:GLN:HE21	1.66	0.58
1:N:50:LEU:O	1:N:53:GLU:HB3	2.04	0.58
1:A:24:ARG:O	1:A:24:ARG:HD3	2.03	0.58
1:J:92:ILE:HD12	1:J:92:ILE:N	2.17	0.58
1:C:74:SER:O	1:C:77:SER:HB3	2.03	0.58
1:A:146:ARG:CG	1:B:120:ARG:HH22	2.16	0.58
1:C:127:LEU:HD23	1:J:133:GLN:HA	1.85	0.58
1:I:141:SER:O	1:I:144:ILE:HG22	2.03	0.58
1:B:72:ILE:HA	1:B:100:MET:CE	2.34	0.58
1:C:100:MET:HE1	1:C:151:MET:SD	2.44	0.58
1:M:92:ILE:HD12	1:M:92:ILE:N	2.19	0.58
1:J:164:GLU:HA	1:J:164:GLU:OE1	2.04	0.58
1:K:122:MET:HA	1:K:174:PHE:O	2.04	0.58
1:L:23:SER:O	1:L:27:LYS:HG3	2.04	0.58
1:A:120:ARG:HH12	1:G:146:ARG:CD	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD13	1:G:84:PHE:CE1	2.38	0.57
1:E:150:LEU:C	1:E:150:LEU:HD23	2.29	0.57
1:F:29:ARG:NH1	1:F:59:LYS:O	2.37	0.57
1:I:172:ARG:NH2	1:J:133:GLN:OE1	2.38	0.57
1:A:125:GLN:NE2	1:H:134:ALA:HB3	2.18	0.57
1:B:125:GLN:NE2	1:I:134:ALA:HB3	2.19	0.57
1:F:134:ALA:HB3	1:M:125:GLN:HE21	1.70	0.57
1:F:189:LYS:HE2	1:F:191:LEU:HD12	1.85	0.57
1:B:29:ARG:HH12	1:B:59:LYS:C	2.11	0.57
1:J:116:LEU:HB3	1:J:117:PRO:HD2	1.86	0.57
1:B:72:ILE:CD1	1:B:126:PRO:HB3	2.33	0.57
1:D:120:ARG:C	1:D:121:ILE:HD12	2.29	0.57
1:A:97:ALA:O	1:A:102:ALA:HB2	2.05	0.57
1:G:166:ILE:O	1:G:170:THR:HG23	2.05	0.57
1:K:159:SER:HA	1:K:185:GLY:O	2.04	0.57
1:F:125:GLN:NE2	1:F:148:LYS:NZ	2.53	0.57
1:L:24:ARG:HH11	1:L:27:LYS:HZ3	1.53	0.57
1:D:176:MET:HB3	1:D:180:GLU:HB2	1.87	0.57
1:F:27:LYS:HB2	1:F:27:LYS:NZ	2.20	0.57
1:I:29:ARG:NH2	1:I:52:LEU:O	2.38	0.57
1:A:163:LEU:HD23	1:A:163:LEU:O	2.04	0.56
1:B:189:LYS:HE2	1:B:191:LEU:HD23	1.86	0.56
1:D:134:ALA:HB3	1:K:125:GLN:HE21	1.70	0.56
1:I:164:GLU:CD	1:I:164:GLU:H	2.12	0.56
1:C:51:PHE:O	1:C:54:ALA:HB3	2.05	0.56
1:F:164:GLU:O	1:F:168:LYS:HG3	2.05	0.56
1:K:190:VAL:O	1:K:192:GLN:N	2.38	0.56
1:N:176:MET:HE1	1:N:186:LEU:HD11	1.85	0.56
1:L:34:SER:HA	1:L:66:ASN:O	2.06	0.56
1:K:92:ILE:HD12	1:K:92:ILE:N	2.21	0.56
1:K:124:HIS:HA	1:K:170:THR:HB	1.88	0.56
1:C:129:GLY:HA2	1:J:130:ALA:O	2.05	0.56
1:G:27:LYS:O	1:G:27:LYS:HD3	2.06	0.56
1:H:53:GLU:OE2	1:H:87:PRO:HD2	2.06	0.56
1:B:29:ARG:NH1	1:B:59:LYS:C	2.64	0.56
1:H:53:GLU:OE2	1:H:85:ILE:HB	2.06	0.56
1:L:117:PRO:HD3	1:L:191:LEU:O	2.06	0.56
1:B:29:ARG:NH1	1:B:59:LYS:HB2	2.21	0.56
1:M:150:LEU:C	1:M:150:LEU:HD23	2.31	0.56
1:G:72:ILE:HD11	1:G:126:PRO:HB3	1.87	0.56
1:L:143:GLU:O	1:L:147:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:ARG:HD3	1:I:24:ARG:C	2.31	0.55
1:A:42:ALA:HA	1:A:78:ILE:HD11	1.88	0.55
1:E:72:ILE:HD11	1:E:126:PRO:HB3	1.87	0.55
1:M:191:LEU:HD13	1:N:84:PHE:CZ	2.41	0.55
1:C:94:ILE:HG13	1:C:94:ILE:O	2.05	0.55
1:I:22:TYR:HE1	1:I:32:LEU:HD12	1.72	0.55
1:I:159:SER:HA	1:I:185:GLY:O	2.07	0.55
1:G:20:ASP:HB3	1:G:23:SER:CB	2.37	0.55
1:H:94:ILE:HG22	1:H:116:LEU:CD1	2.37	0.55
1:I:48:GLN:O	1:I:52:LEU:HG	2.06	0.55
1:A:120:ARG:C	1:A:121:ILE:HD12	2.32	0.55
1:D:98:ALA:HB1	1:D:122:MET:HE3	1.88	0.55
1:L:60:ASP:OD1	1:L:88:ASP:HB2	2.07	0.55
1:N:177:SER:OG	1:N:180:GLU:HG3	2.07	0.55
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.72	0.55
1:I:20:ASP:OD1	1:I:22:TYR:N	2.37	0.55
1:J:42:ALA:O	1:J:46:VAL:HG23	2.07	0.55
1:M:21:ILE:HD11	1:N:51:PHE:HB2	1.87	0.55
1:A:80:ASP:HB3	1:B:116:LEU:HD13	1.88	0.55
1:C:141:SER:O	1:C:145:LEU:HG	2.06	0.54
1:D:134:ALA:HB3	1:K:125:GLN:NE2	2.21	0.54
1:H:29:ARG:NH2	1:H:52:LEU:O	2.40	0.54
1:H:141:SER:O	1:H:144:ILE:HG22	2.08	0.54
1:A:26:LEU:HD13	1:A:48:GLN:HE21	1.71	0.54
1:K:150:LEU:O	1:K:153:SER:HB3	2.07	0.54
1:D:73:THR:HG21	1:E:96:GLN:NE2	2.23	0.54
1:A:124:HIS:C	1:A:124:HIS:CD2	2.83	0.54
1:A:125:GLN:HE21	1:H:134:ALA:HB3	1.72	0.54
1:N:72:ILE:H	1:N:72:ILE:CD1	2.14	0.54
1:A:24:ARG:HD3	1:A:24:ARG:C	2.32	0.54
1:A:94:ILE:HG22	1:A:116:LEU:HD12	1.90	0.54
1:D:125:GLN:NE2	1:K:135:SER:H	2.05	0.54
1:I:92:ILE:N	1:I:92:ILE:HD12	2.23	0.54
1:B:141:SER:O	1:B:144:ILE:HG22	2.07	0.54
1:E:24:ARG:O	1:E:24:ARG:HD3	2.08	0.54
1:F:143:GLU:HA	1:F:146:ARG:HH21	1.72	0.54
1:D:176:MET:HE1	1:D:186:LEU:CD2	2.38	0.54
1:E:80:ASP:HB3	1:F:116:LEU:CD1	2.36	0.54
1:L:178:ALA:O	1:L:181:ALA:HB3	2.08	0.53
1:M:31:VAL:C	1:M:32:LEU:HD12	2.32	0.53
1:E:125:GLN:HE21	1:L:134:ALA:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:GLU:O	1:G:56:ASP:HB2	2.07	0.53
1:N:82:MET:HE3	1:N:89:VAL:CG1	2.38	0.53
1:I:22:TYR:CE1	1:I:32:LEU:HD12	2.44	0.53
1:K:29:ARG:NH1	1:K:52:LEU:HB3	2.21	0.53
1:M:124:HIS:C	1:M:124:HIS:CD2	2.86	0.53
1:E:179:LYS:HZ1	1:E:192:GLN:HE22	1.55	0.53
1:I:53:GLU:HG3	1:I:87:PRO:HD3	1.90	0.53
1:I:189:LYS:HG2	1:I:190:VAL:N	2.24	0.53
1:E:51:PHE:HB2	1:F:21:ILE:HD11	1.89	0.53
1:F:21:ILE:HG23	1:F:22:TYR:N	2.23	0.53
1:K:29:ARG:NH2	1:K:56:ASP:O	2.42	0.53
1:L:64:TYR:CZ	1:L:92:ILE:HD12	2.43	0.53
1:E:82:MET:HE3	1:E:89:VAL:CG1	2.39	0.53
1:I:164:GLU:O	1:I:168:LYS:HG3	2.08	0.53
1:D:92:ILE:N	1:D:92:ILE:HD12	2.24	0.53
1:F:125:GLN:NE2	1:F:148:LYS:HZ2	2.05	0.53
1:M:100:MET:HE1	1:M:103:PHE:CD2	2.43	0.53
1:F:29:ARG:NH2	1:F:52:LEU:O	2.42	0.53
1:M:172:ARG:O	1:M:173:ASP:C	2.52	0.53
1:D:24:ARG:O	1:D:24:ARG:HD3	2.09	0.53
1:D:121:ILE:HG21	1:D:186:LEU:HD23	1.91	0.53
1:E:179:LYS:NZ	1:E:192:GLN:HE22	2.06	0.53
1:D:29:ARG:NH1	1:D:59:LYS:O	2.39	0.52
1:G:98:ALA:HB1	1:G:122:MET:HE3	1.89	0.52
1:C:72:ILE:HG21	1:C:147:LEU:HD13	1.90	0.52
1:E:124:HIS:CD2	1:E:124:HIS:C	2.87	0.52
1:G:21:ILE:HG23	1:G:22:TYR:N	2.24	0.52
1:G:24:ARG:O	1:G:27:LYS:HB3	2.09	0.52
1:K:120:ARG:NH1	1:L:146:ARG:HD2	2.24	0.52
1:L:29:ARG:HD3	1:L:60:ASP:O	2.10	0.52
1:A:71:VAL:HB	1:A:74:SER:HB2	1.90	0.52
1:E:130:ALA:O	1:L:129:GLY:HA2	2.08	0.52
1:N:64:TYR:CZ	1:N:92:ILE:HD13	2.45	0.52
1:E:24:ARG:HD3	1:E:24:ARG:C	2.35	0.52
1:L:21:ILE:HG23	1:L:22:TYR:N	2.24	0.52
1:B:38:ASN:ND2	1:B:41:VAL:H	2.07	0.52
1:F:134:ALA:HB3	1:M:125:GLN:NE2	2.24	0.52
1:K:72:ILE:O	1:K:76:LEU:HG	2.08	0.52
1:H:72:ILE:HA	1:H:100:MET:HE3	1.92	0.52
1:A:71:VAL:O	1:A:74:SER:HB2	2.10	0.52
1:E:37:ILE:HB	1:E:70:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:HIS:C	1:F:124:HIS:CD2	2.88	0.52
1:G:124:HIS:C	1:G:124:HIS:CD2	2.87	0.52
1:A:146:ARG:CD	1:B:120:ARG:HH22	2.22	0.52
1:B:151:MET:O	1:B:155:LEU:HB2	2.10	0.52
1:L:94:ILE:HG22	1:L:116:LEU:CD1	2.40	0.52
1:C:128:GLY:C	1:J:137:ILE:HD11	2.34	0.51
1:H:136:ASP:O	1:H:140:ILE:HG12	2.11	0.51
1:E:174:PHE:HD2	1:E:176:MET:HE2	1.75	0.51
1:F:93:CYS:HB2	1:F:105:LEU:HD22	1.90	0.51
1:B:124:HIS:C	1:B:124:HIS:CD2	2.87	0.51
1:E:164:GLU:CD	1:E:164:GLU:H	2.19	0.51
1:I:29:ARG:NH1	1:I:59:LYS:O	2.43	0.51
1:I:110:LYS:HA	1:I:110:LYS:HE3	1.91	0.51
1:A:129:GLY:HA2	1:H:130:ALA:O	2.10	0.51
1:C:92:ILE:HD12	1:C:92:ILE:N	2.25	0.51
1:K:147:LEU:O	1:K:151:MET:HG2	2.10	0.51
1:M:37:ILE:HB	1:M:70:GLY:HA3	1.90	0.51
1:C:182:LYS:HE3	1:C:188:ASP:O	2.10	0.51
1:K:29:ARG:HD3	1:K:60:ASP:O	2.11	0.51
1:B:135:SER:H	1:I:125:GLN:NE2	2.09	0.51
1:E:179:LYS:HZ1	1:E:192:GLN:HE21	1.57	0.51
1:J:151:MET:HA	1:J:151:MET:HE2	1.91	0.51
1:L:120:ARG:HD2	1:M:143:GLU:OE2	2.10	0.51
1:A:133:GLN:OE1	1:B:172:ARG:NH2	2.43	0.51
1:A:151:MET:O	1:A:155:LEU:HB2	2.11	0.51
1:F:129:GLY:HA2	1:M:130:ALA:O	2.11	0.51
1:K:72:ILE:CD1	1:K:126:PRO:HB3	2.39	0.51
1:D:25:LEU:HD12	1:D:30:ILE:HD12	1.92	0.51
1:F:66:ASN:HA	1:F:96:GLN:O	2.10	0.51
1:F:152:ASN:ND2	1:F:167:ALA:HA	2.26	0.51
1:H:125:GLN:NE2	1:H:148:LYS:HZ1	2.08	0.51
1:B:145:LEU:O	1:B:148:LYS:HB3	2.10	0.51
1:C:124:HIS:C	1:C:124:HIS:CD2	2.89	0.51
1:G:74:SER:O	1:G:77:SER:HB3	2.10	0.51
1:M:21:ILE:HG23	1:M:22:TYR:N	2.26	0.51
1:M:125:GLN:NE2	1:M:148:LYS:NZ	2.59	0.51
1:E:97:ALA:O	1:E:102:ALA:HB2	2.11	0.50
1:D:135:SER:O	1:D:139:ILE:HG13	2.10	0.50
1:H:125:GLN:NE2	1:H:148:LYS:HZ3	2.08	0.50
1:J:118:HIS:CD2	1:K:154:ILE:HD11	2.47	0.50
1:K:42:ALA:O	1:K:46:VAL:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:ALA:HB3	1:L:112:LYS:HB2	1.92	0.50
1:D:117:PRO:HG3	1:D:192:GLN:HB3	1.93	0.50
1:J:57:PRO:HB2	1:J:86:ARG:NH1	2.26	0.50
1:A:136:ASP:O	1:A:140:ILE:HG12	2.11	0.50
1:B:97:ALA:O	1:B:102:ALA:HB2	2.12	0.50
1:C:174:PHE:CD2	1:C:176:MET:HE2	2.46	0.50
1:D:94:ILE:HG22	1:D:116:LEU:HD12	1.93	0.50
1:H:29:ARG:NH1	1:H:59:LYS:O	2.45	0.50
1:E:86:ARG:N	1:E:87:PRO:HD2	2.26	0.50
1:B:55:GLU:O	1:B:56:ASP:HB2	2.11	0.50
1:F:148:LYS:HD2	1:M:134:ALA:HB3	1.94	0.50
1:A:53:GLU:HB2	1:A:85:ILE:HB	1.94	0.50
1:A:84:PHE:CE1	1:B:191:LEU:HD13	2.46	0.50
1:B:38:ASN:HD21	1:B:41:VAL:H	1.58	0.49
1:E:22:TYR:CD1	1:E:32:LEU:HD12	2.48	0.49
1:N:136:ASP:O	1:N:140:ILE:HG12	2.12	0.49
1:B:22:TYR:CE1	1:B:32:LEU:HD12	2.47	0.49
1:F:182:LYS:HA	1:F:187:ILE:HG13	1.94	0.49
1:I:154:ILE:HG22	1:I:158:ASN:ND2	2.28	0.49
1:J:91:THR:C	1:J:92:ILE:HD12	2.36	0.49
1:N:72:ILE:HA	1:N:100:MET:HE3	1.94	0.49
1:C:86:ARG:N	1:C:87:PRO:HD2	2.27	0.49
1:F:164:GLU:HB3	1:F:168:LYS:NZ	2.28	0.49
1:H:28:ASP:O	1:H:29:ARG:HB2	2.12	0.49
1:I:20:ASP:OD1	1:I:20:ASP:C	2.55	0.49
1:J:100:MET:O	1:J:103:PHE:HB3	2.13	0.49
1:K:120:ARG:O	1:K:121:ILE:HD13	2.12	0.49
1:B:92:ILE:N	1:B:92:ILE:HD12	2.27	0.49
1:E:154:ILE:HG22	1:E:158:ASN:ND2	2.27	0.49
1:N:162:SER:OG	1:N:165:GLN:HB2	2.13	0.49
1:E:117:PRO:CG	1:E:192:GLN:HA	2.29	0.49
1:I:189:LYS:HD2	1:I:191:LEU:HD23	1.95	0.49
1:M:29:ARG:HG2	1:M:29:ARG:HH11	1.76	0.49
1:M:100:MET:HE1	1:M:103:PHE:HD2	1.76	0.49
1:D:130:ALA:O	1:K:129:GLY:HA2	2.12	0.49
1:E:176:MET:HE1	1:E:186:LEU:CD1	2.42	0.49
1:G:135:SER:H	1:N:125:GLN:HE22	1.59	0.49
1:K:120:ARG:HH12	1:L:146:ARG:CD	2.25	0.49
1:A:116:LEU:HD13	1:G:80:ASP:HB3	1.94	0.49
1:C:42:ALA:HA	1:C:78:ILE:HD11	1.94	0.49
1:I:124:HIS:C	1:I:124:HIS:CD2	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:VAL:HG13	1:J:48:GLN:OE1	2.12	0.49
1:M:190:VAL:O	1:M:192:GLN:N	2.46	0.49
1:A:72:ILE:O	1:A:100:MET:HE3	2.12	0.49
1:D:21:ILE:HG23	1:D:22:TYR:N	2.27	0.48
1:C:97:ALA:O	1:C:102:ALA:HB2	2.13	0.48
1:M:140:ILE:O	1:M:144:ILE:HD13	2.13	0.48
1:C:24:ARG:HA	1:C:27:LYS:HE3	1.94	0.48
1:E:174:PHE:CD2	1:E:176:MET:HE2	2.47	0.48
1:H:114:PHE:HA	1:H:189:LYS:O	2.14	0.48
1:B:72:ILE:CD1	1:B:151:MET:HE1	2.43	0.48
1:M:53:GLU:OE1	1:M:85:ILE:HG22	2.12	0.48
1:F:27:LYS:HB2	1:F:27:LYS:HZ3	1.78	0.48
1:G:179:LYS:O	1:G:183:GLU:HG3	2.14	0.48
1:K:136:ASP:O	1:K:140:ILE:HG12	2.13	0.48
1:N:79:TYR:O	1:N:82:MET:HB2	2.14	0.48
1:B:38:ASN:ND2	1:B:41:VAL:HG23	2.29	0.48
1:C:130:ALA:O	1:J:129:GLY:HA2	2.12	0.48
1:L:117:PRO:HG3	1:L:192:GLN:HB3	1.95	0.48
1:N:32:LEU:CD2	1:N:64:TYR:HB2	2.41	0.48
1:E:103:PHE:CZ	1:E:154:ILE:HG21	2.49	0.48
1:I:24:ARG:HG3	1:J:51:PHE:CE1	2.49	0.48
1:I:97:ALA:O	1:I:102:ALA:HB2	2.13	0.48
1:A:120:ARG:HD2	1:G:143:GLU:OE2	2.14	0.48
1:J:121:ILE:HD12	1:J:121:ILE:N	2.28	0.48
1:N:164:GLU:HG2	1:N:168:LYS:NZ	2.28	0.48
1:B:21:ILE:CG2	1:B:22:TYR:N	2.77	0.47
1:B:135:SER:H	1:I:125:GLN:HE22	1.62	0.47
1:C:83:ASN:C	1:C:83:ASN:HD22	2.20	0.47
1:C:91:THR:C	1:C:92:ILE:HD12	2.39	0.47
1:C:79:TYR:CE2	1:C:154:ILE:HD13	2.50	0.47
1:C:91:THR:HB	1:C:105:LEU:HD12	1.97	0.47
1:I:144:ILE:CG2	1:I:145:LEU:N	2.77	0.47
1:M:116:LEU:HB3	1:M:117:PRO:HD2	1.97	0.47
1:A:125:GLN:HB2	1:A:126:PRO:HD2	1.96	0.47
1:B:127:LEU:HB3	1:I:133:GLN:HA	1.96	0.47
1:E:51:PHE:CB	1:F:21:ILE:HD11	2.44	0.47
1:I:29:ARG:HD3	1:I:60:ASP:O	2.14	0.47
1:K:21:ILE:HG23	1:K:22:TYR:H	1.80	0.47
1:N:53:GLU:OE2	1:N:53:GLU:HA	2.13	0.47
1:N:124:HIS:C	1:N:124:HIS:CD2	2.91	0.47
1:B:72:ILE:HG12	1:B:151:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:SER:OG	1:E:180:GLU:HG3	2.14	0.47
1:L:103:PHE:HD1	1:L:155:LEU:HD13	1.79	0.47
1:C:125:GLN:NE2	1:C:148:LYS:NZ	2.62	0.47
1:H:96:GLN:HB3	1:I:73:THR:HB	1.96	0.47
1:K:29:ARG:NH1	1:K:52:LEU:HD13	2.29	0.47
1:A:98:ALA:HB1	1:A:122:MET:HE3	1.96	0.47
1:B:72:ILE:HA	1:B:100:MET:HE3	1.96	0.47
1:E:190:VAL:CG1	1:E:192:GLN:HG3	2.43	0.47
1:L:124:HIS:C	1:L:124:HIS:CD2	2.92	0.47
1:N:116:LEU:HB3	1:N:117:PRO:HD2	1.95	0.47
1:N:121:ILE:N	1:N:121:ILE:HD12	2.29	0.47
1:F:130:ALA:HB2	1:F:140:ILE:HG21	1.96	0.47
1:J:141:SER:O	1:J:144:ILE:HG22	2.15	0.47
1:K:93:CYS:HB2	1:K:105:LEU:HD22	1.96	0.47
1:A:93:CYS:SG	1:A:119:SER:HB3	2.55	0.47
1:B:100:MET:HE1	1:B:151:MET:SD	2.54	0.47
1:B:116:LEU:HB3	1:B:117:PRO:HD2	1.96	0.47
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.80	0.47
1:G:125:GLN:NE2	1:G:148:LYS:CE	2.78	0.47
1:H:124:HIS:C	1:H:124:HIS:CD2	2.93	0.47
1:B:182:LYS:HD2	1:B:182:LYS:C	2.40	0.47
1:C:57:PRO:HA	1:C:87:PRO:HD3	1.95	0.47
1:C:66:ASN:HB2	1:C:94:ILE:HG13	1.97	0.47
1:C:93:CYS:HB2	1:C:105:LEU:HD22	1.97	0.46
1:C:150:LEU:O	1:C:153:SER:HB3	2.15	0.46
1:D:68:PRO:HA	1:D:96:GLN:NE2	2.30	0.46
1:D:80:ASP:HB3	1:E:116:LEU:HD13	1.97	0.46
1:D:189:LYS:HE3	1:D:191:LEU:HD23	1.97	0.46
1:F:56:ASP:OD1	1:F:58:GLU:HB2	2.15	0.46
1:J:76:LEU:HD21	1:J:151:MET:HE1	1.97	0.46
1:K:60:ASP:OD2	1:K:112:LYS:NZ	2.40	0.46
1:K:177:SER:OG	1:K:180:GLU:HG3	2.15	0.46
1:M:51:PHE:O	1:M:55:GLU:HG2	2.15	0.46
1:E:64:TYR:CZ	1:E:92:ILE:HD12	2.50	0.46
1:G:98:ALA:HA	1:G:122:MET:O	2.15	0.46
1:I:94:ILE:HG13	1:I:94:ILE:O	2.16	0.46
1:K:60:ASP:OD1	1:K:88:ASP:HB2	2.15	0.46
1:D:85:ILE:HD11	1:D:89:VAL:CG2	2.45	0.46
1:M:122:MET:HG3	1:M:175:TYR:CE2	2.50	0.46
1:N:29:ARG:NH2	1:N:52:LEU:O	2.48	0.46
1:A:86:ARG:HG3	1:A:86:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:79:TYR:CE1	1:J:83:ASN:ND2	2.84	0.46
1:M:116:LEU:HD13	1:N:80:ASP:HB3	1.98	0.46
1:M:126:PRO:HG3	1:M:151:MET:CE	2.45	0.46
1:H:93:CYS:SG	1:H:97:ALA:HB2	2.55	0.46
1:L:56:ASP:OD2	1:L:59:LYS:HB2	2.15	0.46
1:B:52:LEU:O	1:B:55:GLU:HB3	2.16	0.46
1:H:121:ILE:HG13	1:H:181:ALA:CB	2.45	0.46
1:H:125:GLN:HB2	1:H:126:PRO:HD2	1.98	0.46
1:J:123:ILE:HG13	1:J:170:THR:HG22	1.97	0.46
1:K:52:LEU:HD12	1:K:61:ILE:HD13	1.97	0.46
1:M:126:PRO:HG3	1:M:151:MET:HE1	1.97	0.46
1:D:51:PHE:CE1	1:E:24:ARG:HD2	2.51	0.46
1:H:57:PRO:HB3	1:H:86:ARG:NE	2.31	0.46
1:B:94:ILE:O	1:B:94:ILE:HG13	2.15	0.46
1:D:150:LEU:HD11	1:D:154:ILE:HD11	1.98	0.46
1:H:57:PRO:HB3	1:H:86:ARG:CZ	2.45	0.46
1:C:59:LYS:HB3	1:C:59:LYS:NZ	2.31	0.46
1:D:129:GLY:HA2	1:K:130:ALA:O	2.15	0.46
1:D:177:SER:N	1:D:180:GLU:OE1	2.47	0.46
1:E:94:ILE:HG22	1:E:116:LEU:CD1	2.46	0.46
1:I:53:GLU:HG3	1:I:87:PRO:CD	2.46	0.46
1:M:24:ARG:O	1:M:24:ARG:HD3	2.16	0.46
1:B:38:ASN:ND2	1:B:40:SER:N	2.63	0.45
1:D:98:ALA:HA	1:D:122:MET:O	2.17	0.45
1:E:134:ALA:HB3	1:L:125:GLN:HE21	1.81	0.45
1:L:21:ILE:HG23	1:L:22:TYR:H	1.81	0.45
1:B:164:GLU:CD	1:B:164:GLU:N	2.74	0.45
1:F:182:LYS:HD3	1:F:182:LYS:C	2.42	0.45
1:H:33:LEU:HD11	1:H:37:ILE:HG12	1.97	0.45
1:I:93:CYS:SG	1:I:119:SER:HB3	2.56	0.45
1:M:29:ARG:HG2	1:M:52:LEU:HD22	1.97	0.45
1:B:48:GLN:O	1:B:52:LEU:HG	2.16	0.45
1:C:98:ALA:CB	1:C:122:MET:HB3	2.47	0.45
1:D:182:LYS:HE3	1:D:188:ASP:O	2.16	0.45
1:E:141:SER:O	1:E:144:ILE:HG22	2.15	0.45
1:H:60:ASP:OD1	1:H:88:ASP:HB2	2.16	0.45
1:H:72:ILE:HD13	1:H:100:MET:HE2	1.98	0.45
1:N:100:MET:HE1	1:N:151:MET:SD	2.56	0.45
1:A:120:ARG:NH1	1:G:146:ARG:HD2	2.22	0.45
1:D:124:HIS:CD2	1:D:124:HIS:C	2.94	0.45
1:G:56:ASP:C	1:G:58:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:ILE:N	1:G:92:ILE:HD12	2.32	0.45
1:H:44:SER:O	1:H:48:GLN:HG3	2.16	0.45
1:K:120:ARG:HH12	1:L:146:ARG:HD2	1.81	0.45
1:B:30:ILE:HG23	1:B:64:TYR:CD1	2.52	0.45
1:E:155:LEU:HD12	1:E:155:LEU:HA	1.80	0.45
1:H:25:LEU:HD22	1:H:30:ILE:HD12	1.98	0.45
1:L:66:ASN:HA	1:L:96:GLN:O	2.17	0.45
1:D:121:ILE:HD12	1:D:121:ILE:N	2.32	0.45
1:F:88:ASP:OD2	1:F:112:LYS:HE3	2.16	0.45
1:B:22:TYR:HE1	1:B:32:LEU:HD12	1.81	0.45
1:D:189:LYS:HE3	1:D:191:LEU:CD2	2.47	0.45
1:F:80:ASP:OD1	1:G:118:HIS:CD2	2.67	0.45
1:B:150:LEU:O	1:B:154:ILE:HG13	2.16	0.45
1:E:143:GLU:HA	1:E:143:GLU:OE1	2.17	0.45
1:F:148:LYS:HD2	1:M:134:ALA:CB	2.47	0.45
1:I:59:LYS:O	1:I:87:PRO:HB3	2.16	0.45
1:A:130:ALA:O	1:H:129:GLY:HA2	2.16	0.45
1:F:72:ILE:HA	1:F:100:MET:HE3	1.98	0.45
1:G:130:ALA:O	1:N:129:GLY:HA2	2.16	0.45
1:D:34:SER:HA	1:D:66:ASN:O	2.17	0.44
1:E:94:ILE:HG22	1:E:116:LEU:HD12	1.99	0.44
1:G:71:VAL:HB	1:G:74:SER:OG	2.17	0.44
1:G:176:MET:HE1	1:G:186:LEU:HD11	1.99	0.44
1:K:190:VAL:O	1:K:190:VAL:HG12	2.16	0.44
1:L:179:LYS:HE2	1:L:182:LYS:HD2	1.98	0.44
1:M:150:LEU:HD23	1:M:150:LEU:O	2.16	0.44
1:B:72:ILE:HG23	1:B:100:MET:HE1	1.99	0.44
1:C:170:THR:O	1:C:171:ASP:C	2.59	0.44
1:K:21:ILE:CG2	1:K:22:TYR:N	2.79	0.44
1:L:192:GLN:OE1	1:L:192:GLN:N	2.47	0.44
1:B:156:ALA:HB2	1:B:166:ILE:HG13	1.99	0.44
1:D:136:ASP:O	1:D:140:ILE:HG13	2.17	0.44
1:E:82:MET:HE3	1:E:89:VAL:HG11	1.98	0.44
1:E:176:MET:HE1	1:E:186:LEU:HD11	2.00	0.44
1:G:125:GLN:NE2	1:G:148:LYS:HE3	2.32	0.44
1:H:182:LYS:HD3	1:H:182:LYS:C	2.41	0.44
1:I:143:GLU:OE1	1:I:143:GLU:HA	2.16	0.44
1:B:69:GLY:HA3	1:B:99:ALA:HB3	1.99	0.44
1:D:176:MET:HE1	1:D:186:LEU:HD22	2.00	0.44
1:A:51:PHE:CB	1:B:21:ILE:HD11	2.48	0.44
1:A:52:LEU:CD1	1:A:61:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLN:NE2	1:D:132:GLY:N	2.65	0.44
1:E:80:ASP:OD1	1:F:118:HIS:HD2	1.99	0.44
1:G:125:GLN:HE21	1:G:148:LYS:HE3	1.82	0.44
1:L:117:PRO:HG3	1:L:192:GLN:CB	2.47	0.44
1:N:86:ARG:N	1:N:87:PRO:HD2	2.32	0.44
1:A:125:GLN:HG2	1:H:133:GLN:NE2	2.33	0.44
1:C:134:ALA:HB3	1:J:125:GLN:NE2	2.31	0.44
1:D:85:ILE:HB	1:D:87:PRO:HD2	2.00	0.44
1:E:50:LEU:HA	1:E:50:LEU:HD23	1.86	0.44
1:E:164:GLU:O	1:E:168:LYS:HG3	2.17	0.44
1:I:32:LEU:HD23	1:I:64:TYR:HB2	1.99	0.44
1:L:155:LEU:HD12	1:L:155:LEU:HA	1.88	0.44
1:A:80:ASP:OD1	1:B:118:HIS:CD2	2.64	0.44
1:B:38:ASN:ND2	1:B:40:SER:H	2.16	0.44
1:B:72:ILE:HD13	1:B:151:MET:HE1	2.00	0.44
1:C:49:LEU:O	1:C:85:ILE:HG21	2.17	0.44
1:E:143:GLU:HG2	1:F:175:TYR:CD2	2.52	0.44
1:K:103:PHE:HD1	1:K:155:LEU:HD13	1.83	0.44
1:L:150:LEU:O	1:L:154:ILE:HG13	2.17	0.44
1:M:63:LEU:HB3	1:M:91:THR:HG22	1.99	0.44
1:A:163:LEU:HD23	1:A:163:LEU:C	2.43	0.44
1:K:29:ARG:HH11	1:K:61:ILE:HG12	1.82	0.44
1:K:176:MET:HE1	1:K:186:LEU:HD11	1.95	0.44
1:L:24:ARG:O	1:L:27:LYS:HB2	2.18	0.44
1:L:44:SER:O	1:L:48:GLN:HG3	2.18	0.44
1:A:94:ILE:HG22	1:A:116:LEU:CD1	2.48	0.44
1:L:94:ILE:HG22	1:L:116:LEU:HD12	1.99	0.44
1:A:117:PRO:HD3	1:A:191:LEU:O	2.18	0.43
1:B:80:ASP:HB3	1:C:116:LEU:HB3	2.00	0.43
1:E:31:VAL:HG23	1:E:63:LEU:HA	1.99	0.43
1:G:20:ASP:HB3	1:G:23:SER:OG	2.18	0.43
1:A:29:ARG:NH1	1:A:59:LYS:O	2.50	0.43
1:C:79:TYR:HE2	1:C:154:ILE:HD13	1.83	0.43
1:D:33:LEU:HD13	1:D:45:ILE:CD1	2.49	0.43
1:D:82:MET:HE3	1:D:89:VAL:CG1	2.47	0.43
1:E:42:ALA:O	1:E:46:VAL:HG23	2.18	0.43
1:G:29:ARG:NH2	1:G:52:LEU:O	2.51	0.43
1:M:20:ASP:HB3	1:M:23:SER:HB2	2.00	0.43
1:C:153:SER:HA	1:C:163:LEU:CD1	2.48	0.43
1:E:44:SER:O	1:E:48:GLN:HG3	2.18	0.43
1:E:161:GLN:HB2	1:E:166:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ARG:HH11	1:L:27:LYS:CE	2.32	0.43
1:M:24:ARG:HD3	1:M:24:ARG:C	2.44	0.43
1:D:29:ARG:NH2	1:D:56:ASP:O	2.52	0.43
1:E:178:ALA:O	1:E:187:ILE:HD11	2.18	0.43
1:F:165:GLN:HE21	1:F:165:GLN:HA	1.83	0.43
1:A:177:SER:OG	1:A:180:GLU:HG3	2.19	0.43
1:B:143:GLU:OE1	1:B:143:GLU:HA	2.18	0.43
1:B:177:SER:OG	1:B:180:GLU:HG3	2.18	0.43
1:D:144:ILE:HD12	1:K:134:ALA:CB	2.47	0.43
1:E:102:ALA:O	1:E:105:LEU:HB3	2.19	0.43
1:F:143:GLU:CA	1:F:146:ARG:HH21	2.31	0.43
1:J:164:GLU:O	1:J:168:LYS:HE3	2.19	0.43
1:K:116:LEU:HD23	1:K:116:LEU:HA	1.86	0.43
1:D:72:ILE:HD11	1:D:126:PRO:HB3	2.00	0.43
1:E:135:SER:H	1:L:125:GLN:HE22	1.67	0.43
1:F:125:GLN:HE21	1:M:134:ALA:CB	2.26	0.43
1:N:164:GLU:HG2	1:N:168:LYS:HE3	2.01	0.43
1:A:52:LEU:HD12	1:A:61:ILE:CG2	2.48	0.43
1:D:80:ASP:HB3	1:E:116:LEU:CD1	2.48	0.43
1:F:165:GLN:HA	1:F:165:GLN:NE2	2.34	0.43
1:K:189:LYS:HG2	1:K:190:VAL:N	2.33	0.43
1:L:21:ILE:HD11	1:M:51:PHE:CB	2.49	0.43
1:A:29:ARG:NH1	1:A:59:LYS:C	2.76	0.43
1:C:58:GLU:OE2	1:C:58:GLU:HA	2.18	0.43
1:F:98:ALA:HB1	1:F:122:MET:HE3	2.01	0.43
1:F:99:ALA:C	1:F:101:GLY:N	2.75	0.43
1:I:114:PHE:HA	1:I:189:LYS:O	2.18	0.43
1:M:79:TYR:CE1	1:M:107:CYS:SG	3.12	0.43
1:D:125:GLN:HE22	1:K:135:SER:H	1.67	0.43
1:G:152:ASN:OD1	1:G:166:ILE:HG22	2.18	0.43
1:J:74:SER:O	1:J:78:ILE:HG13	2.19	0.43
1:B:51:PHE:CG	1:C:21:ILE:HD11	2.54	0.42
1:B:182:LYS:HE3	1:B:188:ASP:O	2.18	0.42
1:K:51:PHE:O	1:K:54:ALA:HB3	2.19	0.42
1:B:108:GLY:HA3	1:B:113:ARG:HG2	1.99	0.42
1:E:64:TYR:HB3	1:E:94:ILE:HD11	2.01	0.42
1:E:122:MET:HG3	1:E:175:TYR:CE2	2.55	0.42
1:E:134:ALA:HB3	1:L:125:GLN:NE2	2.34	0.42
1:G:37:ILE:HD12	1:G:100:MET:HB3	2.00	0.42
1:K:116:LEU:HD13	1:L:80:ASP:CB	2.41	0.42
1:M:117:PRO:HG2	1:N:80:ASP:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:NH2	1:A:52:LEU:O	2.51	0.42
1:K:124:HIS:C	1:K:124:HIS:CD2	2.97	0.42
1:L:24:ARG:HH11	1:L:27:LYS:NZ	2.15	0.42
1:B:94:ILE:HG22	1:B:116:LEU:CD1	2.49	0.42
1:H:24:ARG:O	1:H:24:ARG:HD3	2.19	0.42
1:H:164:GLU:H	1:H:164:GLU:CD	2.27	0.42
1:A:51:PHE:HB2	1:B:21:ILE:HD11	2.01	0.42
1:M:86:ARG:N	1:M:87:PRO:CD	2.82	0.42
1:M:118:HIS:HD2	1:N:80:ASP:OD1	2.01	0.42
1:A:72:ILE:HD11	1:A:126:PRO:CB	2.48	0.42
1:A:178:ALA:O	1:A:187:ILE:HD11	2.19	0.42
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.89	0.42
1:I:29:ARG:NH2	1:I:56:ASP:O	2.53	0.42
1:A:121:ILE:HD12	1:A:121:ILE:N	2.34	0.42
1:E:130:ALA:CB	1:E:140:ILE:HD12	2.50	0.42
1:E:154:ILE:HG22	1:E:158:ASN:HD21	1.84	0.42
1:F:130:ALA:O	1:M:129:GLY:HA2	2.20	0.42
1:H:117:PRO:HD3	1:H:191:LEU:O	2.20	0.42
1:I:44:SER:O	1:I:48:GLN:HG3	2.19	0.42
1:A:29:ARG:NH1	1:A:59:LYS:CB	2.82	0.42
1:A:125:GLN:HE22	1:A:148:LYS:NZ	2.17	0.42
1:E:86:ARG:H	1:E:87:PRO:HD2	1.85	0.42
1:G:29:ARG:HD3	1:G:60:ASP:O	2.20	0.42
1:H:29:ARG:NH2	1:H:56:ASP:O	2.52	0.42
1:B:30:ILE:HG23	1:B:64:TYR:CE1	2.55	0.42
1:E:93:CYS:HB3	1:E:115:SER:HA	2.02	0.42
1:M:20:ASP:HB3	1:M:23:SER:OG	2.19	0.42
1:A:143:GLU:OE1	1:A:143:GLU:HA	2.20	0.42
1:B:79:TYR:O	1:B:82:MET:HB2	2.19	0.42
1:F:21:ILE:CG2	1:F:22:TYR:N	2.83	0.42
1:G:72:ILE:HD11	1:G:126:PRO:CB	2.50	0.42
1:J:86:ARG:N	1:J:87:PRO:HD2	2.35	0.42
1:M:76:LEU:O	1:M:79:TYR:HB3	2.20	0.42
1:M:110:LYS:HD3	1:M:110:LYS:N	2.35	0.42
1:D:99:ALA:C	1:D:101:GLY:N	2.78	0.41
1:E:125:GLN:NE2	1:L:135:SER:H	2.18	0.41
1:F:36:GLU:HA	1:F:69:GLY:O	2.20	0.41
1:I:151:MET:O	1:I:155:LEU:HB2	2.19	0.41
1:B:72:ILE:HA	1:B:100:MET:HE2	2.02	0.41
1:C:31:VAL:O	1:C:32:LEU:HD13	2.19	0.41
1:D:91:THR:C	1:D:92:ILE:HD12	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ILE:HG23	1:K:64:TYR:CE1	2.55	0.41
1:M:29:ARG:HG2	1:M:29:ARG:NH1	2.34	0.41
1:C:56:ASP:HA	1:C:57:PRO:HD2	1.95	0.41
1:F:20:ASP:OD2	1:F:23:SER:N	2.51	0.41
1:F:91:THR:C	1:F:92:ILE:HD12	2.46	0.41
1:I:177:SER:N	1:I:180:GLU:OE2	2.46	0.41
1:J:38:ASN:OD1	1:J:40:SER:HB3	2.20	0.41
1:K:120:ARG:HH21	1:L:147:LEU:HD23	1.85	0.41
1:L:105:LEU:CD2	1:L:121:ILE:HD12	2.51	0.41
1:M:93:CYS:HB2	1:M:105:LEU:HD13	2.02	0.41
1:M:150:LEU:C	1:M:150:LEU:CD2	2.93	0.41
1:D:86:ARG:N	1:D:87:PRO:HD2	2.35	0.41
1:F:169:ASP:OD2	1:F:184:TYR:OH	2.31	0.41
1:H:177:SER:O	1:H:178:ALA:C	2.63	0.41
1:J:57:PRO:HB2	1:J:86:ARG:HH11	1.85	0.41
1:K:117:PRO:HG3	1:K:192:GLN:HA	2.02	0.41
1:M:59:LYS:HE3	1:M:59:LYS:HB2	1.81	0.41
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.34	0.41
1:C:143:GLU:HA	1:C:143:GLU:OE1	2.20	0.41
1:D:66:ASN:ND2	1:D:95:GLY:HA3	2.35	0.41
1:K:72:ILE:HA	1:K:100:MET:HE2	2.01	0.41
1:M:29:ARG:NE	1:M:59:LYS:HB3	2.35	0.41
1:F:117:PRO:HB3	1:F:192:GLN:HB3	2.02	0.41
1:L:130:ALA:HB2	1:L:140:ILE:HG21	2.01	0.41
1:M:20:ASP:HB3	1:M:23:SER:CB	2.50	0.41
1:N:123:ILE:HG13	1:N:174:PHE:HB3	2.03	0.41
1:A:86:ARG:N	1:A:87:PRO:CD	2.84	0.41
1:C:72:ILE:HA	1:C:100:MET:HE3	2.03	0.41
1:D:127:LEU:HD23	1:K:133:GLN:HA	2.02	0.41
1:F:153:SER:O	1:F:156:ALA:HB3	2.21	0.41
1:N:48:GLN:O	1:N:51:PHE:HB3	2.21	0.41
1:K:79:TYR:CE2	1:K:154:ILE:HD13	2.56	0.41
1:M:79:TYR:CD1	1:M:107:CYS:SG	3.14	0.41
1:C:150:LEU:HD13	1:C:150:LEU:C	2.45	0.41
1:D:176:MET:HA	1:D:180:GLU:OE1	2.20	0.41
1:G:27:LYS:HD3	1:G:27:LYS:C	2.46	0.41
1:G:86:ARG:HE	1:G:86:ARG:HB2	1.70	0.41
1:H:57:PRO:CB	1:H:86:ARG:CZ	2.99	0.41
1:I:24:ARG:C	1:I:24:ARG:CD	2.93	0.41
1:I:42:ALA:O	1:I:46:VAL:HG23	2.21	0.41
1:I:50:LEU:O	1:I:51:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ILE:CD1	1:I:126:PRO:HB3	2.45	0.41
1:J:97:ALA:O	1:J:102:ALA:HB2	2.21	0.41
1:K:29:ARG:HE	1:K:59:LYS:HB2	1.86	0.41
1:N:53:GLU:OE2	1:N:53:GLU:CA	2.69	0.41
1:D:168:LYS:HB2	1:D:168:LYS:NZ	2.36	0.41
1:I:179:LYS:O	1:I:183:GLU:HG3	2.21	0.41
1:K:40:SER:O	1:K:43:SER:HB3	2.21	0.41
1:K:99:ALA:C	1:K:101:GLY:N	2.78	0.41
1:K:143:GLU:OE1	1:K:143:GLU:HA	2.21	0.41
1:L:78:ILE:O	1:L:82:MET:HG3	2.21	0.41
1:N:124:HIS:HA	1:N:170:THR:HB	2.03	0.41
1:E:68:PRO:HA	1:E:98:ALA:HB3	2.03	0.40
1:G:176:MET:HE1	1:G:186:LEU:CD1	2.50	0.40
1:J:42:ALA:HA	1:J:78:ILE:HD11	2.02	0.40
1:J:172:ARG:O	1:J:173:ASP:C	2.64	0.40
1:M:110:LYS:CD	1:M:110:LYS:H	2.33	0.40
1:M:125:GLN:NE2	1:M:148:LYS:HZ1	2.19	0.40
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.84	0.40
1:F:135:SER:H	1:M:125:GLN:HE22	1.70	0.40
1:H:79:TYR:CE2	1:H:154:ILE:HD13	2.57	0.40
1:K:28:ASP:O	1:K:29:ARG:HB2	2.21	0.40
1:L:103:PHE:CD1	1:L:155:LEU:HD13	2.57	0.40
1:A:35:GLY:C	1:A:68:PRO:HD2	2.47	0.40
1:A:125:GLN:NE2	1:A:148:LYS:NZ	2.69	0.40
1:B:125:GLN:HE21	1:B:125:GLN:HB2	1.75	0.40
1:D:161:GLN:HG3	1:D:166:ILE:HD11	2.04	0.40
1:F:103:PHE:HD1	1:F:155:LEU:HD13	1.85	0.40
1:F:152:ASN:HD22	1:F:167:ALA:HA	1.86	0.40
1:H:86:ARG:N	1:H:87:PRO:HD2	2.36	0.40
1:N:42:ALA:HA	1:N:78:ILE:HD11	2.04	0.40
1:K:78:ILE:O	1:K:82:MET:HG3	2.21	0.40
1:F:116:LEU:HB3	1:F:117:PRO:HD2	2.03	0.40
1:G:35:GLY:C	1:G:68:PRO:HD2	2.46	0.40
1:K:86:ARG:N	1:K:87:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	171/196 (87%)	163 (95%)	7 (4%)	1 (1%)	21	48
1	B	171/196 (87%)	157 (92%)	11 (6%)	3 (2%)	6	22
1	C	171/196 (87%)	157 (92%)	13 (8%)	1 (1%)	21	48
1	D	171/196 (87%)	160 (94%)	11 (6%)	0	100	100
1	E	171/196 (87%)	164 (96%)	7 (4%)	0	100	100
1	F	171/196 (87%)	160 (94%)	10 (6%)	1 (1%)	21	48
1	G	171/196 (87%)	161 (94%)	8 (5%)	2 (1%)	10	31
1	H	171/196 (87%)	158 (92%)	13 (8%)	0	100	100
1	I	171/196 (87%)	165 (96%)	6 (4%)	0	100	100
1	J	171/196 (87%)	163 (95%)	8 (5%)	0	100	100
1	K	171/196 (87%)	156 (91%)	13 (8%)	2 (1%)	10	31
1	L	171/196 (87%)	162 (95%)	9 (5%)	0	100	100
1	M	171/196 (87%)	164 (96%)	6 (4%)	1 (1%)	21	48
1	N	171/196 (87%)	162 (95%)	9 (5%)	0	100	100
All	All	2394/2744 (87%)	2252 (94%)	131 (6%)	11 (0%)	24	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	191	LEU
1	K	191	LEU
1	M	191	LEU
1	B	56	ASP
1	C	60	ASP
1	A	191	LEU
1	F	191	LEU
1	G	56	ASP
1	B	57	PRO

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Mol	Chain	Res	Type
1	G	57	PRO
1	K	160	GLY

5.3.2 Protein sidechains ⓘ

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	144/165 (87%)	136 (94%)	8 (6%)	19	48
1	B	144/165 (87%)	135 (94%)	9 (6%)	16	43
1	C	144/165 (87%)	139 (96%)	5 (4%)	32	65
1	D	144/165 (87%)	141 (98%)	3 (2%)	47	78
1	E	144/165 (87%)	142 (99%)	2 (1%)	59	84
1	F	144/165 (87%)	136 (94%)	8 (6%)	19	48
1	G	144/165 (87%)	140 (97%)	4 (3%)	38	71
1	H	144/165 (87%)	138 (96%)	6 (4%)	26	59
1	I	144/165 (87%)	140 (97%)	4 (3%)	38	71
1	J	144/165 (87%)	140 (97%)	4 (3%)	38	71
1	K	144/165 (87%)	139 (96%)	5 (4%)	32	65
1	L	144/165 (87%)	136 (94%)	8 (6%)	19	48
1	M	144/165 (87%)	140 (97%)	4 (3%)	38	71
1	N	144/165 (87%)	139 (96%)	5 (4%)	32	65
All	All	2016/2310 (87%)	1941 (96%)	75 (4%)	30	63

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	53	GLU
1	A	92	ILE
1	A	96	GLN
1	A	146	ARG

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	172	ARG
1	A	192	GLN
1	B	31	VAL
1	B	33	LEU
1	B	38	ASN
1	B	110	LYS
1	B	125	GLN
1	B	127	LEU
1	B	131	GLN
1	B	182	LYS
1	B	186	LEU
1	C	29	ARG
1	C	32	LEU
1	C	53	GLU
1	C	83	ASN
1	C	182	LYS
1	D	58	GLU
1	D	144	ILE
1	D	168	LYS
1	E	24	ARG
1	E	55	GLU
1	F	27	LYS
1	F	29	ARG
1	F	52	LEU
1	F	96	GLN
1	F	157	GLN
1	F	163	LEU
1	F	183	GLU
1	F	191	LEU
1	G	25	LEU
1	G	46	VAL
1	G	100	MET
1	G	163	LEU
1	H	33	LEU
1	H	92	ILE
1	H	96	GLN
1	H	148	LYS
1	H	153	SER
1	H	163	LEU
1	I	28	ASP
1	I	110	LYS

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Mol	Chain	Res	Type
1	I	121	ILE
1	I	155	LEU
1	J	63	LEU
1	J	80	ASP
1	J	86	ARG
1	J	100	MET
1	K	32	LEU
1	K	73	THR
1	K	96	GLN
1	K	155	LEU
1	K	163	LEU
1	L	24	ARG
1	L	29	ARG
1	L	36	GLU
1	L	144	ILE
1	L	155	LEU
1	L	168	LYS
1	L	179	LYS
1	L	192	GLN
1	M	33	LEU
1	M	88	ASP
1	M	110	LYS
1	M	163	LEU
1	N	24	ARG
1	N	33	LEU
1	N	72	ILE
1	N	157	GLN
1	N	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	66	ASN
1	A	83	ASN
1	A	118	HIS
1	A	125	GLN
1	A	131	GLN
1	A	152	ASN
1	B	38	ASN
1	B	96	GLN
1	B	118	HIS

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Mol	Chain	Res	Type
1	B	124	HIS
1	B	125	GLN
1	B	131	GLN
1	B	165	GLN
1	C	83	ASN
1	C	125	GLN
1	C	157	GLN
1	C	165	GLN
1	C	192	GLN
1	D	66	ASN
1	D	118	HIS
1	D	125	GLN
1	D	131	GLN
1	D	158	ASN
1	E	83	ASN
1	E	96	GLN
1	E	124	HIS
1	E	125	GLN
1	E	158	ASN
1	E	192	GLN
1	F	118	HIS
1	F	124	HIS
1	F	125	GLN
1	F	131	GLN
1	F	152	ASN
1	F	165	GLN
1	F	192	GLN
1	G	118	HIS
1	G	125	GLN
1	G	131	GLN
1	H	66	ASN
1	H	124	HIS
1	H	125	GLN
1	H	131	GLN
1	H	152	ASN
1	H	165	GLN
1	I	48	GLN
1	I	118	HIS
1	I	125	GLN
1	I	152	ASN
1	I	158	ASN
1	J	96	GLN

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Mol	Chain	Res	Type
1	J	125	GLN
1	J	165	GLN
1	K	83	ASN
1	K	118	HIS
1	K	125	GLN
1	K	158	ASN
1	L	48	GLN
1	L	118	HIS
1	L	125	GLN
1	L	161	GLN
1	M	48	GLN
1	M	66	ASN
1	M	118	HIS
1	M	125	GLN
1	N	83	ASN
1	N	125	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 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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/196 (88%)	-0.44	1 (0%) 85 80	22, 32, 46, 57	0
1	B	173/196 (88%)	-0.43	1 (0%) 85 80	19, 31, 52, 62	0
1	C	173/196 (88%)	-0.29	1 (0%) 85 80	22, 36, 53, 62	0
1	D	173/196 (88%)	-0.19	0 100 100	26, 39, 59, 74	0
1	E	173/196 (88%)	-0.22	2 (1%) 76 68	24, 36, 54, 67	0
1	F	173/196 (88%)	-0.37	1 (0%) 85 80	22, 34, 52, 62	0
1	G	173/196 (88%)	-0.47	0 100 100	17, 30, 48, 59	0
1	H	173/196 (88%)	-0.44	0 100 100	19, 30, 50, 61	0
1	I	173/196 (88%)	-0.45	0 100 100	19, 32, 53, 60	0
1	J	173/196 (88%)	-0.36	0 100 100	20, 33, 48, 64	0
1	K	173/196 (88%)	-0.18	0 100 100	23, 40, 57, 66	0
1	L	173/196 (88%)	-0.22	0 100 100	23, 38, 57, 64	0
1	M	173/196 (88%)	-0.36	0 100 100	22, 33, 51, 59	0
1	N	173/196 (88%)	-0.32	1 (0%) 85 80	24, 34, 54, 63	0
All	All	2422/2744 (88%)	-0.34	7 (0%) 90 86	17, 34, 54, 74	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	GLN	3.0
1	A	192	GLN	2.7
1	C	192	GLN	2.6
1	B	191	LEU	2.5
1	N	192	GLN	2.2
1	E	183	GLU	2.2
1	F	192	GLN	2.1

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.