



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 1ZOF / pdb_00001zof
Title : Crystal structure of alkyl hydroperoxide-reductase (AhpC) from *Helicobacter Pylori*
Authors : Papinutto, E.; Windle, H.J.; Cendron, L.; Battistutta, R.; Kelleher, D.; Zanolotti, G.
Deposited on : 2005-05-13
Resolution : 2.95 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

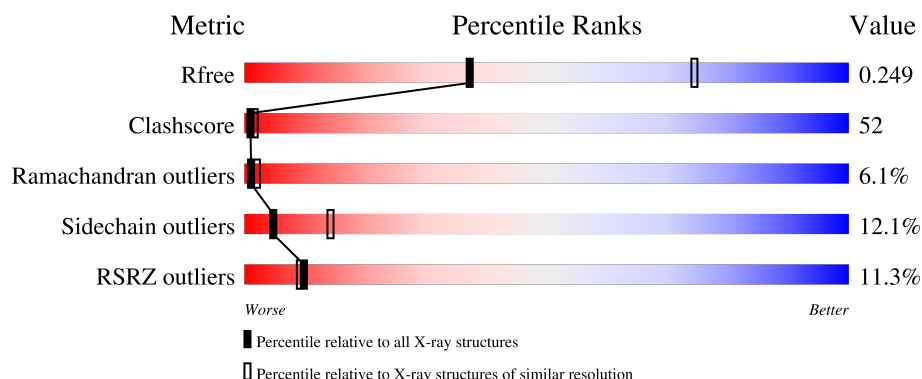
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	198	10% 33% 41% 11% 14%
1	B	198	10% 28% 48% 12% 12%
1	C	198	12% 28% 46% 9% 14%
1	D	198	13% 26% 50% 11% 12%
1	E	198	7% 28% 44% 11% 14%

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Mol	Chain	Length	Quality of chain
1	F	198	10% 30% 46% 10% • 12%
1	G	198	7% 31% 42% 12% • 14%
1	H	198	6% 29% 47% 11% • 12%
1	I	198	15% 30% 42% 12% • 14%
1	J	198	10% 28% 46% 14% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13770 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 alkyl hydroperoxide-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1349	871	226	245	7			
1	B	175	Total	C	N	O	S	0	0	0
			1392	899	236	250	7			
1	C	170	Total	C	N	O	S	0	0	0
			1349	871	226	245	7			
1	D	175	Total	C	N	O	S	0	0	0
			1392	899	236	250	7			
1	E	170	Total	C	N	O	S	0	0	0
			1349	871	226	245	7			
1	F	175	Total	C	N	O	S	0	0	0
			1392	899	236	250	7			
1	G	170	Total	C	N	O	S	0	0	0
			1349	871	226	245	7			
1	H	175	Total	C	N	O	S	0	0	0
			1392	899	236	250	7			
1	I	170	Total	C	N	O	S	0	0	0
			1349	871	226	245	7			
1	J	175	Total	C	N	O	S	0	0	0
			1392	899	236	250	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP P56876
B	2	VAL	LEU	engineered mutation	UNP P56876
C	2	VAL	LEU	engineered mutation	UNP P56876
D	2	VAL	LEU	engineered mutation	UNP P56876
E	2	VAL	LEU	engineered mutation	UNP P56876
F	2	VAL	LEU	engineered mutation	UNP P56876
G	2	VAL	LEU	engineered mutation	UNP P56876
H	2	VAL	LEU	engineered mutation	UNP P56876
I	2	VAL	LEU	engineered mutation	UNP P56876

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Chain	Residue	Modelled	Actual	Comment	Reference
J	2	VAL	LEU	engineered mutation	UNP P56876

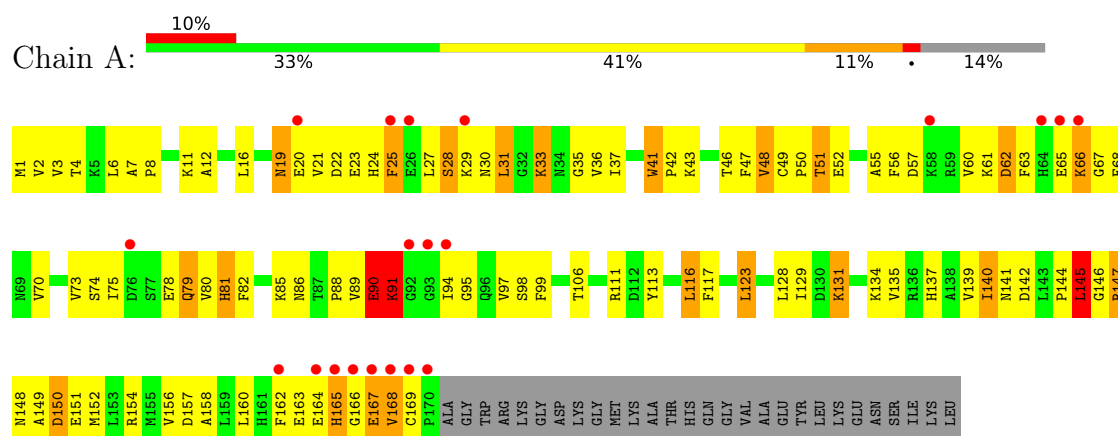
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	8	Total O 8 8	0	0
2	C	9	Total O 9 9	0	0
2	D	6	Total O 6 6	0	0
2	E	9	Total O 9 9	0	0
2	F	7	Total O 7 7	0	0
2	G	2	Total O 2 2	0	0
2	H	2	Total O 2 2	0	0
2	I	2	Total O 2 2	0	0
2	J	6	Total O 6 6	0	0

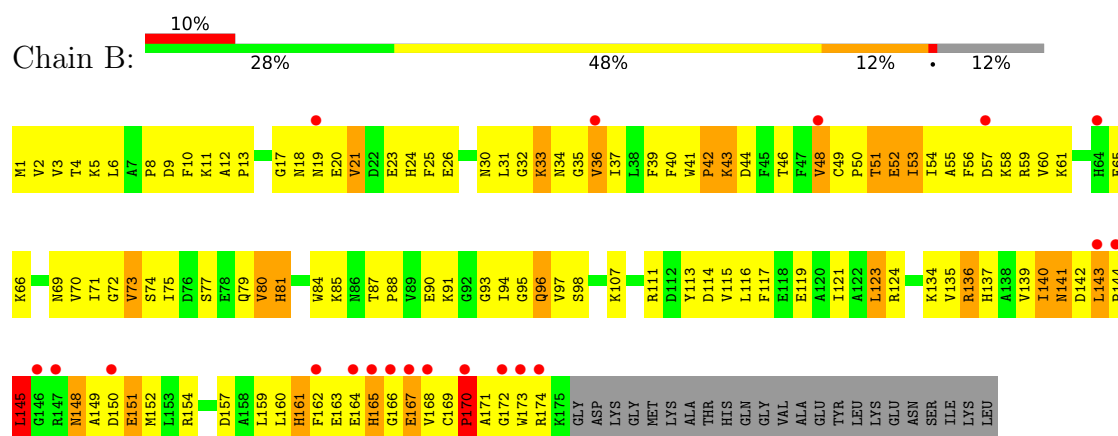
3 Residue-property plots [i](#)

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

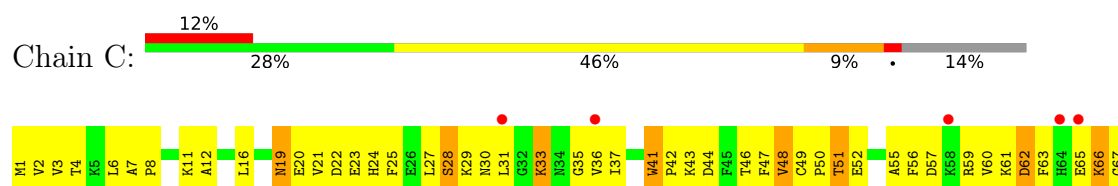
- Molecule 1: alkyl hydroperoxide-reductase

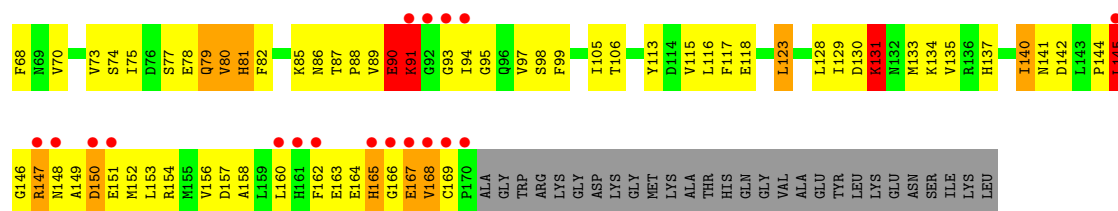


- Molecule 1: alkyl hydroperoxide-reductase

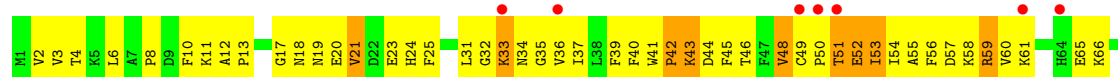


- Molecule 1: alkyl hydroperoxide-reductase

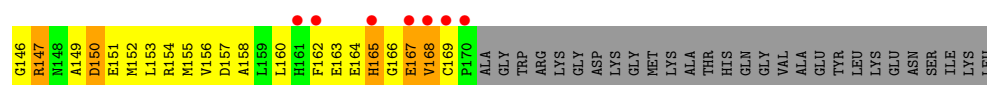
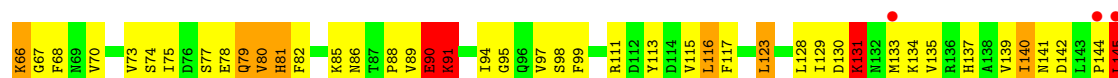
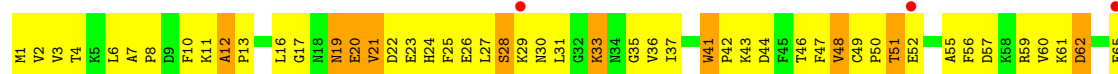




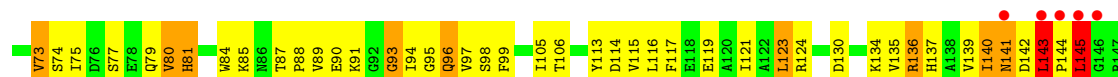
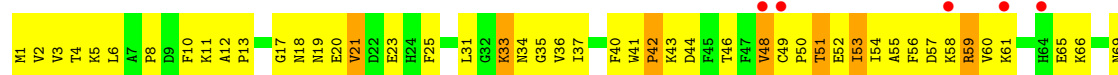
• Molecule 1: alkyl hydroperoxide-reductase



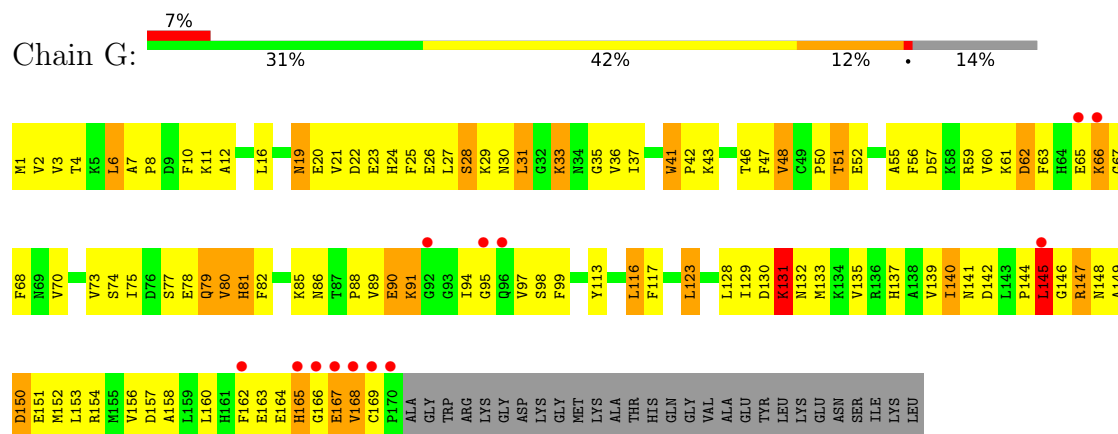
• Molecule 1: alkyl hydroperoxide-reductase



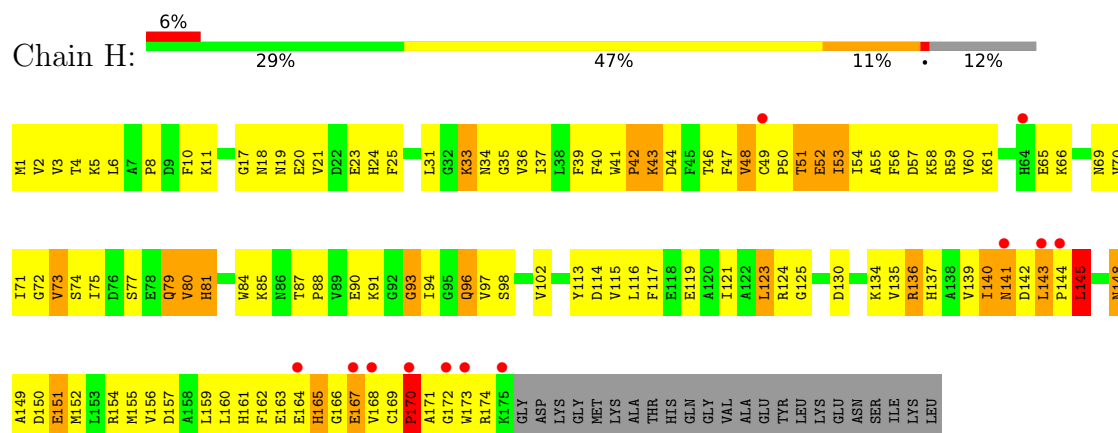
• Molecule 1: alkyl hydroperoxide-reductase



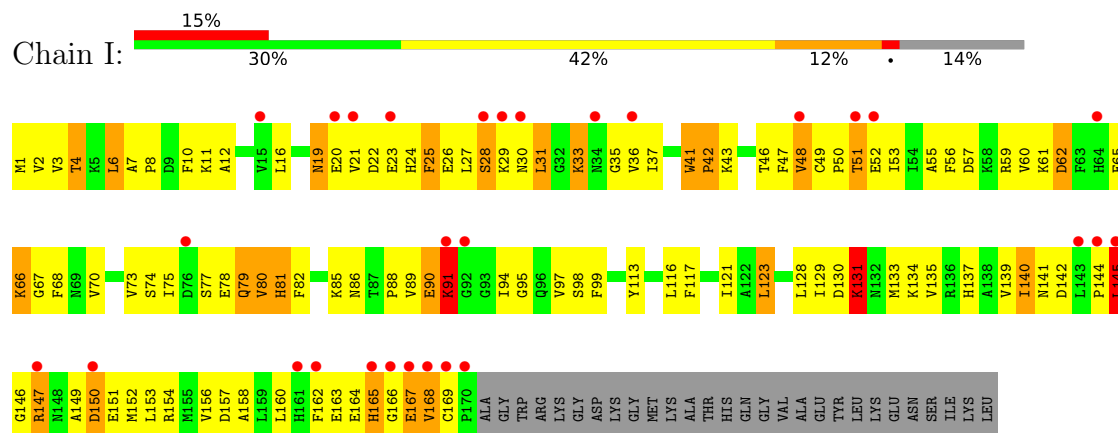
- Molecule 1: alkyl hydroperoxide-reductase



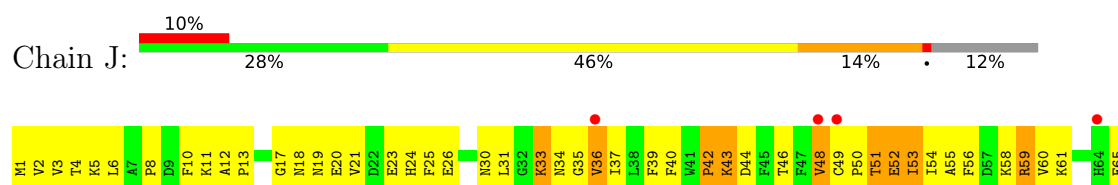
- Molecule 1: alkyl hydroperoxide-reductase

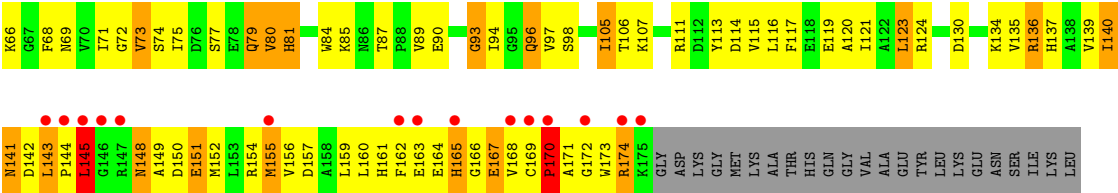


- Molecule 1: alkyl hydroperoxide-reductase



- Molecule 1: alkyl hydroperoxide-reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.86Å 138.42Å 127.54Å 90.00° 125.70° 90.00°	Depositor
Resolution (Å)	52.80 – 2.95 52.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.80-2.95) 99.9 (52.80-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.260 0.227 , 0.249	Depositor DCC
R_{free} test set	4943 reflections (8.17%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13770	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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	0.60	0/1381	1.02	7/1867 (0.4%)
1	B	0.65	0/1426	1.05	5/1927 (0.3%)
1	C	0.61	0/1381	1.02	8/1867 (0.4%)
1	D	0.68	0/1426	1.07	3/1927 (0.2%)
1	E	0.56	0/1381	1.04	9/1867 (0.5%)
1	F	0.59	0/1426	1.05	6/1927 (0.3%)
1	G	0.53	0/1381	1.01	6/1867 (0.3%)
1	H	0.57	0/1426	1.04	3/1927 (0.2%)
1	I	0.55	0/1381	1.03	6/1867 (0.3%)
1	J	0.65	1/1426 (0.1%)	1.04	4/1927 (0.2%)
All	All	0.60	1/14035 (0.0%)	1.04	57/18970 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	155	MET	SD-CE	5.62	1.93	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	12	ALA	N-CA-C	7.58	114.82	108.07
1	D	115	VAL	N-CA-C	-7.15	106.16	113.10
1	A	81	HIS	N-CA-C	-6.99	103.35	110.97
1	I	81	HIS	N-CA-C	-6.83	102.68	111.02
1	F	115	VAL	N-CA-C	-6.72	106.58	113.10
1	G	81	HIS	N-CA-C	-6.58	102.99	111.02
1	B	115	VAL	N-CA-C	-6.55	106.75	113.10
1	C	81	HIS	N-CA-C	-6.45	103.15	111.02
1	J	115	VAL	N-CA-C	-6.39	106.90	113.10
1	A	12	ALA	N-CA-C	6.35	115.44	108.14
1	G	12	ALA	N-CA-C	6.30	115.38	108.14
1	I	12	ALA	N-CA-C	6.17	115.23	108.14
1	C	12	ALA	N-CA-C	6.15	115.21	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	GLU	N-CA-C	-6.08	101.48	110.48
1	E	81	HIS	N-CA-C	-6.04	103.87	111.11
1	E	21	VAL	N-CA-C	5.95	115.30	106.85
1	A	20	GLU	N-CA-C	-5.92	101.72	110.48
1	I	20	GLU	N-CA-C	-5.87	101.79	110.48
1	D	21	VAL	N-CA-C	5.79	116.53	108.89
1	B	43	LYS	N-CA-C	5.76	117.61	108.79
1	H	115	VAL	N-CA-C	-5.71	107.70	113.47
1	H	43	LYS	N-CA-C	5.71	117.53	108.79
1	G	20	GLU	N-CA-C	-5.71	102.03	110.48
1	F	41	TRP	CA-C-N	5.65	126.90	119.84
1	F	41	TRP	C-N-CA	5.65	126.90	119.84
1	C	41	TRP	CA-C-N	5.64	126.89	119.84
1	C	41	TRP	C-N-CA	5.64	126.89	119.84
1	E	115	VAL	N-CA-C	-5.60	107.82	113.20
1	A	41	TRP	CA-C-N	5.56	126.78	119.84
1	A	41	TRP	C-N-CA	5.56	126.78	119.84
1	E	41	TRP	CA-C-N	5.55	126.78	119.84
1	E	41	TRP	C-N-CA	5.55	126.78	119.84
1	E	20	GLU	N-CA-C	-5.54	102.28	110.48
1	B	36	VAL	N-CA-C	5.53	115.60	107.75
1	G	41	TRP	CA-C-N	5.47	126.68	119.84
1	G	41	TRP	C-N-CA	5.47	126.68	119.84
1	I	41	TRP	CA-C-N	5.45	126.66	119.84
1	I	41	TRP	C-N-CA	5.45	126.66	119.84
1	H	21	VAL	N-CA-C	5.45	116.08	108.89
1	B	161	HIS	N-CA-C	-5.35	104.34	111.24
1	G	90	GLU	N-CA-C	-5.33	106.29	112.89
1	C	115	VAL	N-CA-C	-5.31	108.10	113.20
1	B	21	VAL	N-CA-C	5.26	115.83	108.89
1	A	91	LYS	N-CA-C	-5.22	106.75	113.02
1	C	90	GLU	N-CA-C	-5.21	106.43	112.89
1	J	43	LYS	N-CA-C	5.20	116.97	109.07
1	F	21	VAL	N-CA-C	5.17	116.02	108.58
1	D	43	LYS	N-CA-C	5.15	116.90	109.07
1	I	91	LYS	N-CA-C	-5.14	106.85	113.02
1	E	90	GLU	N-CA-C	-5.13	106.53	112.89
1	F	143	LEU	CA-C-N	5.13	124.92	119.28
1	F	143	LEU	C-N-CA	5.13	124.92	119.28
1	A	90	GLU	N-CA-C	-5.12	106.54	112.89
1	E	91	LYS	N-CA-C	-5.11	106.89	113.02
1	J	36	VAL	N-CA-C	5.08	114.97	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	105	ILE	N-CA-C	5.04	116.36	110.62
1	C	91	LYS	N-CA-C	-5.02	107.00	113.02

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	1349	0	1340	138	1
1	B	1392	0	1384	176	0
1	C	1349	0	1340	143	1
1	D	1392	0	1384	175	0
1	E	1349	0	1340	145	0
1	F	1392	0	1384	162	0
1	G	1349	0	1340	132	0
1	H	1392	0	1384	164	0
1	I	1349	0	1340	141	0
1	J	1392	0	1384	164	0
2	A	14	0	0	2	0
2	B	8	0	0	4	0
2	C	9	0	0	1	0
2	D	6	0	0	2	0
2	E	9	0	0	4	0
2	F	7	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	1	0
2	J	6	0	0	1	0
All	All	13770	0	13620	1425	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1425) 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:J:53:ILE:HD12	1:J:53:ILE:H	1.24	1.01
1:B:53:ILE:HD12	1:B:53:ILE:H	1.27	0.99
1:B:3:VAL:HA	1:B:135:VAL:HG23	1.42	0.98
1:H:53:ILE:HD12	1:H:53:ILE:H	1.29	0.98
1:C:137:HIS:HD2	1:D:141:ASN:HB2	1.25	0.97
1:F:3:VAL:HA	1:F:135:VAL:HG23	1.46	0.97
1:H:3:VAL:HA	1:H:135:VAL:HG23	1.47	0.96
1:D:3:VAL:HA	1:D:135:VAL:HG23	1.46	0.96
1:J:3:VAL:HA	1:J:135:VAL:HG23	1.48	0.96
1:G:137:HIS:HD2	1:H:141:ASN:HB2	1.30	0.96
1:F:53:ILE:H	1:F:53:ILE:HD12	1.27	0.96
1:I:137:HIS:HD2	1:J:141:ASN:HB2	1.28	0.95
1:C:160:LEU:HA	1:C:163:GLU:HG2	1.49	0.95
1:A:160:LEU:HA	1:A:163:GLU:HG2	1.49	0.94
1:J:116:LEU:HD11	1:J:119:GLU:HA	1.51	0.93
1:H:169:CYS:HB2	1:H:170:PRO:HD2	1.51	0.93
1:D:53:ILE:HD12	1:D:53:ILE:H	1.35	0.92
1:E:160:LEU:HA	1:E:163:GLU:HG2	1.52	0.92
1:B:169:CYS:HB2	1:B:170:PRO:HD2	1.51	0.92
1:G:160:LEU:HA	1:G:163:GLU:HG2	1.52	0.90
1:D:169:CYS:HB2	1:D:170:PRO:HD2	1.54	0.90
1:F:169:CYS:HB2	1:F:170:PRO:HD2	1.52	0.89
1:D:2:VAL:HG12	1:D:135:VAL:HG21	1.54	0.89
1:D:43:LYS:HD2	1:E:79:GLN:HG3	1.52	0.89
1:I:160:LEU:HA	1:I:163:GLU:HG2	1.51	0.88
1:D:116:LEU:HD11	1:D:119:GLU:HA	1.55	0.88
1:H:2:VAL:HG12	1:H:135:VAL:HG21	1.55	0.88
1:F:18:ASN:OD1	1:F:20:GLU:HG2	1.74	0.87
1:F:116:LEU:HD11	1:F:119:GLU:HA	1.57	0.87
1:F:2:VAL:HG12	1:F:135:VAL:HG21	1.56	0.86
1:B:48:VAL:HG22	1:B:49:CYS:H	1.40	0.86
1:I:37:ILE:HD12	1:I:152:MET:HE3	1.56	0.86
1:G:37:ILE:HD12	1:G:152:MET:HE3	1.58	0.86
1:E:137:HIS:HD2	1:F:141:ASN:HB2	1.41	0.86
1:J:2:VAL:HG12	1:J:135:VAL:HG21	1.57	0.85
1:B:18:ASN:OD1	1:B:20:GLU:HG2	1.77	0.85
1:J:169:CYS:HB2	1:J:170:PRO:HD2	1.55	0.85
1:H:48:VAL:HG22	1:H:49:CYS:H	1.42	0.85
1:J:48:VAL:HG22	1:J:49:CYS:H	1.42	0.85
1:C:37:ILE:HD12	1:C:152:MET:HE3	1.57	0.84
1:D:48:VAL:HG22	1:D:49:CYS:H	1.42	0.84
1:F:48:VAL:HG22	1:F:49:CYS:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:PRO:HB2	1:E:91:LYS:HB2	1.58	0.84
1:D:18:ASN:OD1	1:D:20:GLU:HG2	1.78	0.83
1:E:37:ILE:HD12	1:E:152:MET:HE3	1.59	0.83
1:H:18:ASN:OD1	1:H:20:GLU:HG2	1.78	0.83
1:A:37:ILE:HD12	1:A:152:MET:HE3	1.60	0.83
1:H:116:LEU:HD11	1:H:119:GLU:HA	1.61	0.82
1:A:137:HIS:HD2	1:B:141:ASN:HB2	1.40	0.82
1:C:128:LEU:HB2	1:C:152:MET:HE1	1.61	0.82
1:B:33:LYS:HG3	1:B:34:ASN:ND2	1.94	0.82
1:C:88:PRO:HB2	1:C:91:LYS:HB2	1.61	0.82
1:C:137:HIS:CD2	1:D:141:ASN:HB2	2.13	0.82
1:I:88:PRO:HB2	1:I:91:LYS:HB2	1.60	0.82
1:B:116:LEU:HD11	1:B:119:GLU:HA	1.61	0.82
1:F:136:ARG:HA	1:F:136:ARG:HH11	1.45	0.82
1:G:85:LYS:HA	1:G:94:ILE:HG22	1.60	0.81
1:B:85:LYS:HA	1:B:94:ILE:HG22	1.62	0.81
1:I:137:HIS:CD2	1:J:141:ASN:HB2	2.16	0.81
1:B:42:PRO:HB3	1:B:121:ILE:HD12	1.61	0.80
1:E:128:LEU:HB2	1:E:152:MET:HE1	1.62	0.80
1:I:85:LYS:HA	1:I:94:ILE:HG22	1.63	0.80
1:E:147:ARG:HB3	1:E:147:ARG:HH11	1.47	0.80
1:C:123:LEU:HD23	1:C:140:ILE:HD11	1.64	0.80
1:A:88:PRO:HB2	1:A:91:LYS:HB2	1.63	0.79
1:A:85:LYS:HA	1:A:94:ILE:HG22	1.63	0.79
1:G:123:LEU:HD23	1:G:140:ILE:HD11	1.62	0.79
1:G:137:HIS:CD2	1:H:141:ASN:HB2	2.16	0.79
1:C:85:LYS:HA	1:C:94:ILE:HG22	1.63	0.79
1:D:117:PHE:HB2	1:D:123:LEU:HD13	1.63	0.78
1:H:117:PHE:HB2	1:H:123:LEU:HD13	1.65	0.78
1:B:136:ARG:HH11	1:B:136:ARG:HA	1.49	0.78
1:G:88:PRO:HB2	1:G:91:LYS:HB2	1.64	0.78
1:B:3:VAL:HA	1:B:135:VAL:CG2	2.14	0.78
1:H:36:VAL:HG13	1:H:69:ASN:O	1.84	0.77
1:B:2:VAL:HG12	1:B:135:VAL:HG21	1.65	0.77
1:B:53:ILE:H	1:B:53:ILE:CD1	1.98	0.77
1:F:85:LYS:HA	1:F:94:ILE:HG22	1.65	0.77
1:G:147:ARG:HH11	1:G:147:ARG:HB3	1.48	0.77
1:D:85:LYS:HA	1:D:94:ILE:HG22	1.65	0.77
1:G:128:LEU:HB2	1:G:152:MET:HE1	1.67	0.77
1:A:147:ARG:HH11	1:A:147:ARG:HB3	1.49	0.77
1:F:43:LYS:HD2	1:G:79:GLN:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HD23	1:E:140:ILE:HD11	1.65	0.76
1:D:143:LEU:HB3	1:D:145:LEU:HD11	1.66	0.76
1:F:3:VAL:HA	1:F:135:VAL:CG2	2.16	0.76
1:H:85:LYS:HA	1:H:94:ILE:HG22	1.65	0.76
1:I:123:LEU:HD23	1:I:140:ILE:HD11	1.65	0.76
1:E:85:LYS:HA	1:E:94:ILE:HG22	1.67	0.76
1:A:142:ASP:CG	1:B:136:ARG:HH12	1.93	0.76
1:J:33:LYS:HG3	1:J:34:ASN:ND2	1.99	0.76
1:H:43:LYS:HD2	1:I:79:GLN:HG3	1.68	0.75
1:A:3:VAL:CB	1:B:140:ILE:HD11	2.17	0.74
1:B:117:PHE:HB2	1:B:123:LEU:HD13	1.69	0.74
1:H:136:ARG:HA	1:H:136:ARG:HH11	1.53	0.74
1:H:33:LYS:HB2	1:H:33:LYS:NZ	2.02	0.74
1:A:123:LEU:HD23	1:A:140:ILE:HD11	1.69	0.74
1:E:142:ASP:CG	1:F:136:ARG:HH12	1.95	0.74
1:G:142:ASP:CG	1:H:136:ARG:HH12	1.94	0.74
1:D:6:LEU:HD23	1:D:134:LYS:HD2	1.70	0.74
1:F:117:PHE:HB2	1:F:123:LEU:HD13	1.70	0.74
1:J:18:ASN:OD1	1:J:20:GLU:HG2	1.88	0.74
1:H:143:LEU:HB3	1:H:145:LEU:HD11	1.67	0.74
1:B:36:VAL:HG22	1:B:69:ASN:HB2	1.69	0.74
1:G:33:LYS:HE2	1:G:33:LYS:H	1.52	0.74
1:D:36:VAL:HG22	1:D:69:ASN:HB2	1.70	0.73
1:D:36:VAL:HG11	1:D:71:ILE:HD12	1.69	0.73
1:J:19:ASN:OD1	1:J:85:LYS:HD3	1.88	0.73
1:I:128:LEU:HB2	1:I:152:MET:HE1	1.69	0.73
1:A:128:LEU:HB2	1:A:152:MET:HE1	1.69	0.73
1:F:36:VAL:HG13	1:F:69:ASN:O	1.89	0.73
1:C:147:ARG:HH11	1:C:147:ARG:HB3	1.54	0.73
1:G:33:LYS:HE2	1:G:33:LYS:N	2.04	0.73
1:H:3:VAL:HA	1:H:135:VAL:CG2	2.19	0.73
1:J:6:LEU:HD23	1:J:134:LYS:HD2	1.70	0.73
1:J:53:ILE:H	1:J:53:ILE:CD1	1.99	0.73
1:B:43:LYS:HD2	1:C:79:GLN:HG3	1.68	0.73
1:A:33:LYS:HE2	1:A:33:LYS:N	2.05	0.72
1:E:33:LYS:H	1:E:33:LYS:HE2	1.54	0.72
1:F:6:LEU:HD23	1:F:134:LYS:HD2	1.71	0.72
1:D:42:PRO:HB3	1:D:121:ILE:HD12	1.71	0.72
1:D:48:VAL:HG13	1:D:49:CYS:N	2.05	0.72
1:H:6:LEU:HD23	1:H:134:LYS:HD2	1.70	0.72
1:H:77:SER:OG	1:H:80:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:ARG:HH11	1:I:147:ARG:HB3	1.53	0.72
1:I:169:CYS:HG	1:J:49:CYS:HG	1.37	0.72
1:B:52:GLU:HG2	1:B:124:ARG:NH1	2.04	0.72
1:F:53:ILE:H	1:F:53:ILE:CD1	2.00	0.72
1:F:140:ILE:C	1:F:140:ILE:HD12	2.15	0.72
1:J:123:LEU:HD23	1:J:140:ILE:HD13	1.71	0.72
1:H:52:GLU:HG2	1:H:124:ARG:NH1	2.05	0.71
1:D:117:PHE:HB2	1:D:123:LEU:CD1	2.20	0.71
1:J:87:THR:O	1:J:93:GLY:HA3	1.90	0.71
1:F:140:ILE:HD12	1:F:141:ASN:N	2.05	0.71
1:I:33:LYS:HE2	1:I:33:LYS:N	2.06	0.71
1:A:137:HIS:CD2	1:B:141:ASN:HB2	2.25	0.71
1:F:55:ALA:O	1:F:59:ARG:HD3	1.90	0.71
1:J:33:LYS:HB2	1:J:33:LYS:NZ	2.06	0.71
1:J:85:LYS:HA	1:J:94:ILE:HG22	1.72	0.71
1:A:160:LEU:HA	1:A:163:GLU:CG	2.21	0.71
1:E:137:HIS:CD2	1:F:141:ASN:HB2	2.23	0.71
1:F:117:PHE:HB2	1:F:123:LEU:CD1	2.21	0.71
1:D:55:ALA:O	1:D:59:ARG:HD3	1.90	0.71
1:E:36:VAL:HG12	1:E:37:ILE:H	1.55	0.71
1:F:77:SER:OG	1:F:80:VAL:HG12	1.91	0.71
1:G:36:VAL:HG12	1:G:37:ILE:H	1.55	0.71
1:C:36:VAL:HG12	1:C:37:ILE:H	1.56	0.70
1:B:140:ILE:C	1:B:140:ILE:HD12	2.15	0.70
1:F:48:VAL:HG13	1:F:49:CYS:N	2.04	0.70
1:I:33:LYS:HE2	1:I:33:LYS:H	1.55	0.70
1:D:3:VAL:HA	1:D:135:VAL:CG2	2.19	0.70
1:J:66:LYS:HE2	1:J:157:ASP:OD1	1.91	0.70
1:A:3:VAL:HG21	1:B:140:ILE:HD11	1.73	0.70
1:A:33:LYS:HE2	1:A:33:LYS:H	1.56	0.70
1:H:8:PRO:HG2	1:H:113:TYR:CE1	2.27	0.70
1:J:143:LEU:CG	1:J:144:PRO:HD2	2.22	0.70
1:D:52:GLU:HG2	1:D:124:ARG:NH1	2.07	0.70
1:J:136:ARG:HH11	1:J:136:ARG:HA	1.57	0.70
1:A:140:ILE:HG13	1:B:3:VAL:HG21	1.74	0.70
1:D:61:LYS:O	1:D:65:GLU:HG3	1.92	0.70
1:F:61:LYS:O	1:F:65:GLU:HG3	1.92	0.70
1:H:140:ILE:HD12	1:H:140:ILE:C	2.16	0.70
1:B:6:LEU:HD23	1:B:134:LYS:HD2	1.73	0.69
1:A:3:VAL:HG11	1:B:140:ILE:HD11	1.74	0.69
1:D:143:LEU:CG	1:D:144:PRO:HD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:LEU:HB3	1:J:145:LEU:HD11	1.73	0.69
1:D:140:ILE:HD12	1:D:141:ASN:N	2.07	0.69
1:F:143:LEU:CG	1:F:144:PRO:HD2	2.22	0.69
1:A:36:VAL:HG12	1:A:37:ILE:H	1.56	0.69
1:B:117:PHE:HB2	1:B:123:LEU:CD1	2.22	0.69
1:C:160:LEU:HA	1:C:163:GLU:CG	2.20	0.69
1:D:43:LYS:HD2	1:E:79:GLN:CG	2.21	0.69
1:E:160:LEU:HA	1:E:163:GLU:CG	2.22	0.69
1:H:48:VAL:HG22	1:H:49:CYS:N	2.08	0.69
1:F:52:GLU:HG2	1:F:124:ARG:NH1	2.08	0.69
1:H:48:VAL:HG13	1:H:49:CYS:N	2.06	0.69
1:J:3:VAL:HA	1:J:135:VAL:CG2	2.22	0.69
1:B:48:VAL:HG22	1:B:49:CYS:N	2.07	0.69
1:B:87:THR:O	1:B:93:GLY:HA3	1.93	0.69
1:B:48:VAL:HG13	1:B:49:CYS:N	2.06	0.68
1:I:36:VAL:HG12	1:I:37:ILE:H	1.57	0.68
1:B:143:LEU:CG	1:B:144:PRO:HD2	2.22	0.68
1:C:33:LYS:N	1:C:33:LYS:HE2	2.08	0.68
1:G:140:ILE:HG13	1:H:3:VAL:HG21	1.74	0.68
1:D:136:ARG:HA	1:D:136:ARG:HH11	1.59	0.68
1:E:33:LYS:HE2	1:E:33:LYS:N	2.08	0.68
1:D:56:PHE:CZ	1:D:149:ALA:HA	2.28	0.68
1:I:142:ASP:CG	1:J:136:ARG:HH12	2.02	0.68
1:C:33:LYS:HE2	1:C:33:LYS:H	1.59	0.68
1:D:48:VAL:HG22	1:D:49:CYS:N	2.08	0.68
1:E:74:SER:HB3	1:E:81:HIS:HE1	1.59	0.68
1:I:74:SER:HB3	1:I:81:HIS:HE1	1.58	0.68
1:A:62:ASP:OD2	1:A:62:ASP:N	2.25	0.68
1:B:19:ASN:OD1	1:B:85:LYS:HD3	1.94	0.67
1:I:160:LEU:HA	1:I:163:GLU:CG	2.22	0.67
1:J:48:VAL:HG13	1:J:49:CYS:N	2.09	0.67
1:A:79:GLN:HG3	1:J:43:LYS:HD2	1.75	0.67
1:H:33:LYS:HG3	1:H:34:ASN:ND2	2.10	0.67
1:E:62:ASP:OD2	1:E:62:ASP:N	2.27	0.67
1:F:36:VAL:HG22	1:F:69:ASN:HB2	1.76	0.67
1:B:36:VAL:HG13	1:B:69:ASN:O	1.94	0.67
1:H:140:ILE:HD12	1:H:141:ASN:N	2.09	0.67
1:H:143:LEU:CG	1:H:144:PRO:HD2	2.24	0.67
1:J:55:ALA:O	1:J:59:ARG:HD3	1.94	0.67
1:B:79:GLN:HG3	1:C:43:LYS:HD3	1.77	0.67
1:F:48:VAL:HG22	1:F:49:CYS:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:VAL:HG21	1:J:98:SER:OG	1.94	0.67
1:I:62:ASP:OD2	1:I:62:ASP:N	2.28	0.67
1:E:11:LYS:CE	1:E:24:HIS:HB3	2.25	0.67
1:J:56:PHE:CZ	1:J:149:ALA:HA	2.30	0.67
1:A:33:LYS:HD2	1:A:67:GLY:HA2	1.77	0.66
1:D:60:VAL:HG21	1:D:98:SER:OG	1.95	0.66
1:H:60:VAL:HG21	1:H:98:SER:OG	1.95	0.66
1:D:123:LEU:HD23	1:D:140:ILE:HD13	1.77	0.66
1:J:117:PHE:HB2	1:J:123:LEU:HD13	1.76	0.66
1:G:160:LEU:HA	1:G:163:GLU:CG	2.24	0.66
1:H:87:THR:O	1:H:93:GLY:HA3	1.94	0.66
1:J:140:ILE:HD12	1:J:140:ILE:C	2.20	0.66
1:H:53:ILE:H	1:H:53:ILE:CD1	2.03	0.66
1:I:11:LYS:CE	1:I:24:HIS:HB3	2.25	0.66
1:A:74:SER:HB3	1:A:81:HIS:HE1	1.60	0.66
1:J:48:VAL:HG22	1:J:49:CYS:N	2.10	0.66
1:E:3:VAL:HG11	1:F:140:ILE:HD11	1.78	0.66
1:G:62:ASP:OD2	1:G:62:ASP:N	2.27	0.66
1:C:62:ASP:N	1:C:62:ASP:OD2	2.27	0.66
1:I:3:VAL:HG11	1:J:140:ILE:HD11	1.78	0.66
1:J:53:ILE:HD12	1:J:53:ILE:N	2.05	0.66
1:D:87:THR:O	1:D:93:GLY:HA3	1.96	0.66
1:B:59:ARG:HH21	1:B:150:ASP:HB2	1.61	0.65
1:D:131:LYS:HE2	2:D:202:HOH:O	1.96	0.65
1:H:36:VAL:HG22	1:H:69:ASN:HB2	1.77	0.65
1:C:3:VAL:HG11	1:D:140:ILE:HD11	1.78	0.65
1:D:140:ILE:HD12	1:D:140:ILE:C	2.21	0.65
1:D:53:ILE:H	1:D:53:ILE:CD1	2.09	0.65
1:D:143:LEU:HD23	1:D:144:PRO:HD2	1.79	0.65
1:E:117:PHE:HB2	1:E:123:LEU:HD13	1.78	0.65
1:F:36:VAL:HG12	1:F:37:ILE:N	2.11	0.65
1:B:53:ILE:HD12	1:B:53:ILE:N	2.08	0.65
1:I:167:GLU:O	1:I:169:CYS:N	2.30	0.65
1:E:36:VAL:HG12	1:E:37:ILE:N	2.11	0.65
1:E:140:ILE:HG13	1:F:3:VAL:HG21	1.79	0.65
1:B:61:LYS:O	1:B:65:GLU:HG3	1.97	0.65
1:C:74:SER:HB3	1:C:81:HIS:HE1	1.60	0.65
1:D:33:LYS:HB2	1:D:33:LYS:NZ	2.12	0.65
1:G:3:VAL:HG11	1:H:140:ILE:HD11	1.79	0.65
1:B:143:LEU:HB3	1:B:145:LEU:HD11	1.77	0.65
1:E:169:CYS:HG	1:F:49:CYS:HG	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:VAL:HG12	1:G:37:ILE:N	2.13	0.65
1:H:36:VAL:HG12	1:H:37:ILE:N	2.12	0.65
1:F:33:LYS:HB2	1:F:33:LYS:NZ	2.12	0.64
1:B:56:PHE:CZ	1:B:149:ALA:HA	2.33	0.64
1:C:6:LEU:HD23	1:C:7:ALA:O	1.97	0.64
1:C:36:VAL:HG12	1:C:37:ILE:N	2.12	0.64
1:B:33:LYS:HB2	1:B:33:LYS:NZ	2.12	0.64
1:C:57:ASP:O	1:C:60:VAL:HG22	1.98	0.64
1:F:143:LEU:HB3	1:F:145:LEU:HD11	1.79	0.64
1:A:36:VAL:HG12	1:A:37:ILE:N	2.13	0.64
1:D:169:CYS:HB2	1:D:170:PRO:CD	2.28	0.64
1:B:36:VAL:HG11	1:B:71:ILE:HD12	1.79	0.64
1:F:59:ARG:NH2	1:F:150:ASP:HB2	2.13	0.64
1:C:117:PHE:HB2	1:C:123:LEU:HD13	1.79	0.64
1:F:19:ASN:OD1	1:F:85:LYS:HD3	1.97	0.64
1:G:74:SER:HB3	1:G:81:HIS:HE1	1.62	0.64
1:I:57:ASP:O	1:I:60:VAL:HG22	1.98	0.64
1:I:3:VAL:CB	1:J:140:ILE:HD11	2.28	0.64
1:D:19:ASN:OD1	1:D:85:LYS:HD3	1.98	0.64
1:J:59:ARG:NH2	1:J:150:ASP:HB2	2.13	0.64
1:G:167:GLU:O	1:G:169:CYS:N	2.31	0.63
1:J:36:VAL:HG22	1:J:69:ASN:HB2	1.79	0.63
1:F:59:ARG:HH21	1:F:150:ASP:HB2	1.62	0.63
1:A:11:LYS:CE	1:A:24:HIS:HB3	2.28	0.63
1:I:36:VAL:HG12	1:I:37:ILE:N	2.13	0.63
1:D:11:LYS:HE3	1:D:24:HIS:HB3	1.81	0.63
1:A:3:VAL:CG2	1:B:140:ILE:HD11	2.28	0.63
1:E:167:GLU:O	1:E:169:CYS:N	2.30	0.63
1:G:117:PHE:HB2	1:G:123:LEU:HD13	1.80	0.63
1:C:167:GLU:O	1:C:169:CYS:N	2.32	0.63
1:H:169:CYS:HB2	1:H:170:PRO:CD	2.27	0.63
1:J:36:VAL:HG12	1:J:37:ILE:N	2.13	0.63
1:J:140:ILE:HD12	1:J:141:ASN:N	2.14	0.63
1:C:11:LYS:CE	1:C:24:HIS:HB3	2.29	0.63
1:E:33:LYS:HD2	1:E:67:GLY:HA2	1.81	0.63
1:G:33:LYS:HD2	1:G:67:GLY:HA2	1.81	0.63
1:A:167:GLU:O	1:A:169:CYS:N	2.32	0.63
1:J:61:LYS:O	1:J:65:GLU:HG3	1.99	0.63
1:C:8:PRO:HD2	1:C:113:TYR:CZ	2.33	0.62
1:C:140:ILE:HG13	1:D:3:VAL:HG21	1.80	0.62
1:J:59:ARG:HH21	1:J:150:ASP:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:CYS:HB2	1:B:170:PRO:CD	2.27	0.62
1:F:8:PRO:HG2	1:F:113:TYR:CE1	2.35	0.62
1:D:77:SER:OG	1:D:80:VAL:HG12	2.00	0.62
1:F:143:LEU:HG	1:F:144:PRO:HD2	1.80	0.62
1:C:142:ASP:CG	1:D:136:ARG:HH12	2.06	0.62
1:H:19:ASN:OD1	1:H:85:LYS:HD3	1.99	0.62
1:A:57:ASP:O	1:A:60:VAL:HG22	1.98	0.62
1:H:59:ARG:HH21	1:H:150:ASP:HB2	1.64	0.62
1:H:79:GLN:HG3	1:I:43:LYS:HD3	1.81	0.62
1:A:3:VAL:CG1	1:B:140:ILE:HD11	2.30	0.62
1:E:11:LYS:HE3	1:E:24:HIS:HB3	1.82	0.62
1:B:31:LEU:HA	1:B:36:VAL:HG21	1.81	0.62
1:G:11:LYS:CE	1:G:24:HIS:HB3	2.30	0.62
1:A:19:ASN:HD21	1:A:85:LYS:HE2	1.64	0.62
1:A:78:GLU:OE2	1:A:78:GLU:N	2.32	0.62
1:B:140:ILE:HD12	1:B:141:ASN:N	2.15	0.62
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.64	0.62
1:H:61:LYS:O	1:H:65:GLU:HG3	1.99	0.62
1:I:19:ASN:HD21	1:I:85:LYS:HE2	1.63	0.61
1:B:66:LYS:HE2	1:B:157:ASP:OD1	1.99	0.61
1:F:53:ILE:HD12	1:F:53:ILE:N	2.08	0.61
1:G:48:VAL:HG22	1:H:167:GLU:OE1	2.00	0.61
1:J:117:PHE:HB2	1:J:123:LEU:CD1	2.29	0.61
1:F:60:VAL:HG21	1:F:98:SER:OG	2.01	0.61
1:E:57:ASP:O	1:E:60:VAL:HG22	1.99	0.61
1:F:136:ARG:NH1	1:F:136:ARG:HB3	2.16	0.61
1:H:55:ALA:O	1:H:59:ARG:HD3	2.01	0.61
1:I:11:LYS:HE3	1:I:24:HIS:HB3	1.82	0.61
1:I:23:GLU:HA	1:I:23:GLU:OE1	2.01	0.61
1:I:33:LYS:HD2	1:I:67:GLY:HA2	1.81	0.61
1:J:1:MET:HE2	1:J:5:LYS:HE3	1.81	0.61
1:B:55:ALA:O	1:B:59:ARG:HD3	2.01	0.60
1:F:136:ARG:HH11	1:F:136:ARG:CA	2.13	0.60
1:H:33:LYS:HB2	1:H:33:LYS:HZ2	1.65	0.60
1:H:42:PRO:HB3	1:H:121:ILE:HD12	1.82	0.60
1:I:31:LEU:HA	1:I:36:VAL:CG2	2.31	0.60
1:A:78:GLU:CD	1:A:79:GLN:HE21	2.08	0.60
1:G:11:LYS:HE3	1:G:24:HIS:HB3	1.82	0.60
1:G:141:ASN:HB3	1:H:137:HIS:CD2	2.37	0.60
1:B:36:VAL:HG12	1:B:37:ILE:N	2.16	0.60
1:H:56:PHE:CZ	1:H:149:ALA:HA	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:VAL:O	1:B:169:CYS:HB3	2.00	0.60
1:G:33:LYS:HE3	1:G:67:GLY:HA2	1.82	0.60
1:G:85:LYS:HA	1:G:94:ILE:CG2	2.29	0.60
1:I:85:LYS:HA	1:I:94:ILE:CG2	2.31	0.60
1:J:159:LEU:O	1:J:163:GLU:HB2	2.02	0.60
1:C:33:LYS:HD2	1:C:67:GLY:HA2	1.82	0.60
1:I:41:TRP:CE2	1:I:74:SER:HB2	2.37	0.60
1:J:77:SER:OG	1:J:80:VAL:HG12	2.02	0.60
1:C:19:ASN:HD21	1:C:85:LYS:HE2	1.66	0.60
1:D:59:ARG:HH21	1:D:150:ASP:HB2	1.67	0.60
1:E:31:LEU:HA	1:E:36:VAL:CG2	2.32	0.60
1:A:41:TRP:CE2	1:A:74:SER:HB2	2.36	0.60
1:B:77:SER:OG	1:B:80:VAL:HG12	2.01	0.60
1:D:53:ILE:HD12	1:D:53:ILE:N	2.13	0.60
1:I:168:VAL:HG12	2:I:200:HOH:O	2.02	0.60
1:A:117:PHE:HB2	1:A:123:LEU:HD13	1.84	0.59
1:B:31:LEU:HA	1:B:36:VAL:CG2	2.31	0.59
1:D:33:LYS:HG3	1:D:34:ASN:ND2	2.16	0.59
1:H:143:LEU:HD23	1:H:144:PRO:HD2	1.84	0.59
1:J:164:GLU:C	1:J:166:GLY:H	2.10	0.59
1:C:50:PRO:O	1:C:52:GLU:N	2.34	0.59
1:E:31:LEU:N	1:E:31:LEU:HD22	2.17	0.59
1:F:87:THR:O	1:F:93:GLY:HA3	2.02	0.59
1:G:57:ASP:O	1:G:60:VAL:HG22	2.01	0.59
1:J:36:VAL:HG13	1:J:69:ASN:O	2.02	0.59
1:C:78:GLU:HG2	1:C:79:GLN:NE2	2.18	0.59
1:E:117:PHE:HB2	1:E:123:LEU:CD1	2.33	0.59
1:G:41:TRP:CE2	1:G:74:SER:HB2	2.37	0.59
1:I:31:LEU:N	1:I:31:LEU:HD22	2.18	0.59
1:A:6:LEU:HD23	1:A:7:ALA:O	2.02	0.59
1:A:140:ILE:HD12	1:A:141:ASN:N	2.17	0.59
1:D:169:CYS:CB	1:D:170:PRO:HD2	2.30	0.59
1:G:3:VAL:C	1:G:4:THR:HG23	2.28	0.59
1:C:3:VAL:C	1:C:4:THR:HG23	2.28	0.59
1:D:135:VAL:HG23	1:D:135:VAL:O	2.02	0.59
1:J:151:GLU:HA	1:J:154:ARG:NH1	2.18	0.59
1:A:11:LYS:HE3	1:A:24:HIS:HB3	1.84	0.59
1:D:174:ARG:HG3	1:D:174:ARG:HH11	1.66	0.59
1:G:3:VAL:CB	1:H:140:ILE:HD11	2.32	0.59
1:J:169:CYS:HB2	1:J:170:PRO:CD	2.28	0.59
1:B:33:LYS:HB2	1:B:33:LYS:HZ2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:LEU:HG	1:J:144:PRO:HD2	1.82	0.59
1:I:78:GLU:OE2	1:I:78:GLU:N	2.33	0.59
1:A:85:LYS:HA	1:A:94:ILE:CG2	2.32	0.59
1:H:164:GLU:C	1:H:166:GLY:H	2.11	0.59
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.03	0.58
1:F:174:ARG:HG3	1:F:174:ARG:HH11	1.68	0.58
1:H:143:LEU:HB3	1:H:145:LEU:CD1	2.32	0.58
1:H:169:CYS:CB	1:H:170:PRO:HD2	2.28	0.58
1:I:117:PHE:HB2	1:I:123:LEU:HD13	1.84	0.58
1:B:43:LYS:HD2	1:C:79:GLN:CG	2.33	0.58
1:D:31:LEU:HA	1:D:36:VAL:HG21	1.85	0.58
1:G:31:LEU:HA	1:G:36:VAL:CG2	2.32	0.58
1:J:33:LYS:HB2	1:J:33:LYS:HZ2	1.66	0.58
1:A:68:PHE:CE2	1:A:156:VAL:HG13	2.39	0.58
1:I:117:PHE:HB2	1:I:123:LEU:CD1	2.34	0.58
1:I:144:PRO:O	1:I:146:GLY:N	2.37	0.58
1:J:44:ASP:HA	1:J:84:TRP:CZ3	2.39	0.58
1:A:33:LYS:HE3	1:A:67:GLY:HA2	1.86	0.58
1:C:11:LYS:HE3	1:C:24:HIS:HB3	1.84	0.58
1:E:78:GLU:OE2	1:E:78:GLU:N	2.33	0.58
1:I:3:VAL:C	1:I:4:THR:HG23	2.28	0.58
1:C:85:LYS:HA	1:C:94:ILE:CG2	2.31	0.58
1:D:36:VAL:HG12	1:D:37:ILE:N	2.18	0.58
1:H:31:LEU:HA	1:H:36:VAL:HG21	1.86	0.58
1:G:117:PHE:HB2	1:G:123:LEU:CD1	2.34	0.58
1:H:74:SER:HB3	1:H:81:HIS:HE1	1.68	0.58
1:H:143:LEU:CB	1:H:145:LEU:HD11	2.34	0.58
1:C:6:LEU:HD23	1:C:6:LEU:C	2.29	0.58
1:E:23:GLU:OE1	1:E:23:GLU:HA	2.03	0.58
1:E:41:TRP:CE2	1:E:74:SER:HB2	2.38	0.58
1:F:123:LEU:HD23	1:F:140:ILE:HD13	1.86	0.58
1:G:23:GLU:OE1	1:G:23:GLU:HA	2.03	0.58
1:H:174:ARG:HG3	1:H:174:ARG:HH11	1.68	0.58
1:I:48:VAL:HG22	1:J:167:GLU:OE1	2.04	0.58
1:D:164:GLU:C	1:D:166:GLY:H	2.11	0.58
1:C:144:PRO:O	1:C:146:GLY:N	2.37	0.57
1:G:33:LYS:CE	1:G:67:GLY:HA2	2.34	0.57
1:I:141:ASN:HB3	1:J:137:HIS:CD2	2.39	0.57
1:J:52:GLU:HG2	1:J:124:ARG:NH1	2.18	0.57
1:D:161:HIS:HB3	1:D:165:HIS:HE1	1.69	0.57
1:D:168:VAL:O	1:D:169:CYS:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:LEU:HA	1:J:36:VAL:CG2	2.35	0.57
1:A:3:VAL:C	1:A:4:THR:HG23	2.29	0.57
1:H:36:VAL:CG1	1:H:37:ILE:N	2.67	0.57
1:J:90:GLU:CD	1:J:90:GLU:H	2.12	0.57
1:A:6:LEU:HD23	1:A:6:LEU:C	2.29	0.57
1:A:31:LEU:HA	1:A:36:VAL:CG2	2.34	0.57
1:B:59:ARG:NH2	1:B:150:ASP:HB2	2.18	0.57
1:B:143:LEU:HD23	1:B:144:PRO:HD2	1.87	0.57
1:C:41:TRP:CE2	1:C:74:SER:HB2	2.40	0.57
1:I:33:LYS:HE3	1:I:67:GLY:HA2	1.86	0.57
1:A:89:VAL:HG23	1:B:172:GLY:O	2.05	0.57
1:B:50:PRO:O	1:B:51:THR:C	2.47	0.57
1:F:36:VAL:CG1	1:F:37:ILE:N	2.66	0.57
1:G:19:ASN:HD21	1:G:85:LYS:HE2	1.69	0.57
1:J:40:PHE:CD2	1:J:73:VAL:HG22	2.39	0.57
1:C:152:MET:O	1:C:156:VAL:HG23	2.05	0.57
1:D:69:ASN:HB3	2:D:200:HOH:O	2.03	0.57
1:E:48:VAL:HG22	1:F:167:GLU:OE1	2.04	0.57
1:E:50:PRO:O	1:E:52:GLU:N	2.38	0.57
1:B:139:VAL:HG12	1:B:152:MET:HE3	1.87	0.57
1:C:89:VAL:HG23	1:D:172:GLY:O	2.05	0.57
1:D:143:LEU:HB3	1:D:145:LEU:CD1	2.34	0.57
1:D:143:LEU:CD2	1:D:144:PRO:HD2	2.34	0.57
1:E:3:VAL:C	1:E:4:THR:HG23	2.30	0.57
1:E:144:PRO:O	1:E:146:GLY:N	2.38	0.57
1:G:6:LEU:HD23	1:G:7:ALA:O	2.04	0.57
1:A:50:PRO:O	1:A:52:GLU:N	2.37	0.57
1:A:82:PHE:CE2	1:A:86:ASN:ND2	2.73	0.57
1:B:135:VAL:HG23	1:B:135:VAL:O	2.03	0.57
1:B:143:LEU:CB	1:B:144:PRO:HD2	2.35	0.57
1:F:50:PRO:O	1:F:51:THR:C	2.47	0.57
1:F:66:LYS:HE2	1:F:157:ASP:OD1	2.04	0.57
1:F:135:VAL:HG23	1:F:135:VAL:O	2.04	0.57
1:G:164:GLU:HB2	1:G:165:HIS:ND1	2.20	0.57
1:C:169:CYS:HG	1:D:49:CYS:HG	1.51	0.57
1:D:36:VAL:HG13	1:D:69:ASN:O	2.03	0.57
1:D:148:ASN:HA	1:D:151:GLU:HB3	1.86	0.57
1:D:136:ARG:NH1	1:D:136:ARG:HB3	2.20	0.57
1:B:36:VAL:CG1	1:B:37:ILE:N	2.67	0.56
1:D:66:LYS:HE2	1:D:157:ASP:OD1	2.05	0.56
1:D:90:GLU:H	1:D:90:GLU:CD	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:PRO:O	1:G:52:GLU:N	2.38	0.56
1:H:31:LEU:HA	1:H:36:VAL:CG2	2.34	0.56
1:H:148:ASN:HA	1:H:151:GLU:HB3	1.87	0.56
1:C:31:LEU:HA	1:C:36:VAL:CG2	2.35	0.56
1:A:78:GLU:HG2	1:A:79:GLN:NE2	2.20	0.56
1:A:144:PRO:O	1:A:146:GLY:N	2.38	0.56
1:A:164:GLU:HB2	1:A:165:HIS:ND1	2.20	0.56
1:B:169:CYS:CB	1:B:170:PRO:HD2	2.31	0.56
1:D:152:MET:O	1:D:156:VAL:HG23	2.05	0.56
1:E:33:LYS:HE3	1:E:67:GLY:HA2	1.86	0.56
1:E:35:GLY:HA3	1:E:129:ILE:O	2.06	0.56
1:G:28:SER:C	1:G:31:LEU:HD21	2.31	0.56
1:H:43:LYS:HD2	1:I:79:GLN:CG	2.35	0.56
1:H:159:LEU:O	1:H:163:GLU:HB2	2.05	0.56
1:J:174:ARG:HG3	1:J:174:ARG:HH11	1.69	0.56
1:F:137:HIS:CE1	1:F:155:MET:HG3	2.40	0.56
1:H:50:PRO:O	1:H:51:THR:C	2.48	0.56
1:B:151:GLU:OE1	1:B:151:GLU:C	2.48	0.56
1:C:78:GLU:OE2	1:C:78:GLU:N	2.35	0.56
1:F:164:GLU:C	1:F:166:GLY:H	2.13	0.56
1:G:3:VAL:HG12	1:G:4:THR:HG23	1.88	0.56
1:G:35:GLY:HA3	1:G:129:ILE:O	2.06	0.56
1:I:46:THR:OG1	1:I:48:VAL:HG12	2.06	0.56
1:I:78:GLU:CD	1:I:79:GLN:HE21	2.13	0.56
1:J:159:LEU:O	1:J:159:LEU:HD23	2.05	0.56
1:B:168:VAL:HG22	1:B:169:CYS:N	2.21	0.56
1:C:3:VAL:HG12	1:C:4:THR:HG23	1.87	0.56
1:G:6:LEU:HD23	1:G:6:LEU:C	2.31	0.56
1:H:117:PHE:HB2	1:H:123:LEU:CD1	2.34	0.56
1:J:36:VAL:CG1	1:J:37:ILE:N	2.69	0.56
1:A:33:LYS:CE	1:A:67:GLY:HA2	2.36	0.56
1:F:56:PHE:CZ	1:F:149:ALA:HA	2.41	0.56
1:F:168:VAL:O	1:F:169:CYS:HB3	2.05	0.56
1:H:54:ILE:O	1:H:58:LYS:HG2	2.05	0.56
1:H:168:VAL:HG22	1:H:169:CYS:N	2.20	0.56
1:I:35:GLY:HA3	1:I:129:ILE:O	2.05	0.56
1:C:23:GLU:OE1	1:C:23:GLU:HA	2.06	0.56
1:F:31:LEU:HA	1:F:36:VAL:HG21	1.88	0.56
1:H:66:LYS:HE2	1:H:157:ASP:OD1	2.06	0.56
1:D:85:LYS:HE2	1:D:97:VAL:CG2	2.36	0.56
1:F:169:CYS:CB	1:F:170:PRO:HD2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLU:CD	1:H:90:GLU:H	2.14	0.56
1:J:151:GLU:C	1:J:151:GLU:OE1	2.49	0.56
1:B:52:GLU:HB2	1:B:53:ILE:HD12	1.88	0.55
1:C:68:PHE:CE2	1:C:156:VAL:HG13	2.41	0.55
1:C:78:GLU:CD	1:C:79:GLN:HE21	2.14	0.55
1:E:85:LYS:HE3	1:E:97:VAL:HG22	1.88	0.55
1:F:90:GLU:H	1:F:90:GLU:CD	2.13	0.55
1:J:169:CYS:CB	1:J:170:PRO:HD2	2.31	0.55
1:A:168:VAL:O	1:A:168:VAL:HG13	2.05	0.55
1:D:31:LEU:HA	1:D:36:VAL:CG2	2.35	0.55
1:D:79:GLN:HG3	1:E:43:LYS:HD3	1.88	0.55
1:E:164:GLU:HB2	1:E:165:HIS:ND1	2.22	0.55
1:G:152:MET:O	1:G:156:VAL:HG23	2.06	0.55
1:A:66:LYS:HE2	2:A:199:HOH:O	2.05	0.55
1:B:44:ASP:HA	1:B:84:TRP:CZ3	2.40	0.55
1:E:21:VAL:HG13	1:E:21:VAL:O	2.06	0.55
1:E:152:MET:O	1:E:156:VAL:HG23	2.06	0.55
1:I:3:VAL:CG1	1:J:140:ILE:HD11	2.36	0.55
1:J:42:PRO:HB3	1:J:121:ILE:HD12	1.89	0.55
1:J:161:HIS:HB3	1:J:165:HIS:HE1	1.71	0.55
1:C:117:PHE:HB2	1:C:123:LEU:CD1	2.36	0.55
1:C:164:GLU:HB2	1:C:165:HIS:ND1	2.22	0.55
1:E:78:GLU:HG2	1:E:79:GLN:NE2	2.22	0.55
1:D:88:PRO:CG	1:D:91:LYS:HD2	2.36	0.55
1:G:89:VAL:HG23	1:H:172:GLY:O	2.07	0.55
1:J:143:LEU:HB3	1:J:145:LEU:CD1	2.36	0.55
1:J:143:LEU:CB	1:J:144:PRO:HD2	2.37	0.55
1:B:148:ASN:HA	1:B:151:GLU:HB3	1.88	0.55
1:B:164:GLU:C	1:B:166:GLY:H	2.13	0.55
1:B:173:TRP:HB3	2:B:199:HOH:O	2.06	0.55
1:C:48:VAL:HG22	1:D:167:GLU:OE1	2.07	0.55
1:D:59:ARG:NH2	1:D:150:ASP:HB2	2.22	0.55
1:F:169:CYS:HB2	1:F:170:PRO:CD	2.29	0.55
1:G:78:GLU:HG2	1:G:79:GLN:NE2	2.22	0.55
1:I:6:LEU:C	1:I:6:LEU:HD23	2.32	0.55
1:I:11:LYS:HE2	1:I:24:HIS:HB3	1.89	0.55
1:A:3:VAL:HG21	1:B:140:ILE:CD1	2.37	0.55
1:E:28:SER:C	1:E:31:LEU:HD21	2.32	0.55
1:E:85:LYS:HA	1:E:94:ILE:CG2	2.33	0.55
1:G:3:VAL:HG12	1:G:4:THR:CG2	2.37	0.55
1:A:28:SER:C	1:A:31:LEU:HD21	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLU:CD	1:B:90:GLU:H	2.15	0.55
1:E:74:SER:HB3	1:E:81:HIS:CE1	2.42	0.55
1:G:144:PRO:O	1:G:146:GLY:N	2.40	0.55
1:I:140:ILE:HG13	1:J:3:VAL:HG21	1.88	0.55
1:A:117:PHE:HB2	1:A:123:LEU:CD1	2.37	0.55
1:D:35:GLY:O	1:D:36:VAL:HG23	2.07	0.55
1:F:23:GLU:HA	1:F:23:GLU:OE1	2.06	0.55
1:G:131:LYS:HD2	1:G:131:LYS:N	2.22	0.55
1:H:168:VAL:O	1:H:169:CYS:HB3	2.07	0.55
1:I:3:VAL:HG12	1:I:4:THR:HG23	1.88	0.55
1:I:164:GLU:HB2	1:I:165:HIS:ND1	2.22	0.55
1:G:31:LEU:HD22	1:G:31:LEU:N	2.21	0.55
1:J:50:PRO:O	1:J:51:THR:C	2.49	0.55
1:E:31:LEU:HD22	1:E:31:LEU:H	1.72	0.54
1:E:78:GLU:CD	1:E:79:GLN:HE21	2.14	0.54
1:H:143:LEU:HG	1:H:144:PRO:HD2	1.90	0.54
1:I:131:LYS:HD2	1:I:131:LYS:N	2.22	0.54
1:I:168:VAL:O	1:I:168:VAL:HG13	2.07	0.54
1:B:77:SER:OG	1:B:79:GLN:HG2	2.07	0.54
1:D:143:LEU:CB	1:D:145:LEU:HD11	2.34	0.54
1:E:33:LYS:CE	1:E:67:GLY:HA2	2.38	0.54
1:H:59:ARG:NH2	1:H:150:ASP:HB2	2.21	0.54
1:I:6:LEU:HD23	1:I:7:ALA:O	2.08	0.54
1:J:23:GLU:OE1	1:J:23:GLU:HA	2.07	0.54
1:C:35:GLY:HA3	1:C:129:ILE:O	2.07	0.54
1:D:36:VAL:CG1	1:D:37:ILE:N	2.69	0.54
1:D:50:PRO:O	1:D:51:THR:C	2.51	0.54
1:E:16:LEU:HB3	2:E:203:HOH:O	2.07	0.54
1:G:68:PHE:CE2	1:G:156:VAL:HG13	2.42	0.54
1:G:168:VAL:O	1:G:168:VAL:HG13	2.07	0.54
1:J:152:MET:O	1:J:156:VAL:HG23	2.08	0.54
1:A:3:VAL:HG12	1:A:4:THR:HG23	1.90	0.54
1:C:3:VAL:CB	1:D:140:ILE:HD11	2.36	0.54
1:C:33:LYS:HE3	1:C:67:GLY:HA2	1.88	0.54
1:C:140:ILE:HD12	1:C:141:ASN:N	2.22	0.54
1:B:148:ASN:HD22	1:B:149:ALA:N	2.06	0.54
1:I:3:VAL:HG21	1:J:140:ILE:HD11	1.89	0.54
1:I:68:PHE:CE2	1:I:156:VAL:HG13	2.43	0.54
1:A:21:VAL:O	1:A:21:VAL:HG13	2.08	0.54
1:A:31:LEU:N	1:A:31:LEU:HD22	2.23	0.54
1:I:28:SER:C	1:I:31:LEU:HD21	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:SER:HB3	1:I:81:HIS:CE1	2.41	0.54
1:I:78:GLU:HG2	1:I:79:GLN:NE2	2.23	0.54
1:B:107:LYS:HB2	1:B:111:ARG:NH2	2.23	0.54
1:E:168:VAL:HG13	1:E:168:VAL:O	2.07	0.54
1:G:85:LYS:HE3	1:G:97:VAL:HG22	1.90	0.54
1:A:56:PHE:O	1:A:60:VAL:HG13	2.08	0.54
1:C:168:VAL:HG13	1:C:168:VAL:O	2.06	0.54
1:E:6:LEU:HD23	1:E:7:ALA:O	2.07	0.54
1:F:12:ALA:HB1	1:F:13:PRO:HD2	1.90	0.54
1:H:151:GLU:HA	1:H:154:ARG:NH1	2.23	0.54
1:I:33:LYS:CE	1:I:67:GLY:HA2	2.38	0.54
1:I:89:VAL:HG23	1:J:172:GLY:O	2.08	0.54
1:A:35:GLY:HA3	1:A:129:ILE:O	2.07	0.54
1:B:60:VAL:HG21	1:B:98:SER:OG	2.08	0.54
1:D:85:LYS:HE2	1:D:97:VAL:HG22	1.90	0.54
1:D:88:PRO:HG2	1:D:91:LYS:HD2	1.89	0.54
1:E:140:ILE:HD12	1:E:141:ASN:N	2.23	0.54
1:F:43:LYS:HD2	1:G:79:GLN:CG	2.37	0.54
1:G:78:GLU:CD	1:G:79:GLN:HE21	2.15	0.54
1:A:43:LYS:HD3	1:J:79:GLN:HG3	1.89	0.54
1:E:19:ASN:HD21	1:E:85:LYS:HE2	1.73	0.54
1:F:31:LEU:HA	1:F:36:VAL:CG2	2.38	0.54
1:G:78:GLU:OE2	1:G:78:GLU:N	2.34	0.54
1:I:50:PRO:O	1:I:52:GLU:N	2.40	0.54
1:B:1:MET:HE2	1:B:5:LYS:HE3	1.90	0.53
1:B:136:ARG:HH11	1:B:136:ARG:CA	2.20	0.53
1:C:82:PHE:CE2	1:C:86:ASN:ND2	2.76	0.53
1:F:139:VAL:O	1:F:139:VAL:HG13	2.08	0.53
1:J:139:VAL:HG12	1:J:152:MET:HE3	1.89	0.53
1:J:143:LEU:CB	1:J:145:LEU:HD11	2.38	0.53
1:A:66:LYS:HE2	1:A:157:ASP:OD1	2.08	0.53
1:C:157:ASP:O	1:C:158:ALA:C	2.51	0.53
1:E:66:LYS:HE2	1:E:157:ASP:OD1	2.09	0.53
1:E:68:PHE:CE2	1:E:156:VAL:HG13	2.42	0.53
1:E:89:VAL:HG23	1:F:172:GLY:O	2.08	0.53
1:I:140:ILE:HD12	1:I:141:ASN:N	2.23	0.53
1:J:135:VAL:HG23	1:J:135:VAL:O	2.08	0.53
1:C:28:SER:C	1:C:31:LEU:HD21	2.33	0.53
1:C:74:SER:HB3	1:C:81:HIS:CE1	2.42	0.53
1:F:162:PHE:O	1:F:166:GLY:HA2	2.07	0.53
1:A:142:ASP:OD1	1:B:136:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:HB1	1:B:149:ALA:HB3	1.89	0.53
1:C:128:LEU:CB	1:C:152:MET:HE1	2.36	0.53
1:J:8:PRO:HG2	1:J:113:TYR:CE1	2.44	0.53
1:B:159:LEU:O	1:B:163:GLU:HB2	2.08	0.53
1:C:33:LYS:CE	1:C:67:GLY:HA2	2.39	0.53
1:D:159:LEU:O	1:D:163:GLU:HB2	2.09	0.53
1:F:52:GLU:HB2	1:F:53:ILE:HD12	1.91	0.53
1:J:31:LEU:HA	1:J:36:VAL:HG21	1.89	0.53
1:A:131:LYS:N	1:A:131:LYS:HD2	2.23	0.53
1:B:35:GLY:O	1:B:36:VAL:HG23	2.09	0.53
1:B:143:LEU:HB2	2:B:201:HOH:O	2.08	0.53
1:C:3:VAL:HG12	1:C:4:THR:CG2	2.38	0.53
1:I:3:VAL:HG12	1:I:4:THR:CG2	2.39	0.53
1:J:74:SER:HB3	1:J:81:HIS:HE1	1.74	0.53
1:A:46:THR:OG1	1:A:48:VAL:HG12	2.09	0.53
1:G:66:LYS:HE2	1:G:157:ASP:OD1	2.09	0.53
1:J:77:SER:OG	1:J:79:GLN:HG2	2.09	0.53
1:A:157:ASP:O	1:A:158:ALA:C	2.51	0.52
1:C:31:LEU:N	1:C:31:LEU:HD22	2.24	0.52
1:E:3:VAL:HG12	1:E:4:THR:HG23	1.91	0.52
1:E:11:LYS:HE2	1:E:24:HIS:HB3	1.90	0.52
1:H:52:GLU:HG2	1:H:124:ARG:HH11	1.72	0.52
1:J:162:PHE:O	1:J:166:GLY:HA2	2.08	0.52
1:A:74:SER:HB3	1:A:81:HIS:CE1	2.42	0.52
1:A:147:ARG:HH11	1:A:147:ARG:CB	2.20	0.52
1:C:3:VAL:CG1	1:D:140:ILE:HD11	2.39	0.52
1:D:23:GLU:HA	1:D:23:GLU:OE1	2.09	0.52
1:E:3:VAL:CB	1:F:140:ILE:HD11	2.38	0.52
1:E:131:LYS:HD2	1:E:131:LYS:N	2.23	0.52
1:G:3:VAL:CG1	1:H:140:ILE:HD11	2.39	0.52
1:J:54:ILE:O	1:J:58:LYS:HG2	2.09	0.52
1:B:85:LYS:HE2	1:B:97:VAL:CG2	2.40	0.52
1:F:48:VAL:CG2	1:F:49:CYS:H	2.14	0.52
1:J:137:HIS:CE1	1:J:155:MET:HG3	2.44	0.52
1:C:25:PHE:C	1:C:25:PHE:CD2	2.87	0.52
1:E:128:LEU:CB	1:E:152:MET:HE1	2.36	0.52
1:F:48:VAL:HG13	1:F:49:CYS:H	1.73	0.52
1:F:148:ASN:HA	1:F:151:GLU:HB3	1.90	0.52
1:G:128:LEU:CB	1:G:152:MET:HE1	2.38	0.52
1:G:140:ILE:HD12	1:G:141:ASN:N	2.24	0.52
1:H:136:ARG:HB3	1:H:136:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:LEU:HD22	1:I:31:LEU:H	1.74	0.52
1:G:56:PHE:O	1:G:60:VAL:HG13	2.10	0.52
1:J:161:HIS:HB3	1:J:165:HIS:CE1	2.44	0.52
1:A:49:CYS:HB3	1:A:51:THR:HG23	1.92	0.52
1:B:54:ILE:O	1:B:58:LYS:HG2	2.10	0.52
1:F:77:SER:O	1:F:80:VAL:HG13	2.08	0.52
1:F:159:LEU:O	1:F:163:GLU:HB2	2.09	0.52
1:D:143:LEU:HG	1:D:144:PRO:HD2	1.90	0.52
1:F:168:VAL:HG22	1:F:169:CYS:N	2.25	0.52
1:H:143:LEU:CD2	1:H:144:PRO:HD2	2.39	0.52
1:E:3:VAL:CG1	1:F:140:ILE:HD11	2.39	0.52
1:F:139:VAL:HG12	1:F:152:MET:HE3	1.92	0.52
1:G:142:ASP:OD1	1:H:136:ARG:NH1	2.40	0.52
1:J:168:VAL:O	1:J:169:CYS:HB3	2.10	0.52
1:G:11:LYS:HA	1:G:25:PHE:O	2.09	0.52
1:H:53:ILE:HD12	1:H:53:ILE:N	2.12	0.52
1:I:66:LYS:HE2	1:I:157:ASP:OD1	2.10	0.52
1:B:85:LYS:HE2	1:B:97:VAL:HG22	1.92	0.51
1:B:143:LEU:HG	1:B:144:PRO:HD2	1.90	0.51
1:C:46:THR:OG1	1:C:48:VAL:HG12	2.10	0.51
1:H:168:VAL:HG22	1:H:169:CYS:H	1.76	0.51
1:J:60:VAL:HG23	1:J:61:LYS:HE2	1.91	0.51
1:F:33:LYS:HB2	1:F:33:LYS:HZ2	1.75	0.51
1:D:143:LEU:CB	1:D:144:PRO:HD2	2.40	0.51
1:G:21:VAL:HG13	1:G:21:VAL:O	2.10	0.51
1:H:77:SER:O	1:H:80:VAL:HG13	2.11	0.51
1:I:1:MET:HE2	1:J:114:ASP:O	2.10	0.51
1:A:3:VAL:HB	1:B:140:ILE:HD11	1.93	0.51
1:A:152:MET:O	1:A:156:VAL:HG23	2.10	0.51
1:C:66:LYS:HE2	1:C:157:ASP:OD1	2.09	0.51
1:E:3:VAL:HG12	1:E:4:THR:CG2	2.40	0.51
1:G:46:THR:OG1	1:G:48:VAL:HG12	2.09	0.51
1:H:75:ILE:HD12	1:H:75:ILE:C	2.35	0.51
1:H:88:PRO:CG	1:H:91:LYS:HD2	2.41	0.51
1:E:60:VAL:HG23	1:E:61:LYS:N	2.25	0.51
1:H:57:ASP:O	1:H:60:VAL:HG22	2.10	0.51
1:A:8:PRO:HD2	1:A:113:TYR:CZ	2.45	0.51
1:C:56:PHE:O	1:C:60:VAL:HG13	2.10	0.51
1:C:150:ASP:OD2	1:C:154:ARG:HD2	2.10	0.51
1:E:6:LEU:HD23	1:E:6:LEU:C	2.34	0.51
1:E:47:PHE:C	1:F:173:TRP:HH2	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:CG2	1:B:49:CYS:H	2.13	0.51
1:D:148:ASN:N	1:D:148:ASN:HD22	2.07	0.51
1:E:56:PHE:O	1:E:60:VAL:HG13	2.11	0.51
1:E:157:ASP:O	1:E:158:ALA:C	2.52	0.51
1:G:157:ASP:O	1:G:158:ALA:C	2.53	0.51
1:H:159:LEU:O	1:H:159:LEU:HD23	2.10	0.51
1:I:169:CYS:SG	1:J:49:CYS:SG	3.01	0.51
1:A:3:VAL:HG12	1:A:4:THR:CG2	2.40	0.51
1:C:131:LYS:HD2	1:C:131:LYS:N	2.26	0.51
1:E:11:LYS:HA	1:E:25:PHE:O	2.10	0.51
1:F:77:SER:OG	1:F:79:GLN:HG2	2.11	0.51
1:G:8:PRO:HD2	1:G:113:TYR:CZ	2.46	0.51
1:H:161:HIS:HB3	1:H:165:HIS:HE1	1.75	0.51
1:J:3:VAL:C	1:J:4:THR:HG23	2.36	0.51
1:F:159:LEU:O	1:F:159:LEU:HD23	2.10	0.51
1:J:11:LYS:HE3	1:J:24:HIS:HB3	1.91	0.51
1:B:143:LEU:CD2	1:B:144:PRO:HD2	2.40	0.50
1:F:55:ALA:HB1	1:F:149:ALA:HB3	1.94	0.50
1:H:35:GLY:C	1:H:36:VAL:HG23	2.35	0.50
1:I:152:MET:O	1:I:156:VAL:HG23	2.10	0.50
1:I:157:ASP:O	1:I:158:ALA:C	2.54	0.50
1:B:168:VAL:HG22	1:B:169:CYS:H	1.76	0.50
1:E:46:THR:OG1	1:E:48:VAL:HG12	2.11	0.50
1:F:85:LYS:HA	1:F:94:ILE:CG2	2.40	0.50
1:F:143:LEU:HB3	1:F:145:LEU:CD1	2.42	0.50
1:H:3:VAL:C	1:H:4:THR:HG23	2.36	0.50
1:H:23:GLU:OE1	1:H:23:GLU:HA	2.10	0.50
1:I:85:LYS:HE3	1:I:97:VAL:HG22	1.94	0.50
1:F:40:PHE:CD2	1:F:73:VAL:HG22	2.46	0.50
1:A:131:LYS:HD2	1:A:131:LYS:H	1.75	0.50
1:B:79:GLN:CG	1:C:43:LYS:HD3	2.41	0.50
1:B:143:LEU:CB	1:B:145:LEU:HD11	2.42	0.50
1:C:85:LYS:HE3	1:C:97:VAL:HG22	1.92	0.50
1:D:12:ALA:HB1	1:D:13:PRO:HD2	1.93	0.50
1:J:36:VAL:HG11	1:J:71:ILE:HD12	1.93	0.50
1:A:79:GLN:CG	1:J:43:LYS:HD2	2.41	0.50
1:A:85:LYS:HE3	1:A:97:VAL:HG22	1.93	0.50
1:B:35:GLY:C	1:B:36:VAL:HG23	2.36	0.50
1:H:152:MET:O	1:H:156:VAL:HG23	2.11	0.50
1:I:11:LYS:HA	1:I:25:PHE:O	2.11	0.50
1:B:11:LYS:HA	1:B:25:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HG23	1:B:95:GLY:O	2.11	0.50
1:E:75:ILE:HG13	2:E:199:HOH:O	2.11	0.50
1:J:31:LEU:HD22	1:J:36:VAL:CG2	2.42	0.50
1:A:11:LYS:HE2	1:A:24:HIS:HB3	1.92	0.50
1:A:150:ASP:OD2	1:A:154:ARG:HD2	2.12	0.50
1:E:141:ASN:HB3	1:F:137:HIS:CD2	2.46	0.50
1:E:147:ARG:HH11	1:E:147:ARG:CB	2.20	0.50
1:I:142:ASP:OD1	1:J:136:ARG:NH1	2.42	0.50
1:C:60:VAL:HG23	1:C:61:LYS:N	2.27	0.50
1:D:8:PRO:HG2	1:D:113:TYR:CE1	2.47	0.50
1:F:42:PRO:HD3	1:F:124:ARG:HG3	1.93	0.50
1:F:148:ASN:N	1:F:148:ASN:HD22	2.09	0.50
1:G:60:VAL:HG23	1:G:61:LYS:N	2.26	0.50
1:C:169:CYS:SG	1:D:49:CYS:SG	3.01	0.49
1:F:42:PRO:HB3	1:F:121:ILE:HD12	1.94	0.49
1:J:142:ASP:C	1:J:142:ASP:OD2	2.55	0.49
1:A:48:VAL:HG22	1:B:167:GLU:OE1	2.12	0.49
1:B:2:VAL:O	1:B:135:VAL:CG2	2.60	0.49
1:C:21:VAL:O	1:C:21:VAL:HG13	2.12	0.49
1:C:59:ARG:HG3	1:C:59:ARG:HH11	1.77	0.49
1:G:82:PHE:CE2	1:G:86:ASN:ND2	2.79	0.49
1:H:11:LYS:HA	1:H:25:PHE:O	2.12	0.49
1:B:60:VAL:HG23	1:B:61:LYS:HE2	1.93	0.49
1:D:161:HIS:HB3	1:D:165:HIS:CE1	2.46	0.49
1:E:142:ASP:OD1	1:F:136:ARG:NH1	2.45	0.49
1:F:151:GLU:HA	1:F:154:ARG:NH1	2.26	0.49
1:I:60:VAL:HG23	1:I:61:LYS:N	2.27	0.49
1:A:128:LEU:CB	1:A:152:MET:HE1	2.41	0.49
1:D:148:ASN:N	1:D:148:ASN:ND2	2.61	0.49
1:E:85:LYS:HE3	1:E:97:VAL:H	1.78	0.49
1:F:59:ARG:NH2	1:F:150:ASP:CB	2.76	0.49
1:H:40:PHE:CD2	1:H:73:VAL:HG22	2.47	0.49
1:I:56:PHE:O	1:I:60:VAL:HG13	2.12	0.49
1:E:147:ARG:O	1:E:151:GLU:HG2	2.12	0.49
1:I:27:LEU:C	1:I:29:LYS:H	2.21	0.49
1:J:55:ALA:HB1	1:J:149:ALA:HB3	1.94	0.49
1:A:1:MET:HE2	1:B:114:ASP:O	2.13	0.49
1:D:54:ILE:O	1:D:58:LYS:HG2	2.13	0.49
1:E:16:LEU:HD11	1:E:22:ASP:HB2	1.95	0.49
1:F:143:LEU:CB	1:F:144:PRO:HD2	2.43	0.49
1:H:36:VAL:HG11	1:H:71:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:LEU:HD23	1:H:140:ILE:HD13	1.93	0.49
1:H:136:ARG:HH11	1:H:136:ARG:CA	2.23	0.49
1:J:68:PHE:CE2	1:J:156:VAL:HG13	2.48	0.49
1:A:33:LYS:CD	1:A:67:GLY:HA2	2.41	0.49
1:A:60:VAL:HG23	1:A:61:LYS:N	2.27	0.49
1:D:11:LYS:HA	1:D:25:PHE:O	2.12	0.49
1:E:49:CYS:HB3	1:E:51:THR:HG23	1.94	0.49
1:E:88:PRO:O	1:E:91:LYS:N	2.44	0.49
1:F:57:ASP:O	1:F:60:VAL:HG22	2.12	0.49
1:G:131:LYS:HD2	1:G:131:LYS:H	1.78	0.49
1:H:148:ASN:N	1:H:148:ASN:HD22	2.10	0.49
1:J:75:ILE:C	1:J:75:ILE:HD12	2.38	0.49
1:B:139:VAL:HG13	1:B:139:VAL:O	2.12	0.49
1:D:116:LEU:HD11	1:D:119:GLU:CA	2.35	0.49
1:F:8:PRO:HG2	1:F:113:TYR:CZ	2.48	0.49
1:G:74:SER:HB3	1:G:81:HIS:CE1	2.45	0.49
1:B:1:MET:HE3	1:B:3:VAL:O	2.13	0.49
1:B:61:LYS:HA	1:B:61:LYS:HD3	1.65	0.49
1:D:48:VAL:HG13	1:D:49:CYS:H	1.74	0.49
1:F:35:GLY:C	1:F:36:VAL:HG23	2.38	0.49
1:J:148:ASN:HA	1:J:151:GLU:HB3	1.95	0.49
1:C:6:LEU:HD23	1:C:7:ALA:C	2.37	0.49
1:H:88:PRO:HG2	1:H:91:LYS:HD2	1.95	0.49
1:I:147:ARG:O	1:I:151:GLU:HG2	2.12	0.49
1:J:168:VAL:HG22	1:J:169:CYS:N	2.28	0.49
1:A:25:PHE:C	1:A:25:PHE:CD2	2.91	0.48
1:H:52:GLU:HB2	1:H:53:ILE:HD12	1.94	0.48
1:I:82:PHE:CE2	1:I:86:ASN:ND2	2.81	0.48
1:F:79:GLN:HG3	1:G:43:LYS:HD3	1.95	0.48
1:H:135:VAL:HG23	1:H:135:VAL:O	2.12	0.48
1:I:25:PHE:CD2	1:I:25:PHE:C	2.91	0.48
1:B:143:LEU:HB3	1:B:145:LEU:CD1	2.43	0.48
1:I:131:LYS:HD2	1:I:131:LYS:H	1.78	0.48
1:J:105:ILE:HG23	1:J:106:THR:HG23	1.96	0.48
1:J:140:ILE:C	1:J:140:ILE:CD1	2.83	0.48
1:J:148:ASN:HD22	1:J:149:ALA:N	2.11	0.48
1:J:159:LEU:HD23	1:J:159:LEU:C	2.38	0.48
1:A:151:GLU:OE2	1:B:154:ARG:HD2	2.13	0.48
1:B:75:ILE:C	1:B:75:ILE:HD12	2.38	0.48
1:D:39:PHE:HE2	1:D:70:VAL:HG12	1.77	0.48
1:E:82:PHE:CE2	1:E:86:ASN:ND2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLY:C	1:D:36:VAL:HG23	2.37	0.48
1:G:85:LYS:HE3	1:G:97:VAL:H	1.78	0.48
1:H:46:THR:OG1	1:H:48:VAL:HG12	2.14	0.48
1:B:12:ALA:HB1	1:B:13:PRO:HD2	1.95	0.48
1:B:116:LEU:CD1	1:B:119:GLU:HA	2.40	0.48
1:B:135:VAL:CG2	1:B:135:VAL:O	2.62	0.48
1:C:147:ARG:O	1:C:151:GLU:HG2	2.13	0.48
1:D:151:GLU:OE1	1:D:155:MET:HG2	2.14	0.48
1:G:147:ARG:HH11	1:G:147:ARG:CB	2.20	0.48
1:H:35:GLY:O	1:H:36:VAL:HG23	2.13	0.48
1:I:49:CYS:HB3	1:I:51:THR:HG23	1.95	0.48
1:A:68:PHE:HE2	1:A:156:VAL:HG13	1.77	0.48
1:B:39:PHE:HE2	1:B:70:VAL:HG12	1.79	0.48
1:C:11:LYS:HE2	1:C:24:HIS:HB3	1.95	0.48
1:G:33:LYS:CD	1:G:67:GLY:HA2	2.43	0.48
1:I:33:LYS:CD	1:I:67:GLY:HA2	2.44	0.48
1:I:139:VAL:HG13	1:I:139:VAL:O	2.13	0.48
1:C:162:PHE:O	1:C:163:GLU:C	2.57	0.48
1:F:85:LYS:HE2	1:F:97:VAL:CG2	2.44	0.48
1:H:44:ASP:HA	1:H:84:TRP:CZ3	2.49	0.48
1:J:143:LEU:HB2	2:J:203:HOH:O	2.13	0.48
1:G:31:LEU:HA	1:G:36:VAL:HG21	1.96	0.48
1:A:150:ASP:O	1:A:154:ARG:HG3	2.14	0.47
1:B:151:GLU:HA	1:B:154:ARG:NH1	2.29	0.47
1:B:162:PHE:O	1:B:166:GLY:HA2	2.13	0.47
1:D:151:GLU:HA	1:D:154:ARG:NH1	2.29	0.47
1:F:1:MET:HE2	1:F:5:LYS:HE3	1.95	0.47
1:G:47:PHE:C	1:H:173:TRP:HH2	2.22	0.47
1:H:143:LEU:CB	1:H:144:PRO:HD2	2.44	0.47
1:B:10:PHE:CD1	1:B:10:PHE:C	2.92	0.47
1:B:136:ARG:NH1	1:B:136:ARG:HB3	2.29	0.47
1:C:151:GLU:OE2	1:D:154:ARG:HD2	2.13	0.47
1:H:48:VAL:HG13	1:H:49:CYS:H	1.75	0.47
1:B:159:LEU:O	1:B:159:LEU:HD23	2.14	0.47
1:D:60:VAL:HG23	1:D:61:LYS:HE2	1.96	0.47
1:E:1:MET:HE2	1:F:114:ASP:O	2.14	0.47
1:E:151:GLU:OE2	1:F:154:ARG:HD2	2.15	0.47
1:F:136:ARG:NH1	1:F:136:ARG:CB	2.77	0.47
1:G:128:LEU:N	1:G:152:MET:HE1	2.30	0.47
1:H:79:GLN:CG	1:I:43:LYS:HD3	2.44	0.47
1:H:162:PHE:O	1:H:166:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:LEU:HD11	1:I:22:ASP:HB2	1.96	0.47
1:A:78:GLU:CD	1:A:79:GLN:NE2	2.72	0.47
1:B:17:GLY:C	1:B:19:ASN:H	2.21	0.47
1:B:142:ASP:OD2	1:B:142:ASP:C	2.57	0.47
1:E:25:PHE:C	1:E:25:PHE:CD2	2.92	0.47
1:G:150:ASP:O	1:G:154:ARG:HG3	2.14	0.47
1:I:144:PRO:O	1:I:145:LEU:C	2.57	0.47
1:A:6:LEU:HD23	1:A:7:ALA:C	2.39	0.47
1:A:16:LEU:HD11	1:A:22:ASP:HB2	1.97	0.47
1:A:162:PHE:O	1:A:163:GLU:C	2.57	0.47
1:G:147:ARG:O	1:G:151:GLU:HG2	2.14	0.47
1:C:27:LEU:C	1:C:29:LYS:H	2.22	0.47
1:D:164:GLU:O	1:D:166:GLY:N	2.47	0.47
1:E:27:LEU:C	1:E:29:LYS:H	2.22	0.47
1:E:33:LYS:CD	1:E:67:GLY:HA2	2.44	0.47
1:E:70:VAL:O	1:E:99:PHE:HB2	2.14	0.47
1:H:159:LEU:HD23	1:H:159:LEU:C	2.40	0.47
1:A:142:ASP:OD2	1:B:136:ARG:NH1	2.47	0.47
1:B:26:GLU:O	1:B:30:ASN:ND2	2.47	0.47
1:C:144:PRO:O	1:C:145:LEU:C	2.57	0.47
1:D:55:ALA:HB1	1:D:149:ALA:HB3	1.97	0.47
1:D:136:ARG:HH11	1:D:136:ARG:CA	2.26	0.47
1:F:135:VAL:CG2	1:F:135:VAL:O	2.63	0.47
1:H:39:PHE:O	1:H:72:GLY:HA2	2.14	0.47
1:H:151:GLU:OE1	1:H:155:MET:HG2	2.15	0.47
1:H:151:GLU:OE1	1:H:151:GLU:C	2.58	0.47
1:I:28:SER:C	1:I:29:LYS:HD2	2.39	0.47
1:I:128:LEU:CB	1:I:152:MET:HE1	2.41	0.47
1:I:151:GLU:OE2	1:J:154:ARG:HD2	2.14	0.47
1:B:161:HIS:HB3	1:B:165:HIS:HE1	1.80	0.47
1:E:31:LEU:HA	1:E:36:VAL:HG21	1.97	0.47
1:E:131:LYS:HD2	1:E:131:LYS:H	1.79	0.47
1:F:85:LYS:HE2	1:F:97:VAL:HG22	1.96	0.47
1:I:2:VAL:HG12	1:I:135:VAL:HG11	1.97	0.47
1:I:85:LYS:HE3	1:I:97:VAL:H	1.80	0.47
1:I:147:ARG:HH11	1:I:147:ARG:CB	2.24	0.47
1:J:130:ASP:OD2	1:J:136:ARG:HD3	2.15	0.47
1:A:82:PHE:CZ	1:A:86:ASN:ND2	2.83	0.47
1:A:128:LEU:N	1:A:152:MET:HE1	2.30	0.47
1:F:3:VAL:C	1:F:4:THR:HG23	2.40	0.47
1:F:130:ASP:OD1	1:F:130:ASP:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ARG:HA	1:F:136:ARG:NH1	2.22	0.47
1:G:25:PHE:C	1:G:25:PHE:CD2	2.93	0.47
1:A:144:PRO:O	1:A:145:LEU:C	2.58	0.47
1:D:74:SER:HB3	1:D:81:HIS:HE1	1.80	0.47
1:F:143:LEU:CB	1:F:145:LEU:HD11	2.44	0.47
1:F:148:ASN:N	1:F:148:ASN:ND2	2.63	0.47
1:G:2:VAL:HG12	1:G:135:VAL:HG11	1.97	0.47
1:G:27:LEU:C	1:G:29:LYS:H	2.23	0.47
1:J:26:GLU:O	1:J:30:ASN:ND2	2.46	0.47
1:B:52:GLU:HG2	1:B:124:ARG:HH12	1.80	0.46
1:C:33:LYS:CD	1:C:67:GLY:HA2	2.45	0.46
1:D:21:VAL:O	1:D:21:VAL:HG23	2.15	0.46
1:J:42:PRO:HD3	1:J:124:ARG:HG3	1.96	0.46
1:J:136:ARG:NH1	1:J:136:ARG:HB3	2.29	0.46
1:C:49:CYS:HB3	1:C:51:THR:HG23	1.97	0.46
1:J:164:GLU:O	1:J:166:GLY:N	2.46	0.46
1:C:25:PHE:C	1:C:25:PHE:HD2	2.23	0.46
1:D:145:LEU:H	1:D:145:LEU:HG	1.33	0.46
1:D:168:VAL:HG22	1:D:169:CYS:N	2.31	0.46
1:E:134:LYS:HB2	1:E:134:LYS:HE2	1.68	0.46
1:F:94:ILE:HG23	1:F:95:GLY:O	2.15	0.46
1:B:41:TRP:CE2	1:B:74:SER:HB2	2.50	0.46
1:D:52:GLU:HG2	1:D:124:ARG:HH11	1.77	0.46
1:G:50:PRO:O	1:G:51:THR:C	2.59	0.46
1:G:144:PRO:O	1:G:145:LEU:C	2.58	0.46
1:J:151:GLU:HA	1:J:154:ARG:HH12	1.81	0.46
1:C:147:ARG:HH11	1:C:147:ARG:CB	2.24	0.46
1:E:6:LEU:HD23	1:E:7:ALA:C	2.41	0.46
1:H:139:VAL:O	1:H:139:VAL:HG13	2.16	0.46
1:J:35:GLY:C	1:J:36:VAL:HG23	2.40	0.46
1:B:55:ALA:CB	1:B:149:ALA:HB3	2.46	0.46
1:D:151:GLU:OE1	1:D:151:GLU:C	2.59	0.46
1:F:161:HIS:HB3	1:F:165:HIS:CE1	2.50	0.46
1:G:6:LEU:HD23	1:G:7:ALA:C	2.40	0.46
1:G:11:LYS:HE2	1:G:24:HIS:HB3	1.97	0.46
1:I:47:PHE:C	1:J:173:TRP:HH2	2.24	0.46
1:A:89:VAL:O	1:B:173:TRP:O	2.34	0.46
1:B:48:VAL:HG13	1:B:49:CYS:H	1.76	0.46
1:D:18:ASN:OD1	1:D:18:ASN:C	2.59	0.46
1:F:74:SER:HB3	1:F:81:HIS:HE1	1.81	0.46
1:G:16:LEU:HD11	1:G:22:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:GLY:C	1:H:19:ASN:H	2.24	0.46
1:I:59:ARG:HG3	1:I:59:ARG:HH11	1.80	0.46
1:B:49:CYS:HA	1:B:50:PRO:HD3	1.74	0.46
1:D:159:LEU:O	1:D:159:LEU:HD23	2.16	0.46
1:E:8:PRO:HD2	1:E:113:TYR:CZ	2.51	0.46
1:F:161:HIS:HB3	1:F:165:HIS:HE1	1.80	0.46
1:F:168:VAL:HG22	1:F:169:CYS:H	1.80	0.46
1:G:3:VAL:HG21	1:H:140:ILE:HD11	1.98	0.46
1:G:131:LYS:H	1:G:131:LYS:CD	2.29	0.46
1:I:162:PHE:O	1:I:163:GLU:C	2.58	0.46
1:J:49:CYS:HA	1:J:50:PRO:HD3	1.74	0.46
1:A:147:ARG:O	1:A:151:GLU:HG2	2.14	0.46
1:B:23:GLU:HA	1:B:23:GLU:OE1	2.14	0.46
1:D:75:ILE:C	1:D:75:ILE:HD12	2.41	0.46
1:D:162:PHE:O	1:D:166:GLY:HA2	2.15	0.46
1:E:162:PHE:HA	1:E:165:HIS:O	2.16	0.46
1:H:55:ALA:HB1	1:H:149:ALA:HB3	1.96	0.46
1:H:164:GLU:O	1:H:166:GLY:N	2.46	0.46
1:I:89:VAL:O	1:J:173:TRP:O	2.33	0.46
1:B:136:ARG:HA	1:B:136:ARG:NH1	2.25	0.46
1:D:39:PHE:O	1:D:72:GLY:HA2	2.16	0.46
1:G:139:VAL:HG13	1:G:139:VAL:O	2.15	0.46
1:H:137:HIS:CE1	1:H:155:MET:HG3	2.51	0.46
1:I:31:LEU:HA	1:I:36:VAL:HG21	1.96	0.46
1:I:131:LYS:H	1:I:131:LYS:CD	2.29	0.46
1:B:159:LEU:HD23	1:B:159:LEU:C	2.40	0.45
1:C:31:LEU:HA	1:C:36:VAL:HG21	1.98	0.45
1:D:6:LEU:HD23	1:D:6:LEU:HA	1.79	0.45
1:D:49:CYS:C	1:D:51:THR:H	2.24	0.45
1:D:141:ASN:ND2	1:D:143:LEU:H	2.14	0.45
1:F:44:ASP:HA	1:F:84:TRP:CZ3	2.51	0.45
1:H:74:SER:HB3	1:H:81:HIS:CE1	2.49	0.45
1:H:161:HIS:HB3	1:H:165:HIS:CE1	2.51	0.45
1:I:3:VAL:CG2	1:J:140:ILE:HD11	2.45	0.45
1:J:61:LYS:HA	1:J:61:LYS:HD3	1.67	0.45
1:J:136:ARG:HH11	1:J:136:ARG:CA	2.26	0.45
1:B:123:LEU:HD23	1:B:140:ILE:HD13	1.98	0.45
1:C:55:ALA:HB1	1:C:149:ALA:HB3	1.97	0.45
1:C:130:ASP:C	1:C:130:ASP:OD1	2.59	0.45
1:F:48:VAL:CG1	1:F:49:CYS:N	2.73	0.45
1:F:61:LYS:HA	1:F:61:LYS:HD3	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PHE:C	1:B:173:TRP:HH2	2.24	0.45
1:A:139:VAL:HG13	1:A:139:VAL:O	2.16	0.45
1:C:68:PHE:HE2	1:C:156:VAL:HG13	1.81	0.45
1:C:165:HIS:ND1	1:C:165:HIS:N	2.49	0.45
1:D:49:CYS:HA	1:D:50:PRO:HD3	1.71	0.45
1:F:142:ASP:OD2	1:F:142:ASP:C	2.60	0.45
1:G:169:CYS:HG	1:H:49:CYS:CB	2.29	0.45
1:I:8:PRO:HD2	1:I:113:TYR:CZ	2.51	0.45
1:I:55:ALA:HB1	1:I:149:ALA:HB3	1.98	0.45
1:C:44:ASP:OD1	1:C:81:HIS:ND1	2.46	0.45
1:D:53:ILE:HG23	1:D:99:PHE:HZ	1.81	0.45
1:F:75:ILE:HD12	1:F:75:ILE:C	2.41	0.45
1:G:31:LEU:HD22	1:G:31:LEU:H	1.80	0.45
1:H:11:LYS:HE3	1:H:24:HIS:HB3	1.98	0.45
1:H:39:PHE:HE2	1:H:70:VAL:HG12	1.81	0.45
1:H:96:GLN:HE21	1:H:96:GLN:HB3	1.52	0.45
1:J:3:VAL:O	1:J:4:THR:HG23	2.16	0.45
1:J:55:ALA:CB	1:J:149:ALA:HB3	2.47	0.45
1:A:3:VAL:HG11	1:B:140:ILE:CD1	2.46	0.45
1:A:131:LYS:H	1:A:131:LYS:CD	2.29	0.45
1:A:141:ASN:HB3	1:B:137:HIS:CD2	2.50	0.45
1:E:80:VAL:O	1:E:81:HIS:C	2.60	0.45
1:G:77:SER:OG	1:G:80:VAL:HG13	2.16	0.45
1:H:85:LYS:HE2	1:H:97:VAL:CG2	2.46	0.45
1:J:136:ARG:HA	1:J:136:ARG:NH1	2.28	0.45
1:A:28:SER:C	1:A:29:LYS:HD2	2.41	0.45
1:B:74:SER:HA	2:B:200:HOH:O	2.16	0.45
1:C:70:VAL:O	1:C:99:PHE:HB2	2.17	0.45
1:E:65:GLU:C	1:E:67:GLY:H	2.25	0.45
1:H:142:ASP:OD2	1:H:142:ASP:C	2.59	0.45
1:I:150:ASP:OD2	1:I:154:ARG:HD2	2.17	0.45
1:J:2:VAL:O	1:J:135:VAL:CG2	2.65	0.45
1:A:111:ARG:HG3	1:A:116:LEU:HD12	1.99	0.45
1:B:6:LEU:HD23	1:B:6:LEU:HA	1.83	0.45
1:B:8:PRO:HG2	1:B:113:TYR:CE1	2.52	0.45
1:D:42:PRO:HD3	1:D:124:ARG:HG3	1.99	0.45
1:F:89:VAL:HG23	1:F:90:GLU:N	2.32	0.45
1:H:50:PRO:HB3	1:H:94:ILE:HD11	1.98	0.45
1:H:148:ASN:N	1:H:148:ASN:ND2	2.63	0.45
1:A:85:LYS:HE3	1:A:97:VAL:H	1.81	0.45
1:B:11:LYS:HE3	1:B:24:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLU:O	1:B:166:GLY:N	2.46	0.45
1:B:169:CYS:O	1:B:170:PRO:C	2.60	0.45
1:C:85:LYS:HE3	1:C:97:VAL:H	1.80	0.45
1:E:50:PRO:O	1:E:51:THR:C	2.59	0.45
1:E:162:PHE:O	1:E:163:GLU:C	2.58	0.45
1:F:52:GLU:HG2	1:F:124:ARG:HH11	1.78	0.45
1:H:48:VAL:CG2	1:H:49:CYS:H	2.14	0.45
1:I:3:VAL:HB	1:J:140:ILE:HD11	1.98	0.45
1:I:21:VAL:O	1:I:21:VAL:HG13	2.16	0.45
1:I:88:PRO:O	1:I:91:LYS:N	2.45	0.45
1:I:95:GLY:O	1:I:97:VAL:HG13	2.16	0.45
1:J:116:LEU:C	1:J:116:LEU:HD13	2.42	0.45
1:D:50:PRO:HB3	1:D:94:ILE:HD11	1.98	0.45
1:F:49:CYS:C	1:F:51:THR:H	2.24	0.45
1:F:60:VAL:HG23	1:F:61:LYS:N	2.32	0.45
1:F:96:GLN:HE21	1:F:96:GLN:HB3	1.56	0.45
1:F:159:LEU:HD23	1:F:159:LEU:C	2.42	0.45
1:G:162:PHE:HA	1:G:165:HIS:O	2.16	0.45
1:H:35:GLY:O	1:H:36:VAL:CG2	2.64	0.45
1:B:49:CYS:C	1:B:51:THR:H	2.24	0.45
1:C:2:VAL:HG12	1:C:135:VAL:HG11	1.99	0.45
1:C:88:PRO:O	1:C:91:LYS:N	2.47	0.45
1:C:150:ASP:O	1:C:154:ARG:HG3	2.17	0.45
1:D:104:ASP:OD2	1:D:107:LYS:HA	2.16	0.45
1:E:131:LYS:H	1:E:131:LYS:CD	2.30	0.45
1:F:136:ARG:HB3	1:F:136:ARG:CZ	2.46	0.45
1:G:130:ASP:OD1	1:G:130:ASP:C	2.60	0.45
1:H:8:PRO:HG2	1:H:113:TYR:CZ	2.52	0.45
1:H:49:CYS:HA	1:H:50:PRO:HD3	1.73	0.45
1:J:94:ILE:HD12	1:J:94:ILE:HA	1.82	0.45
1:A:50:PRO:O	1:A:51:THR:C	2.61	0.44
1:C:11:LYS:HA	1:C:25:PHE:O	2.16	0.44
1:D:3:VAL:C	1:D:4:THR:HG23	2.42	0.44
1:D:61:LYS:HA	1:D:61:LYS:HD3	1.74	0.44
1:E:59:ARG:HD3	1:E:153:LEU:HD22	2.00	0.44
1:G:27:LEU:O	1:G:29:LYS:N	2.50	0.44
1:G:59:ARG:HD3	1:G:153:LEU:HD22	1.99	0.44
1:G:75:ILE:C	1:G:75:ILE:HD12	2.41	0.44
1:J:48:VAL:HG13	1:J:49:CYS:H	1.80	0.44
1:J:164:GLU:C	1:J:166:GLY:N	2.76	0.44
1:B:50:PRO:HB3	1:B:94:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HD12	1:C:75:ILE:C	2.43	0.44
1:E:111:ARG:HG3	1:E:116:LEU:HD12	1.99	0.44
1:F:46:THR:OG1	1:F:48:VAL:HG12	2.17	0.44
1:F:59:ARG:O	1:F:60:VAL:C	2.59	0.44
1:J:59:ARG:NH2	1:J:150:ASP:CB	2.78	0.44
1:A:31:LEU:HD22	1:A:31:LEU:H	1.81	0.44
1:A:146:GLY:HA2	2:A:206:HOH:O	2.17	0.44
1:D:11:LYS:CE	1:D:24:HIS:HB3	2.47	0.44
1:D:41:TRP:CE2	1:D:74:SER:HB2	2.53	0.44
1:D:139:VAL:HG13	1:D:139:VAL:O	2.17	0.44
1:E:28:SER:C	1:E:29:LYS:HD2	2.42	0.44
1:E:68:PHE:HE2	1:E:156:VAL:HG13	1.82	0.44
1:F:51:THR:OG1	1:F:52:GLU:N	2.51	0.44
1:H:61:LYS:HA	1:H:61:LYS:HD3	1.76	0.44
1:I:27:LEU:O	1:I:29:LYS:N	2.50	0.44
1:J:169:CYS:O	1:J:170:PRO:C	2.60	0.44
1:A:31:LEU:HA	1:A:36:VAL:HG21	1.99	0.44
1:B:3:VAL:O	1:B:4:THR:OG1	2.28	0.44
1:C:118:GLU:N	2:C:202:HOH:O	2.50	0.44
1:D:77:SER:O	1:D:80:VAL:HG13	2.17	0.44
1:D:96:GLN:HE21	1:D:96:GLN:HB3	1.52	0.44
1:D:135:VAL:CG2	1:D:135:VAL:O	2.63	0.44
1:E:128:LEU:N	1:E:152:MET:HE1	2.32	0.44
1:I:6:LEU:HD23	1:I:7:ALA:C	2.42	0.44
1:I:75:ILE:C	1:I:75:ILE:HD12	2.42	0.44
1:I:162:PHE:HA	1:I:165:HIS:O	2.18	0.44
1:I:163:GLU:HA	1:I:163:GLU:OE1	2.17	0.44
1:J:139:VAL:HG13	1:J:139:VAL:O	2.17	0.44
1:A:11:LYS:HA	1:A:25:PHE:O	2.17	0.44
1:A:27:LEU:C	1:A:29:LYS:H	2.26	0.44
1:B:174:ARG:HH11	1:B:174:ARG:CG	2.30	0.44
1:E:2:VAL:HG12	1:E:135:VAL:HG11	2.00	0.44
1:F:49:CYS:HA	1:F:50:PRO:HD3	1.72	0.44
1:F:55:ALA:CB	1:F:149:ALA:HB3	2.47	0.44
1:G:28:SER:C	1:G:29:LYS:HD2	2.43	0.44
1:H:10:PHE:CD1	1:H:10:PHE:C	2.94	0.44
1:H:59:ARG:O	1:H:60:VAL:C	2.59	0.44
1:I:70:VAL:O	1:I:99:PHE:HB2	2.18	0.44
1:J:85:LYS:HE2	1:J:97:VAL:CG2	2.48	0.44
1:D:59:ARG:O	1:D:60:VAL:C	2.60	0.44
1:E:130:ASP:C	1:E:130:ASP:OD1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:PHE:O	1:G:163:GLU:C	2.59	0.44
1:H:1:MET:HE2	1:H:5:LYS:HE3	1.99	0.44
1:H:169:CYS:CB	1:H:170:PRO:CD	2.92	0.44
1:I:130:ASP:OD1	1:I:130:ASP:C	2.61	0.44
1:I:165:HIS:ND1	1:I:165:HIS:N	2.52	0.44
1:J:74:SER:HB3	1:J:81:HIS:CE1	2.51	0.44
1:A:134:LYS:HB2	1:A:134:LYS:HE2	1.67	0.44
1:B:42:PRO:HD3	1:B:124:ARG:HG3	2.00	0.44
1:C:95:GLY:O	1:C:97:VAL:HG13	2.17	0.44
1:D:142:ASP:OD2	1:D:142:ASP:C	2.61	0.44
1:E:55:ALA:HB1	1:E:149:ALA:HB3	1.99	0.44
1:E:150:ASP:OD2	1:E:154:ARG:HD2	2.17	0.44
1:F:139:VAL:HG12	1:F:152:MET:CE	2.47	0.44
1:H:49:CYS:C	1:H:51:THR:H	2.25	0.44
1:B:59:ARG:O	1:B:60:VAL:C	2.59	0.44
1:C:59:ARG:HD3	1:C:153:LEU:HD22	1.99	0.44
1:C:141:ASN:HB3	1:D:137:HIS:CD2	2.53	0.44
1:D:79:GLN:CG	1:E:43:LYS:HD3	2.48	0.44
1:F:35:GLY:O	1:F:36:VAL:HG23	2.18	0.44
1:G:68:PHE:HE2	1:G:156:VAL:HG13	1.82	0.44
1:H:49:CYS:HB2	1:H:51:THR:HG23	1.98	0.44
1:A:162:PHE:HA	1:A:165:HIS:O	2.18	0.44
1:C:162:PHE:HA	1:C:165:HIS:O	2.18	0.44
1:D:33:LYS:HB2	1:D:33:LYS:HZ2	1.82	0.44
1:F:140:ILE:C	1:F:140:ILE:CD1	2.80	0.44
1:G:1:MET:HE2	1:H:114:ASP:O	2.18	0.44
1:J:135:VAL:CG2	1:J:135:VAL:O	2.65	0.44
1:A:75:ILE:HD12	1:A:75:ILE:C	2.43	0.43
1:C:16:LEU:HD11	1:C:22:ASP:HB2	2.00	0.43
1:D:169:CYS:CB	1:D:170:PRO:CD	2.92	0.43
1:F:54:ILE:O	1:F:58:LYS:HG2	2.17	0.43
1:F:116:LEU:HD11	1:F:119:GLU:CA	2.39	0.43
1:J:50:PRO:HB3	1:J:94:ILE:HD11	2.00	0.43
1:B:35:GLY:O	1:B:36:VAL:CG2	2.65	0.43
1:C:131:LYS:HD2	1:C:131:LYS:H	1.82	0.43
1:D:137:HIS:CE1	1:D:155:MET:HG3	2.52	0.43
1:F:105:ILE:HG23	1:F:106:THR:HG23	2.00	0.43
1:F:169:CYS:O	1:F:170:PRO:C	2.61	0.43
1:H:141:ASN:HD21	1:H:143:LEU:HB2	1.83	0.43
1:I:68:PHE:HE2	1:I:156:VAL:HG13	1.82	0.43
1:I:90:GLU:H	1:I:90:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:89:VAL:HG23	1:J:90:GLU:N	2.32	0.43
1:B:74:SER:HB3	1:B:81:HIS:HE1	1.83	0.43
1:E:139:VAL:O	1:E:139:VAL:HG13	2.18	0.43
1:F:60:VAL:HG23	1:F:61:LYS:HE2	2.00	0.43
1:F:136:ARG:HH11	1:F:136:ARG:CB	2.31	0.43
1:H:135:VAL:CG2	1:H:135:VAL:O	2.67	0.43
1:I:134:LYS:HE2	1:I:134:LYS:HB2	1.66	0.43
1:A:2:VAL:HG12	1:A:135:VAL:HG11	2.00	0.43
1:A:55:ALA:HB1	1:A:149:ALA:HB3	2.00	0.43
1:C:27:LEU:O	1:C:29:LYS:N	2.52	0.43
1:C:62:ASP:O	1:C:63:PHE:C	2.62	0.43
1:C:123:LEU:HB3	1:C:140:ILE:HD13	1.99	0.43
1:D:105:ILE:HG23	1:D:106:THR:HG23	2.01	0.43
1:I:128:LEU:N	1:I:152:MET:HE1	2.33	0.43
1:I:150:ASP:O	1:I:154:ARG:HG3	2.18	0.43
1:A:164:GLU:HB2	1:A:165:HIS:H	1.68	0.43
1:B:60:VAL:HG23	1:B:61:LYS:N	2.33	0.43
1:C:50:PRO:O	1:C:51:THR:C	2.60	0.43
1:D:107:LYS:HB2	1:D:111:ARG:NH2	2.34	0.43
1:E:59:ARG:HG3	1:E:59:ARG:HH11	1.82	0.43
1:E:90:GLU:CD	1:E:90:GLU:H	2.26	0.43
1:E:95:GLY:O	1:E:97:VAL:HG13	2.19	0.43
1:F:33:LYS:HG3	1:F:34:ASN:ND2	2.33	0.43
1:J:59:ARG:O	1:J:60:VAL:C	2.60	0.43
1:J:169:CYS:CB	1:J:170:PRO:CD	2.93	0.43
1:B:59:ARG:NH2	1:B:150:ASP:CB	2.81	0.43
1:D:33:LYS:HB2	1:D:33:LYS:HZ3	1.83	0.43
1:G:82:PHE:CZ	1:G:86:ASN:ND2	2.87	0.43
1:H:55:ALA:CB	1:H:149:ALA:HB3	2.49	0.43
1:B:174:ARG:N	2:B:199:HOH:O	2.48	0.43
1:C:36:VAL:CG1	1:C:37:ILE:H	2.30	0.43
1:C:77:SER:OG	1:C:80:VAL:HG13	2.19	0.43
1:D:48:VAL:CG2	1:D:49:CYS:H	2.14	0.43
1:D:151:GLU:OE1	1:D:155:MET:CG	2.67	0.43
1:D:168:VAL:HG22	1:D:169:CYS:H	1.83	0.43
1:E:75:ILE:C	1:E:75:ILE:HD12	2.44	0.43
1:E:85:LYS:CA	1:E:94:ILE:HG22	2.44	0.43
1:E:162:PHE:CD1	1:E:167:GLU:OE1	2.72	0.43
1:G:3:VAL:HB	1:H:140:ILE:HD11	2.00	0.43
1:I:31:LEU:H	1:I:31:LEU:CD2	2.32	0.43
1:C:123:LEU:HB3	1:C:140:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LYS:HB2	1:C:134:LYS:HE2	1.67	0.43
1:H:47:PHE:CZ	1:I:79:GLN:HA	2.53	0.43
1:J:143:LEU:HD23	1:J:144:PRO:HD2	2.01	0.43
1:A:106:THR:HG22	1:J:120:ALA:HB2	2.01	0.43
1:G:95:GLY:O	1:G:97:VAL:HG13	2.19	0.43
1:H:6:LEU:HD23	1:H:6:LEU:HA	1.78	0.43
1:I:6:LEU:HA	1:I:133:MET:O	2.19	0.43
1:I:50:PRO:O	1:I:51:THR:C	2.61	0.43
1:C:47:PHE:C	1:D:173:TRP:HH2	2.27	0.43
1:E:44:ASP:OD1	1:E:81:HIS:ND1	2.51	0.43
1:F:143:LEU:CD2	1:F:144:PRO:HD2	2.49	0.43
1:G:55:ALA:HB1	1:G:149:ALA:HB3	2.00	0.43
1:I:65:GLU:C	1:I:67:GLY:H	2.26	0.43
1:B:31:LEU:HD22	1:B:36:VAL:CG2	2.49	0.42
1:B:51:THR:OG1	1:B:52:GLU:N	2.52	0.42
1:C:65:GLU:C	1:C:67:GLY:H	2.27	0.42
1:D:49:CYS:HB2	1:D:51:THR:HG23	2.00	0.42
1:F:6:LEU:HD23	1:F:6:LEU:HA	1.81	0.42
1:J:51:THR:OG1	1:J:52:GLU:N	2.52	0.42
1:C:36:VAL:CG1	1:C:37:ILE:N	2.81	0.42
1:C:162:PHE:C	1:C:164:GLU:N	2.77	0.42
1:D:17:GLY:C	1:D:19:ASN:H	2.28	0.42
1:D:88:PRO:HD2	1:D:91:LYS:HD2	1.99	0.42
1:E:31:LEU:H	1:E:31:LEU:CD2	2.32	0.42
1:E:89:VAL:O	1:F:173:TRP:O	2.37	0.42
1:E:144:PRO:O	1:E:145:LEU:C	2.61	0.42
1:J:11:LYS:HA	1:J:25:PHE:O	2.19	0.42
1:C:31:LEU:HD22	1:C:31:LEU:H	1.84	0.42
1:G:142:ASP:OD2	1:H:136:ARG:NH1	2.51	0.42
1:H:130:ASP:OD2	1:H:136:ARG:HD3	2.18	0.42
1:J:49:CYS:C	1:J:51:THR:H	2.26	0.42
1:J:143:LEU:HG	1:J:144:PRO:CD	2.49	0.42
1:A:25:PHE:C	1:A:25:PHE:HD2	2.27	0.42
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.52	0.42
1:C:22:ASP:OD1	1:C:23:GLU:N	2.53	0.42
1:D:60:VAL:HG23	1:D:61:LYS:N	2.34	0.42
1:E:6:LEU:HA	1:E:133:MET:O	2.18	0.42
1:E:12:ALA:HB1	1:E:13:PRO:CD	2.50	0.42
1:E:25:PHE:C	1:E:25:PHE:HD2	2.28	0.42
1:F:77:SER:HG	1:F:80:VAL:HG12	1.84	0.42
1:F:88:PRO:CG	1:F:91:LYS:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:VAL:O	1:H:173:TRP:O	2.37	0.42
1:G:151:GLU:OE2	1:H:154:ARG:HD2	2.20	0.42
1:H:36:VAL:HG13	1:H:69:ASN:C	2.44	0.42
1:H:151:GLU:HA	1:H:154:ARG:HH12	1.84	0.42
1:A:65:GLU:C	1:A:67:GLY:H	2.27	0.42
1:B:44:ASP:HA	1:B:84:TRP:CH2	2.54	0.42
1:B:46:THR:OG1	1:B:48:VAL:HG12	2.20	0.42
1:D:35:GLY:O	1:D:36:VAL:CG2	2.67	0.42
1:D:55:ALA:CB	1:D:149:ALA:HB3	2.49	0.42
1:D:125:GLY:HA2	1:D:140:ILE:HA	2.01	0.42
1:E:150:ASP:O	1:E:154:ARG:HG3	2.18	0.42
1:F:10:PHE:CD1	1:F:10:PHE:C	2.97	0.42
1:G:165:HIS:ND1	1:G:165:HIS:N	2.48	0.42
1:I:123:LEU:HB3	1:I:140:ILE:CD1	2.49	0.42
1:J:10:PHE:CD1	1:J:10:PHE:C	2.97	0.42
1:D:59:ARG:NH2	1:D:150:ASP:CB	2.82	0.42
1:D:116:LEU:HD13	1:D:116:LEU:C	2.44	0.42
1:D:116:LEU:CD1	1:D:119:GLU:HA	2.38	0.42
1:E:27:LEU:O	1:E:29:LYS:N	2.52	0.42
1:H:42:PRO:HD3	1:H:124:ARG:HG3	2.02	0.42
1:J:46:THR:OG1	1:J:48:VAL:HG12	2.19	0.42
1:B:40:PHE:CD2	1:B:73:VAL:HG22	2.54	0.42
1:E:163:GLU:OE1	1:E:163:GLU:HA	2.20	0.42
1:E:168:VAL:O	1:E:169:CYS:C	2.62	0.42
1:F:143:LEU:HD23	1:F:144:PRO:HD2	2.00	0.42
1:J:174:ARG:HH11	1:J:174:ARG:CG	2.32	0.42
1:A:139:VAL:HG23	1:B:137:HIS:NE2	2.34	0.42
1:B:21:VAL:O	1:B:21:VAL:HG23	2.18	0.42
1:B:39:PHE:O	1:B:72:GLY:HA2	2.19	0.42
1:B:139:VAL:HG12	1:B:152:MET:CE	2.49	0.42
1:D:141:ASN:ND2	1:D:142:ASP:N	2.67	0.42
1:D:170:PRO:O	1:D:172:GLY:N	2.52	0.42
1:F:164:GLU:O	1:F:166:GLY:N	2.52	0.42
1:G:162:PHE:CD1	1:G:167:GLU:OE1	2.73	0.42
1:J:12:ALA:HB1	1:J:13:PRO:HD2	2.01	0.42
1:B:88:PRO:HG2	1:B:91:LYS:HD2	2.02	0.42
1:B:161:HIS:HB3	1:B:165:HIS:CE1	2.54	0.42
1:E:22:ASP:OD1	1:E:23:GLU:N	2.53	0.42
1:H:59:ARG:NH2	1:H:150:ASP:CB	2.82	0.42
1:J:21:VAL:O	1:J:21:VAL:HG23	2.19	0.42
1:J:130:ASP:OD1	1:J:130:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:HIS:ND1	1:A:24:HIS:N	2.68	0.42
1:B:3:VAL:C	1:B:4:THR:HG23	2.45	0.42
1:C:24:HIS:ND1	1:C:24:HIS:N	2.67	0.42
1:D:46:THR:OG1	1:D:48:VAL:HG12	2.19	0.42
1:E:10:PHE:O	1:E:26:GLU:HA	2.20	0.42
1:E:78:GLU:CD	1:E:79:GLN:NE2	2.78	0.42
1:E:146:GLY:HA2	2:E:201:HOH:O	2.18	0.42
1:F:21:VAL:O	1:F:21:VAL:HG23	2.20	0.42
1:G:10:PHE:O	1:G:26:GLU:HA	2.20	0.42
1:H:151:GLU:OE1	1:H:155:MET:CG	2.68	0.42
1:I:53:ILE:HG23	1:I:99:PHE:HZ	1.84	0.42
1:I:77:SER:OG	1:I:80:VAL:HG13	2.19	0.42
1:A:57:ASP:O	1:A:60:VAL:HG13	2.20	0.41
1:B:164:GLU:C	1:B:166:GLY:N	2.78	0.41
1:C:168:VAL:O	1:C:169:CYS:C	2.63	0.41
1:D:10:PHE:CD1	1:D:10:PHE:C	2.98	0.41
1:D:137:HIS:CD2	1:D:138:ALA:N	2.87	0.41
1:I:27:LEU:C	1:I:29:LYS:N	2.78	0.41
1:J:17:GLY:C	1:J:19:ASN:H	2.28	0.41
1:A:85:LYS:CA	1:A:94:ILE:HG22	2.42	0.41
1:A:95:GLY:O	1:A:97:VAL:HG13	2.19	0.41
1:C:82:PHE:CZ	1:C:86:ASN:ND2	2.88	0.41
1:C:87:THR:HB	1:C:93:GLY:HA3	2.01	0.41
1:E:20:GLU:HA	1:E:20:GLU:OE2	2.21	0.41
1:E:36:VAL:CG1	1:E:37:ILE:H	2.29	0.41
1:E:82:PHE:CZ	1:E:86:ASN:ND2	2.89	0.41
1:F:17:GLY:C	1:F:19:ASN:H	2.27	0.41
1:G:62:ASP:O	1:G:63:PHE:C	2.64	0.41
1:I:19:ASN:ND2	1:I:85:LYS:HE2	2.34	0.41
1:J:168:VAL:HG22	1:J:169:CYS:H	1.85	0.41
1:A:70:VAL:O	1:A:99:PHE:HB2	2.20	0.41
1:B:57:ASP:O	1:B:60:VAL:HG22	2.20	0.41
1:C:78:GLU:CD	1:C:79:GLN:NE2	2.78	0.41
1:C:169:CYS:HG	1:D:49:CYS:CB	2.33	0.41
1:D:136:ARG:HB3	1:D:136:ARG:CZ	2.49	0.41
1:F:169:CYS:CB	1:F:170:PRO:CD	2.96	0.41
1:G:150:ASP:OD2	1:G:154:ARG:HD2	2.20	0.41
1:A:31:LEU:HD12	1:A:36:VAL:HG23	2.02	0.41
1:C:68:PHE:CD2	1:C:156:VAL:HG13	2.55	0.41
1:C:131:LYS:H	1:C:131:LYS:CD	2.33	0.41
1:D:159:LEU:HD23	1:D:159:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:LEU:C	1:E:128:LEU:HD23	2.46	0.41
1:I:123:LEU:HB3	1:I:140:ILE:HD13	2.03	0.41
1:C:78:GLU:CG	1:C:79:GLN:NE2	2.83	0.41
1:C:128:LEU:N	1:C:152:MET:HE1	2.34	0.41
1:D:57:ASP:O	1:D:60:VAL:HG22	2.20	0.41
1:H:125:GLY:HA2	1:H:140:ILE:HA	2.02	0.41
1:H:139:VAL:HG12	1:H:152:MET:HE3	2.01	0.41
1:H:169:CYS:O	1:H:170:PRO:C	2.63	0.41
1:J:6:LEU:HD23	1:J:6:LEU:HA	1.77	0.41
1:J:116:LEU:HD11	1:J:119:GLU:CA	2.36	0.41
1:C:148:ASN:N	1:C:148:ASN:HD22	2.18	0.41
1:F:94:ILE:HD12	1:F:94:ILE:HA	1.85	0.41
1:G:59:ARG:HG3	1:G:59:ARG:HH11	1.86	0.41
1:G:128:LEU:CA	1:G:152:MET:HE1	2.50	0.41
1:J:18:ASN:OD1	1:J:18:ASN:C	2.64	0.41
1:J:143:LEU:CD2	1:J:144:PRO:HD2	2.50	0.41
1:B:148:ASN:HD22	1:B:149:ALA:H	1.68	0.41
1:C:1:MET:HE2	1:D:114:ASP:O	2.21	0.41
1:D:174:ARG:HH11	1:D:174:ARG:CG	2.30	0.41
1:F:18:ASN:OD1	1:F:18:ASN:C	2.64	0.41
1:F:53:ILE:HG23	1:F:99:PHE:HZ	1.86	0.41
1:F:116:LEU:HD13	1:F:116:LEU:C	2.46	0.41
1:G:65:GLU:C	1:G:67:GLY:H	2.27	0.41
1:G:70:VAL:O	1:G:99:PHE:HB2	2.19	0.41
1:G:148:ASN:HD22	1:G:148:ASN:N	2.19	0.41
1:I:25:PHE:C	1:I:25:PHE:HD2	2.27	0.41
1:B:9:ASP:OD1	1:B:10:PHE:N	2.51	0.41
1:B:75:ILE:HB	1:B:107:LYS:HZ2	1.85	0.41
1:D:45:PHE:CZ	1:D:84:TRP:HA	2.56	0.41
1:E:17:GLY:N	2:E:203:HOH:O	2.37	0.41
1:G:85:LYS:CA	1:G:94:ILE:HG22	2.40	0.41
1:G:116:LEU:HA	1:G:116:LEU:HD23	1.82	0.41
1:A:78:GLU:CG	1:A:79:GLN:NE2	2.83	0.41
1:A:162:PHE:C	1:A:164:GLU:N	2.78	0.41
1:B:41:TRP:CD1	1:B:41:TRP:C	2.99	0.41
1:B:79:GLN:NE2	1:C:43:LYS:NZ	2.69	0.41
1:B:88:PRO:CG	1:B:91:LYS:HD2	2.51	0.41
1:C:27:LEU:C	1:C:29:LYS:N	2.79	0.41
1:C:164:GLU:HB2	1:C:165:HIS:H	1.70	0.41
1:E:22:ASP:OD1	1:E:24:HIS:N	2.53	0.41
1:E:77:SER:OG	1:E:80:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HB3	1:E:140:ILE:HD13	2.02	0.41
1:E:169:CYS:SG	1:F:49:CYS:SG	3.04	0.41
1:F:49:CYS:HB2	1:F:51:THR:HG23	2.02	0.41
1:G:123:LEU:HB3	1:G:140:ILE:HD13	2.03	0.41
1:H:33:LYS:HB2	1:H:33:LYS:HZ3	1.83	0.41
1:H:73:VAL:HB	1:H:102:VAL:HB	2.03	0.41
1:I:78:GLU:CD	1:I:79:GLN:NE2	2.78	0.41
1:I:85:LYS:CA	1:I:94:ILE:HG22	2.41	0.41
1:J:52:GLU:HB2	1:J:53:ILE:HD12	2.02	0.41
1:J:66:LYS:CE	1:J:157:ASP:OD1	2.66	0.41
1:J:148:ASN:HD22	1:J:148:ASN:N	2.18	0.41
1:A:62:ASP:O	1:A:63:PHE:C	2.62	0.41
1:A:68:PHE:CD2	1:A:156:VAL:HG13	2.56	0.41
1:A:163:GLU:HA	1:A:163:GLU:OE1	2.21	0.41
1:B:32:GLY:H	1:B:36:VAL:HG23	1.86	0.41
1:C:6:LEU:CD2	1:C:7:ALA:O	2.67	0.41
1:C:6:LEU:HA	1:C:133:MET:O	2.21	0.41
1:D:136:ARG:NH1	1:D:136:ARG:CB	2.83	0.41
1:D:169:CYS:O	1:D:170:PRO:C	2.63	0.41
1:E:123:LEU:HB3	1:E:140:ILE:CD1	2.51	0.41
1:G:167:GLU:O	1:G:168:VAL:C	2.64	0.41
1:H:41:TRP:CE2	1:H:74:SER:HB2	2.57	0.41
1:H:60:VAL:HG23	1:H:61:LYS:N	2.36	0.41
1:H:60:VAL:HG23	1:H:61:LYS:HE2	2.02	0.41
1:H:136:ARG:HA	1:H:136:ARG:NH1	2.28	0.41
1:I:36:VAL:CG1	1:I:37:ILE:N	2.81	0.41
1:I:162:PHE:CD1	1:I:167:GLU:OE1	2.74	0.41
1:J:39:PHE:O	1:J:72:GLY:HA2	2.20	0.41
1:A:162:PHE:CD1	1:A:167:GLU:OE1	2.74	0.40
1:C:85:LYS:CA	1:C:94:ILE:HG22	2.41	0.40
1:C:167:GLU:O	1:C:168:VAL:C	2.64	0.40
1:D:32:GLY:H	1:D:36:VAL:HG23	1.85	0.40
1:F:11:LYS:HA	1:F:25:PHE:O	2.21	0.40
1:G:88:PRO:O	1:G:91:LYS:N	2.50	0.40
1:H:3:VAL:O	1:H:4:THR:HG23	2.21	0.40
1:H:88:PRO:HB3	1:H:90:GLU:OE2	2.21	0.40
1:I:42:PRO:HB3	1:I:121:ILE:HD12	2.03	0.40
1:A:140:ILE:HD12	1:A:140:ILE:C	2.46	0.40
1:A:167:GLU:O	1:A:168:VAL:C	2.64	0.40
1:B:124:ARG:NH1	1:B:124:ARG:HG2	2.37	0.40
1:C:28:SER:C	1:C:29:LYS:HD2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLU:HA	1:C:163:GLU:OE1	2.20	0.40
1:F:164:GLU:C	1:F:166:GLY:N	2.79	0.40
1:F:174:ARG:HH11	1:F:174:ARG:CG	2.32	0.40
1:G:27:LEU:C	1:G:29:LYS:N	2.79	0.40
1:G:68:PHE:CD2	1:G:156:VAL:HG13	2.56	0.40
1:C:105:ILE:HG23	1:C:106:THR:HG23	2.04	0.40
1:D:2:VAL:O	1:D:135:VAL:CG2	2.70	0.40
1:D:44:ASP:HA	1:D:84:TRP:CZ3	2.56	0.40
1:D:77:SER:OG	1:D:79:GLN:HG2	2.21	0.40
1:G:163:GLU:OE1	1:G:163:GLU:HA	2.21	0.40
1:I:10:PHE:O	1:I:26:GLU:HA	2.21	0.40
1:I:24:HIS:ND1	1:I:24:HIS:N	2.69	0.40
1:A:35:GLY:C	1:A:68:PHE:HD1	2.28	0.40
1:A:148:ASN:N	1:A:148:ASN:HD22	2.20	0.40
1:B:161:HIS:O	1:B:164:GLU:N	2.53	0.40
1:D:40:PHE:CD1	1:D:40:PHE:N	2.90	0.40
1:D:40:PHE:CD2	1:D:73:VAL:HG22	2.57	0.40
1:D:148:ASN:HD22	1:D:149:ALA:N	2.19	0.40
1:E:137:HIS:CD2	1:E:155:MET:HE2	2.57	0.40
1:F:88:PRO:HG2	1:F:91:LYS:HD2	2.02	0.40
1:G:6:LEU:HA	1:G:133:MET:O	2.22	0.40
1:H:145:LEU:H	1:H:145:LEU:HG	1.41	0.40
1:I:22:ASP:OD1	1:I:23:GLU:N	2.55	0.40
1:J:107:LYS:HB2	1:J:111:ARG:NH2	2.37	0.40
1:A:123:LEU:HB3	1:A:140:ILE:CD1	2.52	0.40
1:B:169:CYS:CB	1:B:170:PRO:CD	2.94	0.40
1:E:36:VAL:CG1	1:E:37:ILE:N	2.80	0.40
1:G:130:ASP:C	1:G:132:ASN:H	2.29	0.40
1:I:59:ARG:HD3	1:I:153:LEU:HD22	2.04	0.40
1:J:161:HIS:CB	1:J:165:HIS:HE1	2.33	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:OE2	1:C:90:GLU:OE2[4_555]	2.06	0.14

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	168/198 (85%)	133 (79%)	24 (14%)	11 (6%)	1	1
1	B	173/198 (87%)	138 (80%)	27 (16%)	8 (5%)	2	4
1	C	168/198 (85%)	134 (80%)	22 (13%)	12 (7%)	1	1
1	D	173/198 (87%)	141 (82%)	22 (13%)	10 (6%)	1	2
1	E	168/198 (85%)	134 (80%)	22 (13%)	12 (7%)	1	1
1	F	173/198 (87%)	138 (80%)	27 (16%)	8 (5%)	2	4
1	G	168/198 (85%)	133 (79%)	23 (14%)	12 (7%)	1	1
1	H	173/198 (87%)	136 (79%)	28 (16%)	9 (5%)	1	3
1	I	168/198 (85%)	133 (79%)	23 (14%)	12 (7%)	1	1
1	J	173/198 (87%)	140 (81%)	23 (13%)	10 (6%)	1	2
All	All	1705/1980 (86%)	1360 (80%)	241 (14%)	104 (6%)	1	2

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	145	LEU
1	A	168	VAL
1	B	48	VAL
1	B	170	PRO
1	C	51	THR
1	C	145	LEU
1	C	168	VAL
1	D	48	VAL
1	D	170	PRO
1	E	51	THR
1	E	145	LEU
1	E	168	VAL
1	F	48	VAL

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Mol	Chain	Res	Type
1	F	170	PRO
1	G	51	THR
1	G	145	LEU
1	G	168	VAL
1	H	48	VAL
1	H	170	PRO
1	I	51	THR
1	I	145	LEU
1	I	168	VAL
1	J	48	VAL
1	J	170	PRO
1	A	28	SER
1	A	30	ASN
1	A	166	GLY
1	A	167	GLU
1	B	145	LEU
1	B	165	HIS
1	B	171	ALA
1	C	30	ASN
1	C	166	GLY
1	C	167	GLU
1	D	145	LEU
1	D	165	HIS
1	D	171	ALA
1	E	19	ASN
1	E	28	SER
1	E	30	ASN
1	E	166	GLY
1	E	167	GLU
1	F	145	LEU
1	F	171	ALA
1	G	19	ASN
1	G	28	SER
1	G	30	ASN
1	G	166	GLY
1	G	167	GLU
1	H	145	LEU
1	H	165	HIS
1	H	171	ALA
1	I	28	SER
1	I	30	ASN
1	I	166	GLY

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Mol	Chain	Res	Type
1	I	167	GLU
1	J	145	LEU
1	J	165	HIS
1	J	171	ALA
1	A	19	ASN
1	A	66	LYS
1	C	19	ASN
1	C	28	SER
1	C	131	LYS
1	F	51	THR
1	F	165	HIS
1	I	19	ASN
1	B	52	GLU
1	C	66	LYS
1	C	150	ASP
1	D	42	PRO
1	E	66	LYS
1	E	131	LYS
1	E	150	ASP
1	G	66	LYS
1	G	131	LYS
1	H	42	PRO
1	H	52	GLU
1	I	66	LYS
1	I	131	LYS
1	I	150	ASP
1	J	42	PRO
1	J	51	THR
1	A	150	ASP
1	B	51	THR
1	D	51	THR
1	D	52	GLU
1	D	96	GLN
1	F	42	PRO
1	G	150	ASP
1	H	51	THR
1	J	52	GLU
1	A	42	PRO
1	C	42	PRO
1	D	93	GLY
1	J	96	GLN
1	B	42	PRO

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Mol	Chain	Res	Type
1	F	93	GLY
1	J	93	GLY
1	E	42	PRO
1	I	42	PRO
1	G	42	PRO
1	H	93	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	147/168 (88%)	129 (88%)	18 (12%)	5	14
1	B	150/168 (89%)	133 (89%)	17 (11%)	5	17
1	C	147/168 (88%)	131 (89%)	16 (11%)	6	18
1	D	150/168 (89%)	132 (88%)	18 (12%)	5	14
1	E	147/168 (88%)	131 (89%)	16 (11%)	6	18
1	F	150/168 (89%)	132 (88%)	18 (12%)	5	14
1	G	147/168 (88%)	129 (88%)	18 (12%)	5	14
1	H	150/168 (89%)	132 (88%)	18 (12%)	5	14
1	I	147/168 (88%)	127 (86%)	20 (14%)	3	11
1	J	150/168 (89%)	130 (87%)	20 (13%)	4	12
All	All	1485/1680 (88%)	1306 (88%)	179 (12%)	5	14

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	31	LEU
1	A	33	LYS
1	A	48	VAL
1	A	62	ASP
1	A	73	VAL
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	80	VAL
1	A	90	GLU
1	A	91	LYS
1	A	98	SER
1	A	116	LEU
1	A	123	LEU
1	A	131	LYS
1	A	140	ILE
1	A	145	LEU
1	A	147	ARG
1	A	165	HIS
1	B	33	LYS
1	B	53	ILE
1	B	73	VAL
1	B	80	VAL
1	B	81	HIS
1	B	96	GLN
1	B	123	LEU
1	B	136	ARG
1	B	140	ILE
1	B	141	ASN
1	B	143	LEU
1	B	145	LEU
1	B	148	ASN
1	B	151	GLU
1	B	160	LEU
1	B	167	GLU
1	B	170	PRO
1	C	33	LYS
1	C	48	VAL
1	C	62	ASP
1	C	73	VAL
1	C	79	GLN
1	C	80	VAL
1	C	90	GLU
1	C	91	LYS
1	C	98	SER
1	C	116	LEU
1	C	123	LEU
1	C	131	LYS
1	C	140	ILE
1	C	145	LEU

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Mol	Chain	Res	Type
1	C	147	ARG
1	C	165	HIS
1	D	33	LYS
1	D	53	ILE
1	D	59	ARG
1	D	73	VAL
1	D	80	VAL
1	D	81	HIS
1	D	96	GLN
1	D	123	LEU
1	D	136	ARG
1	D	140	ILE
1	D	141	ASN
1	D	143	LEU
1	D	145	LEU
1	D	148	ASN
1	D	151	GLU
1	D	160	LEU
1	D	167	GLU
1	D	170	PRO
1	E	33	LYS
1	E	48	VAL
1	E	62	ASP
1	E	73	VAL
1	E	79	GLN
1	E	80	VAL
1	E	90	GLU
1	E	91	LYS
1	E	98	SER
1	E	116	LEU
1	E	123	LEU
1	E	131	LYS
1	E	140	ILE
1	E	145	LEU
1	E	147	ARG
1	E	165	HIS
1	F	33	LYS
1	F	53	ILE
1	F	59	ARG
1	F	73	VAL
1	F	80	VAL
1	F	81	HIS

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Mol	Chain	Res	Type
1	F	96	GLN
1	F	123	LEU
1	F	136	ARG
1	F	140	ILE
1	F	141	ASN
1	F	143	LEU
1	F	145	LEU
1	F	148	ASN
1	F	151	GLU
1	F	160	LEU
1	F	167	GLU
1	F	170	PRO
1	G	6	LEU
1	G	31	LEU
1	G	33	LYS
1	G	48	VAL
1	G	62	ASP
1	G	73	VAL
1	G	79	GLN
1	G	80	VAL
1	G	90	GLU
1	G	91	LYS
1	G	98	SER
1	G	116	LEU
1	G	123	LEU
1	G	131	LYS
1	G	140	ILE
1	G	145	LEU
1	G	147	ARG
1	G	165	HIS
1	H	33	LYS
1	H	53	ILE
1	H	73	VAL
1	H	79	GLN
1	H	80	VAL
1	H	81	HIS
1	H	96	GLN
1	H	123	LEU
1	H	136	ARG
1	H	140	ILE
1	H	141	ASN
1	H	143	LEU

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Mol	Chain	Res	Type
1	H	145	LEU
1	H	148	ASN
1	H	151	GLU
1	H	160	LEU
1	H	167	GLU
1	H	170	PRO
1	I	4	THR
1	I	6	LEU
1	I	25	PHE
1	I	31	LEU
1	I	33	LYS
1	I	48	VAL
1	I	62	ASP
1	I	73	VAL
1	I	79	GLN
1	I	80	VAL
1	I	90	GLU
1	I	91	LYS
1	I	98	SER
1	I	116	LEU
1	I	123	LEU
1	I	131	LYS
1	I	140	ILE
1	I	145	LEU
1	I	147	ARG
1	I	165	HIS
1	J	33	LYS
1	J	53	ILE
1	J	59	ARG
1	J	73	VAL
1	J	79	GLN
1	J	80	VAL
1	J	81	HIS
1	J	96	GLN
1	J	123	LEU
1	J	136	ARG
1	J	140	ILE
1	J	141	ASN
1	J	143	LEU
1	J	145	LEU
1	J	148	ASN
1	J	151	GLU

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Mol	Chain	Res	Type
1	J	160	LEU
1	J	167	GLU
1	J	170	PRO
1	J	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	79	GLN
1	A	137	HIS
1	A	148	ASN
1	B	34	ASN
1	B	69	ASN
1	B	79	GLN
1	B	141	ASN
1	B	148	ASN
1	B	161	HIS
1	B	165	HIS
1	C	19	ASN
1	C	79	GLN
1	C	137	HIS
1	C	148	ASN
1	D	34	ASN
1	D	69	ASN
1	D	79	GLN
1	D	137	HIS
1	D	141	ASN
1	D	148	ASN
1	D	161	HIS
1	D	165	HIS
1	E	19	ASN
1	E	79	GLN
1	E	137	HIS
1	E	148	ASN
1	F	34	ASN
1	F	69	ASN
1	F	79	GLN
1	F	141	ASN
1	F	148	ASN
1	F	161	HIS
1	F	165	HIS

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Mol	Chain	Res	Type
1	G	19	ASN
1	G	79	GLN
1	G	132	ASN
1	G	137	HIS
1	G	148	ASN
1	H	34	ASN
1	H	69	ASN
1	H	79	GLN
1	H	141	ASN
1	H	148	ASN
1	H	161	HIS
1	H	165	HIS
1	I	19	ASN
1	I	79	GLN
1	I	132	ASN
1	I	137	HIS
1	I	148	ASN
1	J	34	ASN
1	J	69	ASN
1	J	79	GLN
1	J	141	ASN
1	J	148	ASN
1	J	161	HIS
1	J	165	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	170/198 (85%)	0.96	20 (11%) 9 8	35, 59, 103, 126	0
1	B	175/198 (88%)	0.65	20 (11%) 10 9	28, 51, 94, 105	0
1	C	170/198 (85%)	0.97	23 (13%) 7 6	35, 59, 103, 126	0
1	D	175/198 (88%)	0.68	26 (14%) 5 5	28, 51, 94, 105	0
1	E	170/198 (85%)	0.82	13 (7%) 20 18	35, 59, 103, 126	0
1	F	175/198 (88%)	0.60	20 (11%) 10 9	28, 51, 94, 105	0
1	G	170/198 (85%)	0.84	13 (7%) 20 18	35, 59, 103, 126	0
1	H	175/198 (88%)	0.56	12 (6%) 23 19	28, 51, 94, 105	0
1	I	170/198 (85%)	0.99	29 (17%) 4 3	35, 59, 103, 126	0
1	J	175/198 (88%)	0.73	19 (10%) 10 9	28, 51, 94, 105	0
All	All	1725/1980 (87%)	0.78	195 (11%) 10 9	28, 56, 95, 126	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	169	CYS	7.0
1	E	169	CYS	6.2
1	C	170	PRO	5.3
1	C	169	CYS	4.9
1	I	170	PRO	4.8
1	D	143	LEU	4.7
1	J	168	VAL	4.6
1	A	169	CYS	4.6
1	A	170	PRO	4.6
1	I	168	VAL	4.4
1	E	170	PRO	4.3
1	A	165	HIS	4.2
1	J	49	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	168	VAL	4.1
1	G	170	PRO	4.0
1	A	166	GLY	4.0
1	F	144	PRO	3.9
1	B	165	HIS	3.9
1	C	145	LEU	3.9
1	I	91	LYS	3.8
1	G	168	VAL	3.8
1	C	168	VAL	3.7
1	H	170	PRO	3.6
1	C	165	HIS	3.5
1	D	144	PRO	3.5
1	J	165	HIS	3.5
1	F	49	CYS	3.5
1	D	166	GLY	3.3
1	J	146	GLY	3.3
1	E	168	VAL	3.3
1	D	163	GLU	3.3
1	B	64	HIS	3.2
1	D	168	VAL	3.2
1	J	155	MET	3.2
1	J	144	PRO	3.2
1	H	143	LEU	3.2
1	C	162	PHE	3.2
1	F	165	HIS	3.1
1	H	144	PRO	3.1
1	J	170	PRO	3.1
1	D	173	TRP	3.1
1	F	146	GLY	3.1
1	G	145	LEU	3.0
1	E	165	HIS	3.0
1	D	49	CYS	3.0
1	D	174	ARG	3.0
1	F	169	CYS	3.0
1	C	161	HIS	3.0
1	B	146	GLY	3.0
1	B	144	PRO	3.0
1	D	165	HIS	3.0
1	I	165	HIS	3.0
1	B	166	GLY	2.9
1	D	141	ASN	2.9
1	E	144	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	169	CYS	2.9
1	C	147	ARG	2.9
1	D	145	LEU	2.9
1	I	28	SER	2.9
1	G	165	HIS	2.9
1	B	168	VAL	2.9
1	I	144	PRO	2.9
1	B	164	GLU	2.9
1	G	169	CYS	2.9
1	G	162	PHE	2.8
1	C	64	HIS	2.8
1	C	65	GLU	2.8
1	B	143	LEU	2.8
1	E	29	LYS	2.8
1	I	29	LYS	2.8
1	C	94	ILE	2.8
1	D	64	HIS	2.8
1	A	76	ASP	2.8
1	B	167	GLU	2.7
1	A	168	VAL	2.7
1	C	31	LEU	2.7
1	I	145	LEU	2.7
1	J	36	VAL	2.7
1	D	175	LYS	2.7
1	F	174	ARG	2.7
1	G	92	GLY	2.7
1	I	51	THR	2.7
1	A	26	GLU	2.6
1	H	167	GLU	2.6
1	A	64	HIS	2.6
1	B	174	ARG	2.6
1	C	160	LEU	2.6
1	I	166	GLY	2.6
1	F	175	LYS	2.6
1	H	168	VAL	2.6
1	H	64	HIS	2.6
1	C	58	LYS	2.6
1	I	162	PHE	2.6
1	A	66	LYS	2.5
1	F	61	LYS	2.5
1	C	92	GLY	2.5
1	J	64	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	172	GLY	2.5
1	J	48	VAL	2.5
1	C	151	GLU	2.5
1	E	167	GLU	2.5
1	C	93	GLY	2.5
1	F	155	MET	2.5
1	B	150	ASP	2.5
1	D	36	VAL	2.5
1	A	25	PHE	2.5
1	I	20	GLU	2.5
1	J	174	ARG	2.5
1	J	145	LEU	2.4
1	D	162	PHE	2.4
1	D	51	THR	2.4
1	F	64	HIS	2.4
1	I	30	ASN	2.4
1	C	91	LYS	2.4
1	D	167	GLU	2.4
1	F	58	LYS	2.4
1	F	143	LEU	2.4
1	I	143	LEU	2.4
1	H	141	ASN	2.4
1	H	49	CYS	2.4
1	G	66	LYS	2.4
1	H	164	GLU	2.4
1	I	23	GLU	2.4
1	G	96	GLN	2.4
1	A	94	ILE	2.4
1	B	147	ARG	2.4
1	J	175	LYS	2.4
1	B	162	PHE	2.4
1	E	162	PHE	2.4
1	D	171	ALA	2.4
1	F	170	PRO	2.4
1	A	92	GLY	2.3
1	I	150	ASP	2.3
1	B	173	TRP	2.3
1	E	145	LEU	2.3
1	A	58	LYS	2.3
1	C	36	VAL	2.3
1	I	21	VAL	2.3
1	H	172	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	65	GLU	2.3
1	J	143	LEU	2.3
1	I	48	VAL	2.3
1	G	95	GLY	2.3
1	D	50	PRO	2.3
1	B	172	GLY	2.3
1	G	65	GLU	2.2
1	B	19	ASN	2.2
1	F	141	ASN	2.2
1	I	64	HIS	2.2
1	A	164	GLU	2.2
1	G	167	GLU	2.2
1	I	52	GLU	2.2
1	I	15	VAL	2.2
1	H	173	TRP	2.2
1	J	162	PHE	2.2
1	F	167	GLU	2.2
1	C	150	ASP	2.2
1	D	146	GLY	2.2
1	D	172	GLY	2.2
1	A	162	PHE	2.2
1	D	169	CYS	2.2
1	C	167	GLU	2.2
1	E	52	GLU	2.2
1	J	163	GLU	2.2
1	C	148	ASN	2.1
1	B	36	VAL	2.1
1	F	145	LEU	2.1
1	F	171	ALA	2.1
1	A	20	GLU	2.1
1	A	65	GLU	2.1
1	I	167	GLU	2.1
1	B	57	ASP	2.1
1	I	147	ARG	2.1
1	J	147	ARG	2.1
1	I	161	HIS	2.1
1	B	48	VAL	2.1
1	D	89	VAL	2.1
1	I	92	GLY	2.1
1	D	33	LYS	2.1
1	E	161	HIS	2.1
1	I	36	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	167	GLU	2.1
1	H	175	LYS	2.0
1	F	48	VAL	2.0
1	I	34	ASN	2.0
1	A	93	GLY	2.0
1	C	166	GLY	2.0
1	F	162	PHE	2.0
1	I	76	ASP	2.0
1	B	170	PRO	2.0
1	D	170	PRO	2.0
1	G	166	GLY	2.0
1	A	29	LYS	2.0
1	D	61	LYS	2.0
1	E	133	MET	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.