



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:34 AM UTC

PDB ID : 1PKU / pdb_00001pku
Title : Crystal Structure of Nucleoside Diphosphate Kinase from Rice
Authors : Huang, J.-Y.; Chang, C.-Y.; Chang, T.; Chen, C.-J.
Deposited on : 2003-06-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

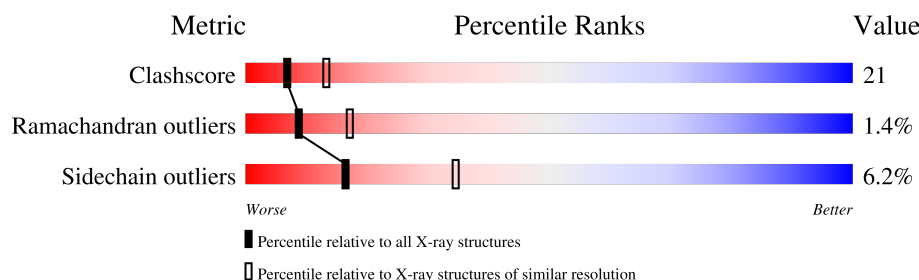
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	150	57% 37% 5% .
1	B	150	59% 39% ..
1	C	150	55% 39% 5% .
1	D	150	59% 36% . ..
1	E	150	52% 43% 5% .
1	F	150	64% 31% . ..
1	G	150	51% 44% 5% .
1	H	150	54% 39% 6% .

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Mol	Chain	Length	Quality of chain
1	I	150	54%39%5% ..
1	J	150	57%37%. ..
1	K	150	55%39%5% .
1	L	150	42%51%5% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14578 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 Nucleoside Diphosphate Kinase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	B	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	C	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	D	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	E	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	F	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	G	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	H	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	I	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	J	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	K	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			
1	L	149	Total	C	N	O	S	0	0	0
			1196	771	209	211	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ARG	-	cloning artifact	UNP Q07661
B	3	ARG	-	cloning artifact	UNP Q07661
C	3	ARG	-	cloning artifact	UNP Q07661
D	3	ARG	-	cloning artifact	UNP Q07661
E	3	ARG	-	cloning artifact	UNP Q07661

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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	ARG	-	cloning artifact	UNP Q07661
G	3	ARG	-	cloning artifact	UNP Q07661
H	3	ARG	-	cloning artifact	UNP Q07661
I	3	ARG	-	cloning artifact	UNP Q07661
J	3	ARG	-	cloning artifact	UNP Q07661
K	3	ARG	-	cloning artifact	UNP Q07661
L	3	ARG	-	cloning artifact	UNP Q07661

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	30	Total O 30 30	0	0
2	B	25	Total O 25 25	0	0
2	C	31	Total O 31 31	0	0
2	D	19	Total O 19 19	0	0
2	E	14	Total O 14 14	0	0
2	F	21	Total O 21 21	0	0
2	G	6	Total O 6 6	0	0
2	H	9	Total O 9 9	0	0
2	I	16	Total O 16 16	0	0
2	J	15	Total O 15 15	0	0
2	K	27	Total O 27 27	0	0
2	L	13	Total O 13 13	0	0

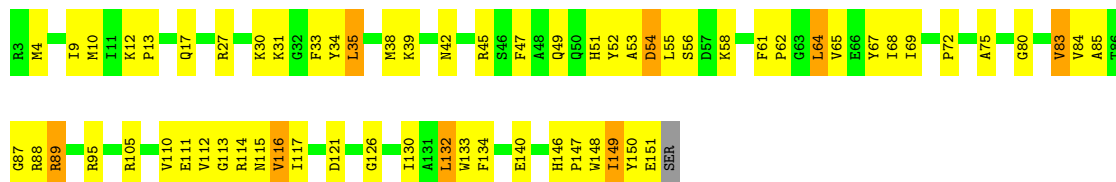
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

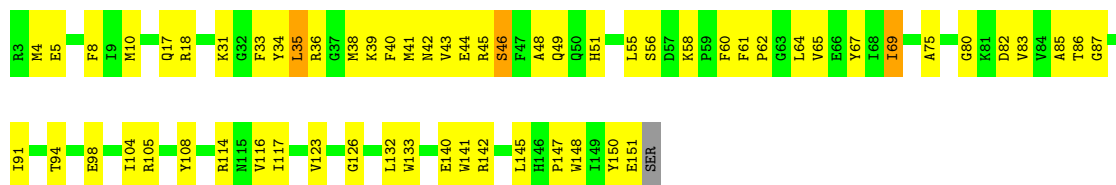
• Molecule 1: Nucleoside Diphosphate Kinase I

Chain A: 



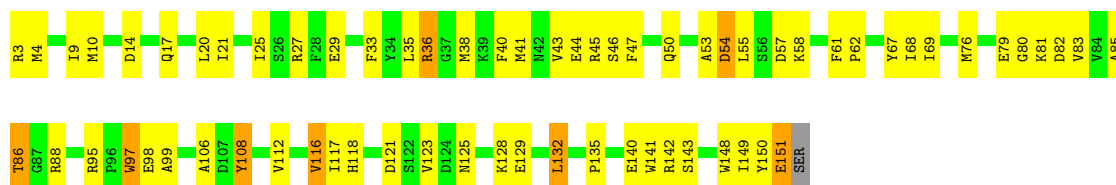
• Molecule 1: Nucleoside Diphosphate Kinase I

Chain B: 



• Molecule 1: Nucleoside Diphosphate Kinase I

Chain C: 



• Molecule 1: Nucleoside Diphosphate Kinase I

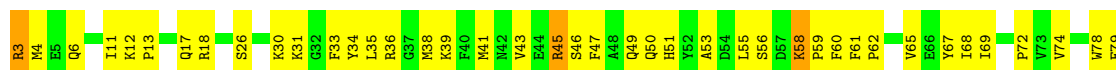
Chain D: 





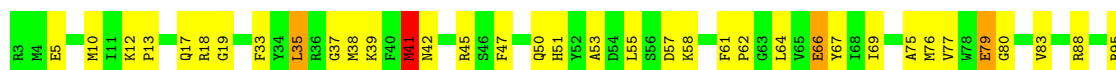
• Molecule 1: Nucleoside Diphosphate Kinase I

Chain E: 52% 43% 5%



• Molecule 1: Nucleoside Diphosphate Kinase I

Chain F: 64% 31%



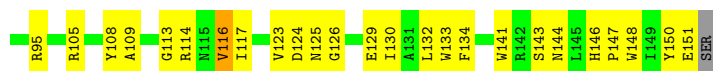
• Molecule 1: Nucleoside Diphosphate Kinase I

Chain G: 51% 44% 5%



• Molecule 1: Nucleoside Diphosphate Kinase I

Chain H: 54% 39% 6%



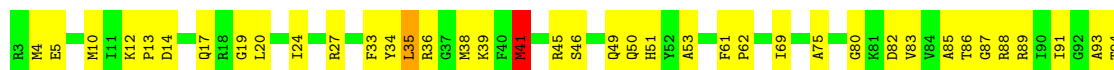
• Molecule 1: Nucleoside Diphosphate Kinase I

Chain I: 54% 39% 5%

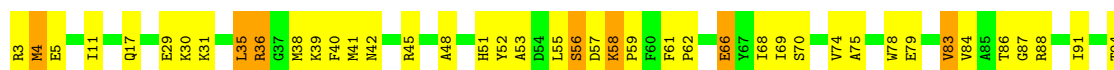




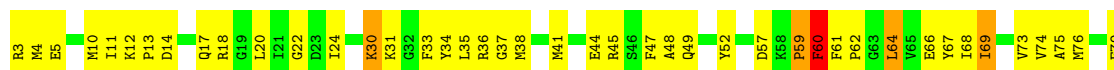
• Molecule 1: Nucleoside Diphosphate Kinase I



• Molecule 1: Nucleoside Diphosphate Kinase I



• Molecule 1: Nucleoside Diphosphate Kinase I



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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.95Å 182.94Å 188.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14578	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	0.50	0/1229	1.00	7/1661 (0.4%)
1	B	0.48	0/1229	1.02	6/1661 (0.4%)
1	C	0.49	0/1229	0.99	5/1661 (0.3%)
1	D	0.49	0/1229	0.98	6/1661 (0.4%)
1	E	0.49	0/1229	0.98	6/1661 (0.4%)
1	F	0.49	0/1229	1.02	7/1661 (0.4%)
1	G	0.46	0/1229	1.03	7/1661 (0.4%)
1	H	0.42	0/1229	1.01	8/1661 (0.5%)
1	I	0.47	0/1229	0.96	2/1661 (0.1%)
1	J	0.48	0/1229	0.97	5/1661 (0.3%)
1	K	0.47	0/1229	1.00	7/1661 (0.4%)
1	L	0.48	0/1229	0.99	2/1661 (0.1%)
All	All	0.48	0/14748	1.00	68/19932 (0.3%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	116	VAL	N-CA-C	8.51	127.03	109.34
1	H	4	MET	N-CA-C	8.18	120.07	108.54
1	E	116	VAL	N-CA-C	8.14	126.27	109.34
1	G	58	LYS	CA-C-N	7.84	128.56	119.47
1	G	58	LYS	C-N-CA	7.84	128.56	119.47
1	H	116	VAL	N-CA-C	7.51	124.97	109.34
1	F	41	MET	N-CA-C	7.42	119.43	108.60
1	I	116	VAL	N-CA-C	7.32	124.57	109.34
1	B	116	VAL	N-CA-C	7.31	124.55	109.34
1	J	41	MET	N-CA-C	7.22	120.14	109.24
1	F	116	VAL	N-CA-C	7.21	124.33	109.34
1	F	58	LYS	CA-C-N	6.99	128.58	119.84
1	F	58	LYS	C-N-CA	6.99	128.58	119.84
1	C	58	LYS	CA-C-N	6.96	126.78	119.05
1	C	58	LYS	C-N-CA	6.96	126.78	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	VAL	N-CA-C	6.85	123.58	109.34
1	A	116	VAL	N-CA-C	6.82	123.53	109.34
1	G	116	VAL	N-CA-C	6.79	123.46	109.34
1	C	41	MET	N-CA-C	6.67	118.26	108.86
1	C	116	VAL	N-CA-C	6.58	123.02	109.34
1	A	4	MET	N-CA-C	-6.55	103.61	112.26
1	G	136	GLU	N-CA-C	-6.55	100.79	110.48
1	D	58	LYS	CA-C-N	6.52	126.75	119.32
1	D	58	LYS	C-N-CA	6.52	126.75	119.32
1	K	70	SER	N-CA-C	6.51	121.37	113.17
1	D	41	MET	N-CA-C	6.33	118.17	108.42
1	B	98	GLU	N-CA-C	-6.28	105.39	114.12
1	B	58	LYS	CA-C-N	6.10	125.65	119.19
1	B	58	LYS	C-N-CA	6.10	125.65	119.19
1	D	87	GLY	N-CA-C	-6.03	105.05	112.77
1	D	83	VAL	CB-CA-C	-5.95	104.36	111.97
1	I	4	MET	N-CA-C	5.93	118.13	110.65
1	J	116	VAL	N-CA-C	5.92	121.66	109.34
1	G	104	ILE	N-CA-C	5.88	116.62	110.62
1	A	149	ILE	N-CA-C	-5.82	107.82	113.53
1	H	45	ARG	N-CA-C	5.77	118.06	111.02
1	F	67	TYR	N-CA-C	5.70	117.17	111.07
1	H	87	GLY	N-CA-C	-5.70	105.89	112.73
1	K	58	LYS	CA-C-N	5.69	125.22	119.19
1	K	58	LYS	C-N-CA	5.69	125.22	119.19
1	E	117	ILE	N-CA-C	5.65	115.68	107.88
1	C	4	MET	N-CA-C	-5.54	104.05	111.87
1	E	45	ARG	N-CA-C	5.51	117.72	111.11
1	H	41	MET	N-CA-C	5.49	117.41	109.07
1	B	126	GLY	N-CA-C	-5.44	106.20	112.73
1	F	79	GLU	N-CA-C	5.44	117.66	109.23
1	L	116	VAL	N-CA-C	5.39	120.56	109.34
1	K	42	ASN	N-CA-C	-5.39	100.39	109.07
1	J	98	GLU	N-CA-C	-5.37	106.66	114.12
1	E	58	LYS	CA-C-N	5.36	126.54	119.84
1	E	58	LYS	C-N-CA	5.36	126.54	119.84
1	K	112	VAL	N-CA-C	5.33	115.53	110.42
1	J	125	ASN	N-CA-C	-5.30	106.07	112.54
1	A	83	VAL	CB-CA-C	-5.28	105.21	111.97
1	E	67	TYR	N-CA-C	5.27	117.11	111.36
1	L	60	PHE	N-CA-C	5.24	121.97	110.80
1	A	58	LYS	CA-C-N	5.23	125.53	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LYS	C-N-CA	5.23	125.53	119.47
1	H	109	ALA	N-CA-C	5.21	118.06	109.72
1	F	117	ILE	N-CA-C	5.17	116.35	108.80
1	B	41	MET	N-CA-C	5.16	116.68	108.79
1	G	98	GLU	N-CA-C	-5.16	105.74	113.89
1	J	117	ILE	N-CA-C	5.13	115.76	108.42
1	K	56	SER	N-CA-C	5.12	118.31	111.75
1	A	87	GLY	N-CA-C	-5.10	106.24	112.77
1	H	58	LYS	CA-C-N	5.08	126.19	119.84
1	H	58	LYS	C-N-CA	5.08	126.19	119.84
1	G	109	ALA	N-CA-C	5.05	117.97	109.95

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	1196	0	1178	58	0
1	B	1196	0	1178	56	0
1	C	1196	0	1178	58	0
1	D	1196	0	1178	47	0
1	E	1196	0	1178	62	0
1	F	1196	0	1178	42	0
1	G	1196	0	1178	64	0
1	H	1196	0	1178	58	0
1	I	1196	0	1178	59	0
1	J	1196	0	1178	56	0
1	K	1196	0	1178	53	0
1	L	1196	0	1178	72	0
2	A	30	0	0	2	0
2	B	25	0	0	1	0
2	C	31	0	0	3	0
2	D	19	0	0	0	0
2	E	14	0	0	1	0
2	F	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	6	0	0	0	0
2	H	9	0	0	2	0
2	I	16	0	0	0	0
2	J	15	0	0	1	0
2	K	27	0	0	1	0
2	L	13	0	0	0	0
All	All	14578	0	14136	608	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 21.

All (608) 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:3:ARG:HG3	1:E:4:MET:H	1.12	1.10
1:E:3:ARG:HH11	1:E:3:ARG:HA	1.15	1.06
1:E:3:ARG:HA	1:E:3:ARG:NH1	1.73	1.04
1:E:88:ARG:HD2	1:E:121:ASP:HA	1.40	0.99
1:J:12:LYS:NZ	1:J:115:ASN:HD21	1.62	0.98
1:G:142:ARG:HH11	1:G:142:ARG:HB3	1.28	0.94
1:E:150:TYR:O	1:E:151:GLU:HB2	1.68	0.91
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.33	0.89
1:H:108:TYR:HE2	1:K:30:LYS:HD3	1.33	0.88
1:J:82:ASP:OD1	1:J:86:THR:HG23	1.75	0.87
1:G:113:GLY:O	1:G:114:ARG:HD3	1.77	0.84
1:J:61:PHE:HB3	1:J:62:PRO:HD3	1.58	0.84
1:A:89:ARG:HH11	1:A:89:ARG:HB3	1.44	0.82
1:H:61:PHE:HB3	1:H:62:PRO:HD3	1.61	0.82
1:H:126:GLY:O	1:H:130:ILE:HG13	1.81	0.80
1:J:125:ASN:O	1:J:129:GLU:HG3	1.81	0.80
1:K:17:GLN:HG3	1:L:148:TRP:CE2	2.18	0.79
1:L:48:ALA:HB2	1:L:69:ILE:HD13	1.63	0.78
1:E:3:ARG:HG3	1:E:4:MET:N	1.92	0.78
1:G:17:GLN:HG3	1:I:148:TRP:CE2	2.19	0.78
1:L:125:ASN:O	1:L:129:GLU:HG3	1.83	0.77
1:H:86:THR:HG22	1:H:89:ARG:HH21	1.50	0.77
1:H:108:TYR:CE2	1:K:30:LYS:HD3	2.20	0.76
1:E:80:GLY:O	1:E:83:VAL:HG23	1.85	0.76
1:L:44:GLU:C	1:L:69:ILE:HD11	2.11	0.76
1:L:61:PHE:HB3	1:L:62:PRO:HD3	1.67	0.76
1:A:64:LEU:O	1:A:68:ILE:HG12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:PHE:HE2	1:F:132:LEU:HD22	1.52	0.75
1:J:88:ARG:HD2	1:J:121:ASP:HA	1.69	0.75
1:C:97:TRP:H	1:C:97:TRP:CD1	2.00	0.75
1:G:80:GLY:O	1:G:83:VAL:HG23	1.86	0.74
1:E:61:PHE:HB3	1:E:62:PRO:HD3	1.68	0.74
1:E:125:ASN:O	1:E:129:GLU:HG3	1.86	0.74
1:B:61:PHE:HB3	1:B:62:PRO:HD3	1.68	0.74
1:A:61:PHE:HB3	1:A:62:PRO:HD3	1.70	0.73
1:G:105:ARG:CD	1:G:115:ASN:HB2	2.19	0.73
1:H:148:TRP:CE2	1:L:17:GLN:HG3	2.24	0.73
1:J:12:LYS:HZ2	1:J:115:ASN:HD21	1.37	0.72
1:D:97:TRP:H	1:D:97:TRP:CD1	2.04	0.72
1:G:113:GLY:C	1:G:114:ARG:HD3	2.14	0.72
1:H:113:GLY:O	1:H:114:ARG:HD3	1.89	0.72
1:D:91:ILE:HG23	1:D:117:ILE:HG23	1.70	0.72
1:D:80:GLY:O	1:D:83:VAL:HG22	1.89	0.72
1:A:149:ILE:HG13	1:A:150:TYR:CD1	2.24	0.72
1:C:135:PRO:HB2	1:I:132:LEU:HD23	1.72	0.71
1:L:47:PHE:HE1	1:L:132:LEU:HD22	1.55	0.71
1:A:52:TYR:HE2	1:A:68:ILE:HG13	1.55	0.71
1:C:61:PHE:HB3	1:C:62:PRO:HD3	1.72	0.71
1:L:95:ARG:HD2	1:L:97:TRP:CH2	2.26	0.71
1:B:94:THR:HA	1:B:105:ARG:NH1	2.06	0.70
1:B:150:TYR:O	1:B:151:GLU:HB2	1.90	0.70
1:G:145:LEU:HD11	1:K:145:LEU:HD11	1.74	0.70
1:D:140:GLU:H	1:D:140:GLU:CD	1.99	0.70
1:B:150:TYR:HD2	1:F:111:GLU:OE2	1.75	0.70
1:L:149:ILE:HG13	1:L:150:TYR:CD1	2.26	0.70
1:I:45:ARG:O	1:I:49:GLN:HG3	1.91	0.69
1:I:42:ASN:HD21	1:L:140:GLU:H	1.39	0.69
1:K:66:GLU:O	1:K:69:ILE:HG22	1.93	0.69
1:B:148:TRP:CE2	1:F:17:GLN:HG3	2.28	0.69
1:E:59:PRO:O	1:E:62:PRO:HD2	1.94	0.68
1:C:36:ARG:HH11	1:C:79:GLU:CD	2.01	0.68
1:J:33:PHE:CE1	1:J:83:VAL:HG12	2.29	0.67
1:A:80:GLY:O	1:A:83:VAL:HG23	1.94	0.67
1:C:125:ASN:O	1:C:129:GLU:HG3	1.95	0.67
1:A:45:ARG:HA	1:A:69:ILE:HD11	1.77	0.67
1:C:40:PHE:CD2	1:F:35:LEU:HD13	2.30	0.67
1:L:64:LEU:HD12	1:L:64:LEU:H	1.60	0.66
1:D:82:ASP:OD2	1:D:86:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ARG:CG	1:E:4:MET:H	1.95	0.66
1:B:80:GLY:O	1:B:83:VAL:HG13	1.96	0.65
1:I:125:ASN:O	1:I:129:GLU:HG3	1.96	0.65
1:B:31:LYS:HA	1:F:107:ASP:O	1.97	0.65
1:C:150:TYR:O	1:C:151:GLU:HB2	1.95	0.65
1:E:51:HIS:CD2	1:E:133:TRP:HE1	2.15	0.65
1:L:34:TYR:OH	1:L:149:ILE:HD11	1.97	0.65
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.05	0.64
1:G:10:MET:O	1:G:117:ILE:HG13	1.98	0.64
1:K:51:HIS:HD2	1:K:133:TRP:HE1	1.46	0.64
1:G:140:GLU:H	1:H:42:ASN:ND2	1.95	0.64
1:K:88:ARG:HH21	1:K:121:ASP:HB3	1.62	0.64
1:J:45:ARG:O	1:J:49:GLN:HG3	1.97	0.64
1:L:5:GLU:HG3	1:L:83:VAL:HG22	1.79	0.64
1:G:5:GLU:O	1:G:79:GLU:HG3	1.96	0.64
1:G:142:ARG:HH11	1:G:142:ARG:CB	2.08	0.64
1:B:17:GLN:HG3	1:E:148:TRP:CE2	2.33	0.64
1:B:31:LYS:HE2	1:B:86:THR:HG21	1.81	0.63
1:J:12:LYS:HZ1	1:J:115:ASN:HD21	1.44	0.63
1:J:45:ARG:HG3	1:J:69:ILE:CD1	2.28	0.63
1:G:124:ASP:O	1:G:128:LYS:HG3	1.98	0.63
1:K:36:ARG:HD3	1:K:79:GLU:OE2	1.99	0.62
1:I:24:ILE:HG21	1:I:117:ILE:HD12	1.80	0.62
1:L:4:MET:HE2	1:L:150:TYR:CE2	2.34	0.62
1:G:82:ASP:O	1:G:86:THR:HG23	2.00	0.62
1:G:9:ILE:CG2	1:G:117:ILE:HD11	2.30	0.62
1:B:10:MET:O	1:B:117:ILE:HG13	2.00	0.61
1:C:38:MET:SD	1:F:38:MET:HE3	2.39	0.61
1:K:36:ARG:HH21	1:K:141:TRP:H	1.48	0.61
1:F:80:GLY:O	1:F:83:VAL:HG13	2.00	0.61
1:G:61:PHE:HB3	1:G:62:PRO:HD3	1.80	0.61
1:K:39:LYS:HG3	1:K:41:MET:HE3	1.82	0.61
1:A:52:TYR:CE2	1:A:68:ILE:HG13	2.34	0.61
1:C:54:ASP:O	1:C:55:LEU:HD23	2.00	0.61
1:D:88:ARG:NH2	1:D:121:ASP:HB3	2.15	0.61
1:H:82:ASP:OD1	1:H:86:THR:HG23	2.00	0.61
1:G:41:MET:HE2	1:G:133:TRP:CZ3	2.36	0.61
1:D:45:ARG:HA	1:D:69:ILE:HD11	1.83	0.61
1:G:31:LYS:HE3	1:J:109:ALA:O	2.01	0.61
1:L:31:LYS:HG2	1:L:33:PHE:CE2	2.36	0.61
1:C:36:ARG:HD3	1:C:79:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:LEU:HD21	1:L:145:LEU:HG	1.83	0.60
1:C:17:GLN:HG3	1:D:148:TRP:CE2	2.35	0.60
1:I:97:TRP:CD1	1:I:97:TRP:H	2.17	0.60
1:E:26:SER:OG	1:E:30:LYS:HE3	2.01	0.60
1:L:64:LEU:H	1:L:64:LEU:CD1	2.14	0.60
1:L:95:ARG:HB2	1:L:98:GLU:HB3	1.82	0.60
1:E:95:ARG:HD3	1:E:97:TRP:CZ2	2.36	0.60
1:J:12:LYS:NZ	1:J:115:ASN:ND2	2.42	0.60
1:A:89:ARG:HH11	1:A:89:ARG:CB	2.13	0.60
1:K:56:SER:HA	1:K:61:PHE:CD1	2.36	0.60
1:F:61:PHE:HB3	1:F:62:PRO:HD3	1.83	0.60
1:H:150:TYR:O	1:H:151:GLU:HB2	2.00	0.60
1:G:142:ARG:HB3	1:G:142:ARG:NH1	2.10	0.60
1:K:61:PHE:HB3	1:K:62:PRO:HD3	1.83	0.60
1:A:45:ARG:O	1:A:49:GLN:HG3	2.02	0.59
1:E:123:VAL:O	1:E:127:LYS:HG3	2.02	0.59
1:I:105:ARG:HE	1:I:115:ASN:HB2	1.67	0.59
1:B:18:ARG:HD2	1:E:149:ILE:HG22	1.82	0.59
1:L:64:LEU:HD12	1:L:64:LEU:N	2.16	0.59
1:L:45:ARG:O	1:L:49:GLN:HG3	2.02	0.59
1:B:114:ARG:NH1	1:E:147:PRO:O	2.36	0.59
1:C:29:GLU:OE2	1:F:19:GLY:HA2	2.02	0.59
1:H:125:ASN:O	1:H:129:GLU:HG3	2.02	0.59
1:G:89:ARG:HG2	1:G:89:ARG:HH11	1.68	0.59
1:C:82:ASP:O	1:C:86:THR:HG23	2.02	0.59
1:D:12:LYS:HE3	1:D:118:HIS:HB2	1.85	0.58
1:G:40:PHE:CD2	1:H:35:LEU:HD13	2.38	0.58
1:B:43:VAL:HB	1:B:69:ILE:HD12	1.85	0.58
1:F:5:GLU:HG3	1:F:83:VAL:HG22	1.85	0.58
1:H:55:LEU:C	1:H:57:ASP:H	2.11	0.58
1:L:99:ALA:CB	1:L:106:ALA:HB2	2.33	0.58
1:G:88:ARG:NH2	1:G:121:ASP:HB3	2.17	0.58
1:H:56:SER:HA	1:H:61:PHE:CD1	2.38	0.58
1:J:39:LYS:HE3	1:J:41:MET:HE3	1.85	0.58
1:L:48:ALA:CB	1:L:69:ILE:HD13	2.31	0.58
1:J:51:HIS:HD2	1:J:133:TRP:HE1	1.50	0.58
1:G:17:GLN:HG3	1:I:148:TRP:NE1	2.18	0.58
1:H:151:GLU:HA	1:H:151:GLU:OE1	2.02	0.58
1:K:51:HIS:CD2	1:K:133:TRP:HE1	2.22	0.58
1:L:97:TRP:CD1	1:L:97:TRP:H	2.20	0.58
1:B:105:ARG:NH2	1:B:117:ILE:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:CG2	1:C:117:ILE:HD11	2.34	0.58
1:D:94:THR:HA	1:D:105:ARG:NH1	2.19	0.58
1:D:61:PHE:HB3	1:D:62:PRO:HD3	1.86	0.58
1:L:105:ARG:NE	1:L:115:ASN:HB2	2.19	0.58
1:E:68:ILE:HG12	1:E:68:ILE:O	2.03	0.57
1:J:14:ASP:OD1	1:J:116:VAL:HA	2.04	0.57
1:L:38:MET:HA	1:L:75:ALA:O	2.04	0.57
1:A:10:MET:O	1:A:117:ILE:HG13	2.04	0.57
1:H:17:GLN:HG3	1:K:148:TRP:CE2	2.39	0.57
1:A:68:ILE:HD11	2:A:156:HOH:O	2.04	0.57
1:G:89:ARG:HG2	1:G:89:ARG:NH1	2.19	0.57
1:I:47:PHE:CE1	1:I:132:LEU:HD22	2.39	0.57
1:B:82:ASP:OD2	1:F:97:TRP:HB2	2.04	0.57
1:I:150:TYR:O	1:I:151:GLU:HB2	2.05	0.57
1:L:48:ALA:HB2	1:L:69:ILE:CD1	2.33	0.57
1:B:44:GLU:OE2	1:B:46:SER:HB3	2.03	0.57
1:D:55:LEU:O	1:D:58:LYS:HG2	2.04	0.57
1:I:51:HIS:CD2	1:I:133:TRP:HE1	2.22	0.57
1:I:88:ARG:NH2	1:I:121:ASP:HB3	2.20	0.57
1:K:36:ARG:NH2	1:K:141:TRP:H	2.03	0.57
1:C:3:ARG:HB2	2:C:158:HOH:O	2.05	0.56
1:E:94:THR:HG22	1:E:112:VAL:HG13	1.87	0.56
1:G:11:ILE:HB	1:G:74:VAL:HB	1.86	0.56
1:D:125:ASN:O	1:D:129:GLU:HG3	2.05	0.56
1:L:89:ARG:HG2	1:L:89:ARG:HH11	1.70	0.56
1:A:35:LEU:HD13	1:B:40:PHE:CD2	2.40	0.56
1:A:39:LYS:HE2	1:A:134:PHE:CE1	2.39	0.56
1:B:5:GLU:CG	1:B:83:VAL:HG22	2.35	0.56
1:C:108:TYR:CE2	1:D:30:LYS:HD3	2.41	0.56
1:H:82:ASP:OD1	1:H:85:ALA:HB3	2.05	0.56
1:H:147:PRO:O	1:L:114:ARG:NH1	2.38	0.56
1:K:31:LYS:HE2	1:K:86:THR:HG21	1.87	0.56
1:L:99:ALA:HB3	1:L:106:ALA:HB2	1.87	0.56
1:B:33:PHE:CD1	1:B:83:VAL:HG12	2.40	0.56
1:L:20:LEU:O	1:L:24:ILE:HG12	2.04	0.56
1:A:140:GLU:H	1:B:42:ASN:ND2	2.04	0.56
1:I:38:MET:SD	1:L:38:MET:HE3	2.46	0.56
1:E:39:LYS:HD2	1:E:41:MET:HE3	1.87	0.56
1:F:41:MET:C	1:F:41:MET:HE3	2.30	0.56
1:G:22:GLY:HA3	1:H:26:SER:OG	2.06	0.56
1:I:4:MET:HE3	1:I:79:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:35:LEU:HD23	1:K:78:TRP:CE2	2.40	0.56
1:K:99:ALA:HB3	1:K:106:ALA:HB2	1.88	0.55
1:D:124:ASP:O	1:D:128:LYS:HG3	2.06	0.55
1:G:33:PHE:CE1	1:G:83:VAL:HG22	2.40	0.55
1:L:37:GLY:O	1:L:76:MET:HA	2.06	0.55
1:H:36:ARG:NH1	1:H:79:GLU:OE2	2.40	0.55
1:I:95:ARG:HD3	1:I:97:TRP:CH2	2.41	0.55
1:B:8:PHE:HE1	1:B:75:ALA:HB1	1.72	0.55
1:K:87:GLY:O	1:K:91:ILE:HG13	2.07	0.55
1:G:41:MET:HE2	1:G:133:TRP:HZ3	1.72	0.55
1:G:150:TYR:O	1:G:151:GLU:HB2	2.05	0.55
1:D:52:TYR:HE2	1:D:68:ILE:HG13	1.72	0.55
1:D:60:PHE:O	1:D:64:LEU:HD13	2.07	0.55
1:J:35:LEU:HD13	1:K:40:PHE:CD2	2.42	0.55
1:K:3:ARG:HG3	1:K:4:MET:N	2.22	0.55
1:C:50:GLN:HA	1:C:50:GLN:NE2	2.23	0.54
1:A:12:LYS:HB3	1:A:13:PRO:HD2	1.89	0.54
1:K:83:VAL:HG23	1:K:84:VAL:H	1.72	0.54
1:A:34:TYR:OH	1:A:149:ILE:HD11	2.08	0.54
1:F:12:LYS:HB3	1:F:13:PRO:HD2	1.89	0.54
1:A:31:LYS:HG2	1:A:33:PHE:CE2	2.42	0.54
1:C:69:ILE:O	1:C:69:ILE:HG22	2.07	0.54
1:A:80:GLY:O	1:A:83:VAL:CG2	2.55	0.54
1:D:10:MET:HE1	1:D:133:TRP:CH2	2.43	0.54
1:I:40:PHE:CE1	1:I:72:PRO:HB2	2.42	0.54
1:A:42:ASN:HD21	1:B:140:GLU:H	1.56	0.54
1:E:56:SER:HA	1:E:61:PHE:CD1	2.43	0.54
1:K:146:HIS:N	1:K:147:PRO:HD2	2.23	0.54
1:L:10:MET:HE3	1:L:73:VAL:HG11	1.90	0.54
1:L:123:VAL:HG12	1:L:127:LYS:HE3	1.90	0.54
1:B:33:PHE:CE1	1:B:83:VAL:HG12	2.42	0.54
1:A:88:ARG:NH2	1:A:121:ASP:HB3	2.23	0.54
1:B:56:SER:HA	1:B:61:PHE:CD1	2.43	0.54
1:C:47:PHE:CE1	1:C:132:LEU:HD22	2.43	0.53
1:H:36:ARG:HG3	1:H:36:ARG:HH11	1.73	0.53
1:B:82:ASP:OD1	1:B:85:ALA:HB3	2.08	0.53
1:I:86:THR:O	1:I:89:ARG:HB3	2.08	0.53
1:J:38:MET:HA	1:J:75:ALA:O	2.09	0.53
1:J:45:ARG:HG3	1:J:69:ILE:HD12	1.90	0.53
1:A:148:TRP:CE2	1:D:17:GLN:HG3	2.43	0.53
1:B:48:ALA:HB2	1:B:69:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:HA	1:C:69:ILE:HD11	1.91	0.53
1:J:88:ARG:NH1	1:J:121:ASP:HB3	2.23	0.53
1:F:33:PHE:CE1	1:F:83:VAL:HG12	2.43	0.53
1:D:87:GLY:O	1:D:91:ILE:HG13	2.08	0.53
1:H:36:ARG:HH12	1:H:79:GLU:CD	2.16	0.53
1:A:39:LYS:HA	1:B:38:MET:O	2.08	0.53
1:H:113:GLY:C	1:H:114:ARG:HD3	2.33	0.53
1:L:33:PHE:CD1	1:L:83:VAL:HG12	2.44	0.53
1:A:114:ARG:NH1	1:A:114:ARG:CG	2.69	0.53
1:D:83:VAL:O	1:D:87:GLY:N	2.40	0.53
1:G:45:ARG:O	1:G:49:GLN:HG3	2.09	0.53
1:L:14:ASP:O	1:L:18:ARG:HB2	2.09	0.53
1:B:5:GLU:HG3	1:B:83:VAL:HG22	1.91	0.52
1:G:72:PRO:HD3	1:H:141:TRP:HB3	1.91	0.52
1:G:80:GLY:C	1:G:83:VAL:HG23	2.33	0.52
1:I:3:ARG:HG2	1:I:4:MET:H	1.74	0.52
1:L:126:GLY:O	1:L:130:ILE:HG13	2.09	0.52
1:A:95:ARG:HA	1:A:112:VAL:HG22	1.91	0.52
1:C:99:ALA:CB	1:C:106:ALA:HB2	2.39	0.52
1:B:80:GLY:C	1:B:83:VAL:HG13	2.35	0.52
1:A:110:VAL:HG21	1:C:149:ILE:HG22	1.92	0.52
1:B:56:SER:HA	1:B:61:PHE:CG	2.45	0.52
1:G:140:GLU:H	1:H:42:ASN:HD21	1.57	0.52
1:G:6:GLN:HA	1:G:78:TRP:O	2.10	0.52
1:L:4:MET:HE2	1:L:150:TYR:HE2	1.75	0.52
1:E:43:VAL:O	1:E:69:ILE:HG23	2.09	0.51
1:F:10:MET:HE2	1:F:133:TRP:CZ2	2.45	0.51
1:B:48:ALA:HB3	1:B:65:VAL:HG13	1.91	0.51
1:I:3:ARG:CG	1:I:4:MET:H	2.23	0.51
1:A:12:LYS:HB3	1:A:13:PRO:CD	2.41	0.51
1:A:17:GLN:HG3	1:C:148:TRP:CE2	2.45	0.51
1:C:117:ILE:HG12	1:C:118:HIS:N	2.25	0.51
1:E:36:ARG:HH21	1:E:79:GLU:CD	2.17	0.51
1:H:114:ARG:NH1	1:K:147:PRO:O	2.42	0.51
1:B:45:ARG:HG2	1:B:49:GLN:HE21	1.76	0.51
1:G:114:ARG:NH1	1:I:147:PRO:O	2.44	0.51
1:E:17:GLN:HG3	1:F:148:TRP:CE2	2.46	0.51
1:G:126:GLY:O	1:G:130:ILE:HG13	2.10	0.51
1:C:44:GLU:OE1	1:C:46:SER:HB2	2.11	0.51
1:D:126:GLY:O	1:D:130:ILE:HG13	2.10	0.51
1:I:126:GLY:O	1:I:130:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:MET:CE	1:D:133:TRP:CH2	2.93	0.51
1:J:51:HIS:CD2	1:J:133:TRP:HE1	2.28	0.51
1:J:80:GLY:C	1:J:83:VAL:HG13	2.36	0.51
1:G:38:MET:HB2	1:G:76:MET:HG2	1.93	0.51
1:C:43:VAL:O	1:C:69:ILE:HG23	2.11	0.51
1:I:44:GLU:HG3	1:I:47:PHE:H	1.75	0.51
1:K:39:LYS:HE3	1:K:41:MET:HE1	1.93	0.51
1:D:33:PHE:CD1	1:D:80:GLY:HA3	2.46	0.50
1:J:96:PRO:HB3	1:J:109:ALA:O	2.10	0.50
1:A:38:MET:HA	1:A:75:ALA:O	2.11	0.50
1:E:33:PHE:CE1	1:E:83:VAL:HG22	2.46	0.50
1:E:39:LYS:CD	1:E:41:MET:HE3	2.42	0.50
1:C:82:ASP:OD2	1:C:85:ALA:HB3	2.11	0.50
1:F:146:HIS:N	1:F:147:PRO:HD2	2.27	0.50
1:G:105:ARG:O	1:G:109:ALA:HB3	2.12	0.50
1:L:11:ILE:HB	1:L:74:VAL:HB	1.93	0.50
1:F:53:ALA:C	1:F:55:LEU:H	2.19	0.50
1:D:51:HIS:CD2	1:D:133:TRP:HE1	2.30	0.50
1:L:91:ILE:HG23	1:L:117:ILE:CG2	2.42	0.50
1:A:110:VAL:HG23	1:A:111:GLU:N	2.27	0.49
1:C:20:LEU:HD22	1:C:108:TYR:CD2	2.47	0.49
1:E:36:ARG:HD2	2:E:155:HOH:O	2.12	0.49
1:H:44:GLU:C	1:H:69:ILE:HD11	2.37	0.49
1:A:51:HIS:HD2	1:A:133:TRP:HE1	1.58	0.49
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.25	0.49
1:D:9:ILE:CG2	1:D:117:ILE:HD11	2.43	0.49
1:A:110:VAL:HG22	2:A:157:HOH:O	2.11	0.49
1:F:39:LYS:HG3	1:F:75:ALA:HB3	1.93	0.49
1:G:145:LEU:HG	1:K:145:LEU:HD21	1.93	0.49
1:I:35:LEU:HD23	1:I:78:TRP:CE2	2.47	0.49
1:J:93:ALA:O	1:J:95:ARG:N	2.42	0.49
1:L:82:ASP:CG	1:L:85:ALA:HB3	2.37	0.49
1:C:17:GLN:HG3	1:D:148:TRP:CD2	2.48	0.49
1:E:6:GLN:HA	1:E:78:TRP:O	2.13	0.49
1:F:38:MET:HA	1:F:75:ALA:O	2.12	0.49
1:C:88:ARG:HD3	1:C:121:ASP:HA	1.94	0.49
1:D:132:LEU:HD23	1:D:132:LEU:O	2.13	0.49
1:D:52:TYR:CE2	1:D:68:ILE:HG13	2.48	0.49
1:F:33:PHE:CD1	1:F:83:VAL:HG12	2.48	0.49
1:G:80:GLY:N	1:G:83:VAL:HG21	2.28	0.49
1:H:36:ARG:NH1	1:H:79:GLU:CD	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:MET:HA	1:G:74:VAL:O	2.13	0.49
1:E:46:SER:O	1:E:50:GLN:HG3	2.12	0.48
1:I:89:ARG:HG3	1:I:89:ARG:HH11	1.78	0.48
1:D:56:SER:HA	1:D:61:PHE:CD1	2.48	0.48
1:L:105:ARG:HE	1:L:115:ASN:HB2	1.76	0.48
1:E:95:ARG:HD2	1:E:98:GLU:OE2	2.13	0.48
1:L:96:PRO:C	1:L:98:GLU:H	2.21	0.48
1:A:51:HIS:CD2	1:A:133:TRP:HE1	2.30	0.48
1:C:27:ARG:HH22	1:C:108:TYR:HE1	1.61	0.48
1:C:88:ARG:HH11	1:C:121:ASP:HB2	1.77	0.48
1:H:86:THR:HG21	2:H:154:HOH:O	2.14	0.48
1:J:19:GLY:HA2	1:K:29:GLU:OE2	2.13	0.48
1:K:36:ARG:NH2	1:K:141:TRP:O	2.46	0.48
1:L:82:ASP:OD2	1:L:85:ALA:HB3	2.14	0.48
1:B:67:TYR:C	1:B:69:ILE:H	2.20	0.48
1:H:146:HIS:N	1:H:147:PRO:HD2	2.29	0.48
1:I:97:TRP:CD1	1:I:97:TRP:N	2.79	0.48
1:C:140:GLU:H	1:F:42:ASN:HD21	1.60	0.48
1:F:41:MET:HE3	1:F:41:MET:O	2.14	0.48
1:K:3:ARG:HG3	1:K:4:MET:H	1.77	0.48
1:B:60:PHE:O	1:B:64:LEU:HB2	2.14	0.48
1:E:58:LYS:HD3	1:E:60:PHE:CZ	2.49	0.48
1:I:56:SER:HA	1:I:61:PHE:CD1	2.48	0.48
1:I:56:SER:HA	1:I:61:PHE:CG	2.49	0.48
1:I:82:ASP:OD2	1:I:86:THR:HG23	2.12	0.48
1:K:124:ASP:O	1:K:128:LYS:HD3	2.13	0.48
1:L:94:THR:O	1:L:96:PRO:HD3	2.14	0.48
1:C:21:ILE:O	1:C:25:ILE:HG13	2.14	0.48
1:H:12:LYS:O	1:H:16:VAL:HG23	2.14	0.48
1:L:149:ILE:HG13	1:L:150:TYR:HD1	1.73	0.48
1:D:69:ILE:HG22	1:D:69:ILE:O	2.13	0.48
1:L:33:PHE:CE1	1:L:83:VAL:HG12	2.49	0.47
1:B:145:LEU:HD22	1:F:18:ARG:HG2	1.96	0.47
1:H:62:PRO:O	1:H:66:GLU:HG2	2.14	0.47
1:L:113:GLY:O	1:L:114:ARG:HD3	2.14	0.47
1:H:114:ARG:HG3	1:H:114:ARG:HH11	1.79	0.47
1:J:12:LYS:HZ1	1:J:115:ASN:ND2	2.09	0.47
1:J:33:PHE:CD1	1:J:83:VAL:HG12	2.49	0.47
1:K:3:ARG:CG	1:K:4:MET:N	2.74	0.47
1:J:110:VAL:HG23	1:J:111:GLU:HG3	1.97	0.47
1:A:114:ARG:HD3	1:C:148:TRP:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:GLY:O	1:F:76:MET:HA	2.15	0.47
1:A:151:GLU:OE2	1:A:151:GLU:HA	2.15	0.47
1:C:88:ARG:CD	1:C:121:ASP:HA	2.44	0.47
1:I:61:PHE:N	1:I:62:PRO:CD	2.78	0.47
1:J:80:GLY:O	1:J:83:VAL:HG13	2.14	0.47
1:C:82:ASP:CG	1:C:85:ALA:HB3	2.40	0.47
1:F:12:LYS:HB3	1:F:13:PRO:CD	2.44	0.47
1:F:95:ARG:HB2	1:F:98:GLU:HB2	1.96	0.47
1:K:66:GLU:C	1:K:69:ILE:HG22	2.39	0.47
1:A:31:LYS:HG2	1:A:33:PHE:CD2	2.49	0.47
1:A:27:ARG:HA	1:A:30:LYS:HE2	1.97	0.46
1:G:67:TYR:OH	1:G:114:ARG:HD2	2.15	0.46
1:G:88:ARG:HH21	1:G:121:ASP:HB3	1.78	0.46
1:J:12:LYS:CE	1:J:115:ASN:HD21	2.27	0.46
1:K:108:TYR:CE2	1:L:30:LYS:HD3	2.49	0.46
1:A:69:ILE:O	1:A:69:ILE:HG22	2.15	0.46
1:H:17:GLN:HG3	1:K:148:TRP:NE1	2.30	0.46
1:C:99:ALA:HB3	1:C:106:ALA:HB2	1.97	0.46
1:D:68:ILE:HD13	1:D:68:ILE:N	2.30	0.46
1:E:45:ARG:HA	1:E:69:ILE:HD11	1.96	0.46
1:E:80:GLY:N	1:E:83:VAL:HG21	2.30	0.46
1:I:146:HIS:N	1:I:147:PRO:HD2	2.31	0.46
1:L:146:HIS:N	1:L:147:PRO:HD2	2.31	0.46
1:F:79:GLU:C	1:F:83:VAL:HG11	2.40	0.46
1:H:36:ARG:HD2	2:H:156:HOH:O	2.14	0.46
1:I:26:SER:OG	1:L:22:GLY:HA3	2.15	0.46
1:L:100:ALA:O	1:L:103:THR:HG23	2.15	0.46
1:C:36:ARG:NH1	1:C:79:GLU:OE2	2.49	0.46
1:D:140:GLU:CD	1:D:140:GLU:N	2.68	0.46
1:C:20:LEU:HD22	1:C:108:TYR:CE2	2.51	0.46
1:G:52:TYR:CE2	1:G:68:ILE:HD12	2.50	0.46
1:I:17:GLN:HG3	1:J:148:TRP:CE2	2.50	0.46
1:I:93:ALA:O	1:I:105:ARG:HD2	2.15	0.46
1:I:109:ALA:HB2	1:I:116:VAL:HG23	1.97	0.46
1:K:100:ALA:O	1:K:103:THR:HG23	2.16	0.46
1:A:113:GLY:O	1:A:114:ARG:HG3	2.15	0.46
1:B:94:THR:HA	1:B:105:ARG:HH11	1.77	0.46
1:C:53:ALA:C	1:C:55:LEU:H	2.24	0.46
1:K:95:ARG:HD2	1:K:97:TRP:CZ2	2.50	0.46
1:A:105:ARG:CZ	1:A:115:ASN:HD22	2.29	0.46
1:D:45:ARG:O	1:D:49:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:HB2	1:C:150:TYR:HE2	1.80	0.46
1:K:11:ILE:HB	1:K:74:VAL:HB	1.98	0.46
1:J:128:LYS:HB2	1:J:128:LYS:NZ	2.30	0.46
1:K:17:GLN:HG3	1:L:148:TRP:NE1	2.30	0.46
1:K:45:ARG:HD2	2:K:158:HOH:O	2.16	0.46
1:L:123:VAL:CG1	1:L:127:LYS:HE3	2.46	0.46
1:B:34:TYR:HB3	1:B:36:ARG:HH11	1.81	0.45
1:G:105:ARG:HD2	1:G:115:ASN:HB2	1.93	0.45
1:A:146:HIS:N	1:A:147:PRO:HD2	2.31	0.45
1:C:86:THR:HG21	2:C:167:HOH:O	2.16	0.45
1:E:49:GLN:HG2	1:E:61:PHE:HZ	1.81	0.45
1:J:39:LYS:HA	1:K:38:MET:O	2.16	0.45
1:E:140:GLU:H	1:E:140:GLU:HG2	1.44	0.45
1:G:38:MET:HA	1:G:75:ALA:O	2.15	0.45
1:G:148:TRP:CE2	1:J:17:GLN:HG3	2.51	0.45
1:I:14:ASP:OD1	1:I:67:TYR:OH	2.31	0.45
1:J:10:MET:O	1:J:117:ILE:HG13	2.16	0.45
1:K:55:LEU:O	1:K:58:LYS:HB2	2.15	0.45
1:L:12:LYS:HB3	1:L:13:PRO:CD	2.46	0.45
1:L:91:ILE:HG23	1:L:117:ILE:HG23	1.99	0.45
1:A:126:GLY:O	1:A:130:ILE:HG13	2.16	0.45
1:C:95:ARG:HA	1:C:112:VAL:HG22	1.99	0.45
1:E:80:GLY:C	1:E:83:VAL:HG23	2.42	0.45
1:E:146:HIS:HB3	1:E:147:PRO:CD	2.47	0.45
1:D:129:GLU:O	1:D:133:TRP:HD1	2.00	0.45
1:E:11:ILE:HB	1:E:74:VAL:HB	1.99	0.45
1:F:39:LYS:HE3	1:F:134:PHE:CE2	2.52	0.45
1:J:38:MET:O	1:K:39:LYS:HA	2.16	0.45
1:E:53:ALA:C	1:E:55:LEU:N	2.75	0.45
1:L:95:ARG:HB2	1:L:98:GLU:CB	2.47	0.45
1:J:12:LYS:HZ2	1:J:115:ASN:ND2	2.09	0.45
1:K:94:THR:O	1:K:96:PRO:HD3	2.17	0.45
1:L:86:THR:O	1:L:90:ILE:HG13	2.17	0.45
1:A:67:TYR:HD1	1:A:68:ILE:HD13	1.81	0.45
1:F:136:GLU:HA	1:I:42:ASN:HB3	1.99	0.45
1:I:35:LEU:C	1:I:35:LEU:HD13	2.42	0.45
1:J:27:ARG:NH2	1:J:108:TYR:HE1	2.15	0.45
1:K:38:MET:HA	1:K:75:ALA:O	2.17	0.45
1:K:48:ALA:HB1	1:K:68:ILE:HD11	1.99	0.45
1:D:22:GLY:O	1:D:23:ASP:C	2.60	0.44
1:F:47:PHE:O	1:F:50:GLN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:HG23	1:F:134:PHE:CE1	2.52	0.44
1:H:77:VAL:HG23	1:H:134:PHE:CE2	2.53	0.44
1:I:81:LYS:HD3	1:I:82:ASP:HB2	1.99	0.44
1:L:44:GLU:O	1:L:69:ILE:HD11	2.17	0.44
1:D:117:ILE:HG12	1:D:118:HIS:N	2.33	0.44
1:G:147:PRO:O	1:J:114:ARG:NH1	2.50	0.44
1:K:52:TYR:O	1:K:53:ALA:C	2.61	0.44
1:L:139:ALA:C	1:L:140:GLU:HG3	2.42	0.44
1:E:3:ARG:O	1:E:4:MET:SD	2.75	0.44
1:F:117:ILE:HG12	1:F:118:HIS:N	2.33	0.44
1:J:146:HIS:N	1:J:147:PRO:HD2	2.33	0.44
1:B:4:MET:HA	2:B:157:HOH:O	2.17	0.44
1:E:65:VAL:O	1:E:69:ILE:HG13	2.17	0.44
1:G:37:GLY:O	1:G:76:MET:HA	2.17	0.44
1:G:89:ARG:HH11	1:G:89:ARG:CG	2.31	0.44
1:H:35:LEU:HB2	1:H:78:TRP:CZ3	2.53	0.44
1:A:85:ALA:O	1:A:89:ARG:HG3	2.18	0.44
1:I:142:ARG:HH11	1:I:142:ARG:HG3	1.82	0.44
1:K:35:LEU:HD23	1:K:78:TRP:CZ2	2.52	0.44
1:D:36:ARG:HB3	1:D:138:LEU:HD13	1.99	0.44
1:H:48:ALA:CB	1:H:65:VAL:HG13	2.48	0.44
1:L:60:PHE:O	1:L:61:PHE:C	2.60	0.44
1:E:12:LYS:HB3	1:E:13:PRO:HD2	1.99	0.44
1:I:136:GLU:OE2	1:I:136:GLU:N	2.47	0.44
1:A:67:TYR:CE2	1:A:114:ARG:NH2	2.86	0.44
1:B:104:ILE:O	1:B:108:TYR:HD1	2.00	0.44
1:H:48:ALA:HB2	1:H:69:ILE:HD13	2.00	0.44
1:H:105:ARG:NH2	1:H:117:ILE:O	2.43	0.44
1:J:12:LYS:HB3	1:J:13:PRO:HD2	2.00	0.44
1:A:9:ILE:CG2	1:A:117:ILE:HD11	2.48	0.43
1:B:4:MET:HG3	1:B:4:MET:O	2.18	0.43
1:B:80:GLY:N	1:B:83:VAL:HG11	2.33	0.43
1:J:144:ASN:O	1:L:144:ASN:HB3	2.17	0.43
1:K:140:GLU:O	1:K:141:TRP:HB3	2.18	0.43
1:E:86:THR:HA	1:E:89:ARG:NH1	2.32	0.43
1:F:45:ARG:HG3	1:F:45:ARG:HH11	1.83	0.43
1:I:61:PHE:HB3	1:I:62:PRO:HD3	2.00	0.43
1:I:101:PRO:CG	1:J:89:ARG:HG2	2.48	0.43
1:J:115:ASN:C	1:J:115:ASN:HD22	2.26	0.43
1:D:141:TRP:CG	1:E:72:PRO:HG3	2.53	0.43
1:E:47:PHE:CE2	1:E:132:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:ALA:C	1:F:55:LEU:N	2.74	0.43
1:H:55:LEU:O	1:H:57:ASP:N	2.47	0.43
1:I:51:HIS:HD2	1:I:133:TRP:HE1	1.66	0.43
1:J:4:MET:O	1:J:4:MET:HG3	2.17	0.43
1:L:3:ARG:C	1:L:4:MET:SD	3.01	0.43
1:A:72:PRO:HD3	1:B:141:TRP:HB3	1.99	0.43
1:D:47:PHE:CZ	1:D:132:LEU:HD22	2.53	0.43
1:E:53:ALA:C	1:E:55:LEU:H	2.26	0.43
1:F:117:ILE:HG12	1:F:118:HIS:H	1.83	0.43
1:I:55:LEU:C	1:I:57:ASP:H	2.27	0.43
1:A:140:GLU:H	1:B:42:ASN:HD21	1.65	0.43
1:A:149:ILE:HG22	1:D:18:ARG:HD2	2.00	0.43
1:G:9:ILE:HG23	1:G:117:ILE:HD11	1.99	0.43
1:H:5:GLU:O	1:H:79:GLU:HG3	2.18	0.43
1:I:21:ILE:O	1:I:22:GLY:C	2.61	0.43
1:J:61:PHE:HB3	1:J:62:PRO:CD	2.39	0.43
1:B:67:TYR:C	1:B:69:ILE:N	2.77	0.43
1:C:36:ARG:NH2	1:C:141:TRP:O	2.51	0.43
1:D:39:LYS:HA	1:E:38:MET:O	2.19	0.43
1:G:17:GLN:HE22	1:H:143:SER:HA	1.84	0.43
1:J:5:GLU:HG3	1:J:83:VAL:HG22	2.01	0.43
1:J:87:GLY:O	1:J:91:ILE:HG13	2.19	0.43
1:A:114:ARG:HD3	1:C:148:TRP:O	2.18	0.43
1:D:117:ILE:CG1	1:D:118:HIS:N	2.81	0.43
1:H:144:ASN:OD1	1:I:148:TRP:NE1	2.46	0.43
1:I:81:LYS:HD3	1:I:81:LYS:C	2.44	0.43
1:E:149:ILE:HG13	1:E:150:TYR:CD1	2.54	0.43
1:J:82:ASP:OD2	1:J:85:ALA:HB3	2.19	0.43
1:L:52:TYR:CE2	1:L:68:ILE:HG13	2.54	0.43
1:D:37:GLY:O	1:D:76:MET:HA	2.19	0.42
1:G:95:ARG:HA	1:G:112:VAL:HG22	2.00	0.42
1:L:18:ARG:NH1	1:L:18:ARG:HG2	2.34	0.42
1:B:147:PRO:O	1:F:114:ARG:NH1	2.52	0.42
1:E:86:THR:O	1:E:90:ILE:HG13	2.19	0.42
1:F:45:ARG:HG3	1:F:45:ARG:NH1	2.34	0.42
1:C:10:MET:O	1:C:117:ILE:HG13	2.20	0.42
1:E:43:VAL:HG13	1:E:47:PHE:HD1	1.84	0.42
1:H:45:ARG:NH1	1:H:66:GLU:OE2	2.52	0.42
1:E:34:TYR:OH	1:E:149:ILE:HD11	2.19	0.42
1:E:12:LYS:HB3	1:E:13:PRO:CD	2.49	0.42
1:G:27:ARG:HA	1:G:30:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:LEU:CD1	1:L:64:LEU:N	2.79	0.42
1:L:88:ARG:HH21	1:L:121:ASP:HB3	1.85	0.42
1:B:82:ASP:CG	1:B:85:ALA:HB3	2.45	0.42
1:C:14:ASP:HB3	1:C:67:TYR:OH	2.20	0.42
1:F:45:ARG:NH2	1:F:66:GLU:OE2	2.52	0.42
1:H:10:MET:HE2	1:H:133:TRP:CZ2	2.55	0.42
1:H:123:VAL:HG23	1:H:124:ASP:N	2.34	0.42
1:I:38:MET:HA	1:I:75:ALA:O	2.19	0.42
1:I:105:ARG:NE	1:I:115:ASN:HB2	2.32	0.42
1:D:142:ARG:NH1	1:D:142:ARG:HG3	2.35	0.42
1:E:31:LYS:HG2	1:E:33:PHE:CE2	2.55	0.42
1:G:80:GLY:N	1:G:83:VAL:CG2	2.83	0.42
1:H:55:LEU:C	1:H:57:ASP:N	2.77	0.42
1:I:12:LYS:HB3	1:I:13:PRO:HD2	2.01	0.42
1:J:49:GLN:O	1:J:53:ALA:N	2.53	0.42
1:A:53:ALA:C	1:A:55:LEU:H	2.27	0.42
1:B:5:GLU:HG3	1:B:83:VAL:CG2	2.49	0.42
1:B:55:LEU:O	1:B:61:PHE:HB2	2.19	0.42
1:E:95:ARG:HB3	1:E:97:TRP:CE2	2.55	0.42
1:G:35:LEU:O	1:H:40:PHE:CE2	2.73	0.42
1:K:150:TYR:O	1:K:151:GLU:HB3	2.20	0.42
1:C:143:SER:HA	1:F:17:GLN:HE22	1.85	0.42
1:E:49:GLN:HG2	1:E:61:PHE:CZ	2.55	0.42
1:K:99:ALA:CB	1:K:106:ALA:HB2	2.49	0.42
1:C:38:MET:HG3	1:C:76:MET:HG2	2.02	0.42
1:C:80:GLY:O	1:C:83:VAL:HG13	2.20	0.42
1:D:72:PRO:HD3	1:E:141:TRP:HB3	2.02	0.42
1:G:86:THR:O	1:G:90:ILE:HG13	2.20	0.42
1:J:36:ARG:HD2	2:J:156:HOH:O	2.20	0.42
1:K:121:ASP:OD1	1:K:122:SER:N	2.53	0.42
1:G:8:PHE:HB3	1:G:129:GLU:OE1	2.19	0.41
1:H:12:LYS:HB3	1:H:13:PRO:CD	2.50	0.41
1:I:91:ILE:HG22	1:I:105:ARG:NH1	2.35	0.41
1:A:65:VAL:O	1:A:69:ILE:HG13	2.19	0.41
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.82	0.41
1:B:114:ARG:HA	1:B:114:ARG:HD3	1.75	0.41
1:F:88:ARG:HE	1:F:121:ASP:CB	2.33	0.41
1:G:45:ARG:HB2	1:G:45:ARG:NH1	2.36	0.41
1:G:146:HIS:N	1:G:147:PRO:HD2	2.36	0.41
1:H:80:GLY:O	1:H:83:VAL:HG13	2.19	0.41
1:I:53:ALA:C	1:I:55:LEU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:SER:O	1:J:50:GLN:HG3	2.20	0.41
1:L:14:ASP:OD2	1:L:67:TYR:OH	2.36	0.41
1:B:51:HIS:CD2	1:B:133:TRP:HE1	2.39	0.41
1:B:94:THR:HG22	1:B:105:ARG:HH12	1.85	0.41
1:B:8:PHE:CE1	1:B:75:ALA:HB1	2.52	0.41
1:I:80:GLY:O	1:I:83:VAL:HG22	2.21	0.41
1:A:47:PHE:HE1	1:A:132:LEU:HD22	1.86	0.41
1:C:69:ILE:HG21	1:L:135:PRO:CG	2.50	0.41
1:D:11:ILE:HD13	1:D:21:ILE:HA	2.03	0.41
1:F:51:HIS:CD2	1:F:133:TRP:HE1	2.38	0.41
1:I:16:VAL:HG13	1:I:21:ILE:HD11	2.03	0.41
1:J:34:TYR:OH	1:J:146:HIS:CD2	2.73	0.41
1:E:18:ARG:NH1	1:E:108:TYR:O	2.52	0.41
1:I:10:MET:O	1:I:117:ILE:HG13	2.20	0.41
1:A:38:MET:O	1:B:39:LYS:HA	2.20	0.41
1:I:105:ARG:HE	1:I:115:ASN:CB	2.31	0.41
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.87	0.41
1:C:142:ARG:HG2	1:C:142:ARG:HH11	1.85	0.41
1:G:17:GLN:HG3	1:I:148:TRP:CD1	2.56	0.41
1:G:145:LEU:CD1	1:K:145:LEU:HD11	2.48	0.41
1:H:6:GLN:HG2	1:H:79:GLU:HG3	2.03	0.41
1:H:36:ARG:HA	1:H:36:ARG:HD3	1.90	0.41
1:H:68:ILE:O	1:H:68:ILE:HG12	2.21	0.41
1:J:115:ASN:ND2	1:J:115:ASN:C	2.78	0.41
1:B:44:GLU:CD	1:B:46:SER:H	2.29	0.41
1:B:87:GLY:O	1:B:91:ILE:HG13	2.21	0.41
1:C:57:ASP:HB2	2:C:173:HOH:O	2.20	0.41
1:C:95:ARG:HB2	1:C:98:GLU:HG3	2.02	0.41
1:E:39:LYS:CE	1:E:41:MET:HE3	2.51	0.41
1:E:146:HIS:C	1:E:148:TRP:H	2.28	0.41
1:G:39:LYS:HA	1:H:38:MET:O	2.21	0.41
1:H:3:ARG:O	1:H:4:MET:SD	2.79	0.41
1:L:117:ILE:HG12	1:L:118:HIS:N	2.36	0.41
1:C:33:PHE:CD1	1:C:83:VAL:HG12	2.56	0.40
1:C:61:PHE:O	1:C:62:PRO:C	2.63	0.40
1:E:94:THR:HA	1:E:105:ARG:NH1	2.36	0.40
1:G:105:ARG:HD3	1:G:115:ASN:O	2.21	0.40
1:C:50:GLN:HA	1:C:50:GLN:HE21	1.86	0.40
1:H:43:VAL:HB	1:H:69:ILE:HD12	2.03	0.40
1:I:36:ARG:HE	1:I:79:GLU:CD	2.29	0.40
1:L:12:LYS:HB3	1:L:13:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:ARG:HE	1:L:79:GLU:CD	2.29	0.40
1:H:55:LEU:HD13	1:H:60:PHE:HE1	1.86	0.40
1:K:58:LYS:HA	1:K:59:PRO:HD3	1.88	0.40
1:G:58:LYS:HA	1:G:59:PRO:HD3	1.83	0.40
1:J:20:LEU:O	1:J:24:ILE:HG13	2.21	0.40
1:E:60:PHE:O	1:E:61:PHE:C	2.63	0.40
1:J:151:GLU:CD	1:J:151:GLU:O	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/150 (98%)	136 (92%)	7 (5%)	4 (3%)	4	6
1	B	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
1	C	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	17
1	D	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	34
1	E	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	34
1	F	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	18	34
1	G	147/150 (98%)	132 (90%)	12 (8%)	3 (2%)	6	10
1	H	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	10
1	I	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	10
1	J	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	6	10
1	K	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
1	L	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	10
All	All	1764/1800 (98%)	1625 (92%)	115 (6%)	24 (1%)	9	17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	E	116	VAL
1	G	116	VAL
1	H	5	GLU
1	H	116	VAL
1	C	116	VAL
1	H	56	SER
1	A	56	SER
1	C	54	ASP
1	G	93	ALA
1	G	137	GLY
1	I	56	SER
1	J	94	THR
1	L	59	PRO
1	L	60	PHE
1	L	116	VAL
1	J	95	ARG
1	J	116	VAL
1	A	54	ASP
1	F	116	VAL
1	I	116	VAL
1	I	21	ILE
1	A	84	VAL
1	D	116	VAL

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	123/124 (99%)	118 (96%)	5 (4%)	27	53
1	B	123/124 (99%)	117 (95%)	6 (5%)	22	45
1	C	123/124 (99%)	113 (92%)	10 (8%)	11	23
1	D	123/124 (99%)	116 (94%)	7 (6%)	18	39
1	E	123/124 (99%)	118 (96%)	5 (4%)	27	53
1	F	123/124 (99%)	115 (94%)	8 (6%)	15	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	123/124 (99%)	115 (94%)	8 (6%)	15	32
1	H	123/124 (99%)	115 (94%)	8 (6%)	15	32
1	I	123/124 (99%)	114 (93%)	9 (7%)	13	27
1	J	123/124 (99%)	117 (95%)	6 (5%)	22	45
1	K	123/124 (99%)	115 (94%)	8 (6%)	15	32
1	L	123/124 (99%)	111 (90%)	12 (10%)	7	16
All	All	1476/1488 (99%)	1384 (94%)	92 (6%)	16	34

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	54	ASP
1	A	64	LEU
1	A	89	ARG
1	A	132	LEU
1	B	35	LEU
1	B	46	SER
1	B	69	ILE
1	B	123	VAL
1	B	132	LEU
1	B	142	ARG
1	C	35	LEU
1	C	36	ARG
1	C	68	ILE
1	C	86	THR
1	C	97	TRP
1	C	108	TYR
1	C	123	VAL
1	C	128	LYS
1	C	132	LEU
1	C	151	GLU
1	D	5	GLU
1	D	35	LEU
1	D	54	ASP
1	D	68	ILE
1	D	83	VAL
1	D	97	TRP
1	D	140	GLU
1	E	3	ARG

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Mol	Chain	Res	Type
1	E	35	LEU
1	E	132	LEU
1	E	140	GLU
1	E	151	GLU
1	F	35	LEU
1	F	41	MET
1	F	57	ASP
1	F	64	LEU
1	F	66	GLU
1	F	69	ILE
1	F	132	LEU
1	F	140	GLU
1	G	35	LEU
1	G	50	GLN
1	G	64	LEU
1	G	68	ILE
1	G	86	THR
1	G	101	PRO
1	G	132	LEU
1	G	142	ARG
1	H	10	MET
1	H	35	LEU
1	H	44	GLU
1	H	50	GLN
1	H	54	ASP
1	H	69	ILE
1	H	95	ARG
1	H	132	LEU
1	I	13	PRO
1	I	44	GLU
1	I	54	ASP
1	I	64	LEU
1	I	69	ILE
1	I	83	VAL
1	I	97	TRP
1	I	123	VAL
1	I	132	LEU
1	J	35	LEU
1	J	41	MET
1	J	115	ASN
1	J	128	LYS
1	J	132	LEU

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Mol	Chain	Res	Type
1	J	140	GLU
1	K	4	MET
1	K	5	GLU
1	K	35	LEU
1	K	36	ARG
1	K	57	ASP
1	K	66	GLU
1	K	83	VAL
1	K	132	LEU
1	L	30	LYS
1	L	35	LEU
1	L	41	MET
1	L	57	ASP
1	L	59	PRO
1	L	64	LEU
1	L	66	GLU
1	L	69	ILE
1	L	88	ARG
1	L	97	TRP
1	L	132	LEU
1	L	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	HIS
1	A	146	HIS
1	B	42	ASN
1	B	49	GLN
1	B	50	GLN
1	B	51	HIS
1	B	146	HIS
1	C	49	GLN
1	C	50	GLN
1	C	146	HIS
1	D	42	ASN
1	D	49	GLN
1	D	50	GLN
1	D	51	HIS
1	D	146	HIS
1	E	50	GLN

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Mol	Chain	Res	Type
1	E	51	HIS
1	E	118	HIS
1	E	125	ASN
1	E	146	HIS
1	F	42	ASN
1	F	51	HIS
1	G	42	ASN
1	G	50	GLN
1	G	118	HIS
1	G	146	HIS
1	H	42	ASN
1	H	49	GLN
1	H	125	ASN
1	I	42	ASN
1	I	50	GLN
1	I	51	HIS
1	I	118	HIS
1	J	51	HIS
1	J	115	ASN
1	J	146	HIS
1	K	42	ASN
1	K	49	GLN
1	K	50	GLN
1	K	51	HIS
1	K	125	ASN
1	K	146	HIS
1	L	42	ASN
1	L	50	GLN
1	L	51	HIS
1	L	146	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.