



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 08:47 AM EDT

PDB ID : 1A81
Title : CRYSTAL STRUCTURE OF THE TANDEM SH2 DOMAIN OF THE SYK KINASE BOUND TO A DUALY TYROSINE-PHOSPHORYLATED ITAM
Authors : Fuetterer, K.; Waksman, G.
Deposited on : 1998-03-31
Resolution : 3.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

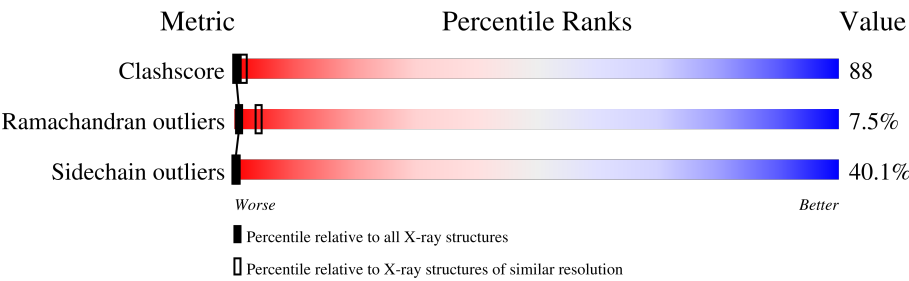
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)





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	254	<div><div>19%</div><div>45%</div><div>33%</div><div>.</div></div>
1	C	254	<div><div>19%</div><div>47%</div><div>32%</div><div>.</div></div>
1	E	254	<div><div>17%</div><div>43%</div><div>26%</div><div>.</div><div>13%</div></div>
1	G	254	<div><div>19%</div><div>39%</div><div>26%</div><div>.</div><div>13%</div></div>
1	I	254	<div><div>17%</div><div>46%</div><div>34%</div><div>.</div></div>
1	K	254	<div><div>17%</div><div>44%</div><div>24%</div><div>.</div><div>13%</div></div>
2	B	18	<div><div>22%</div><div>33%</div><div>33%</div><div>11%</div></div>
2	D	18	<div><div>17%</div><div>50%</div><div>28%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	18	
2	H	18	
2	J	18	
2	L	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	J	181	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12201 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 SYK KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2015	1279	360	370	6			
1	C	254	Total	C	N	O	S	0	0	0
			2015	1279	360	370	6			
1	E	220	Total	C	N	O	S	0	0	0
			1742	1106	314	316	6			
1	G	220	Total	C	N	O	S	0	0	0
			1738	1103	313	316	6			
1	I	254	Total	C	N	O	S	0	0	0
			2011	1276	359	370	6			
1	K	220	Total	C	N	O	S	0	0	0
			1738	1103	313	316	6			

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			
2	D	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			
2	F	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			
2	H	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			
2	J	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			
2	L	18	Total	C	N	O	P	0	0	0
			157	93	27	35	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	PTR	TYR	conflict	UNP P07766

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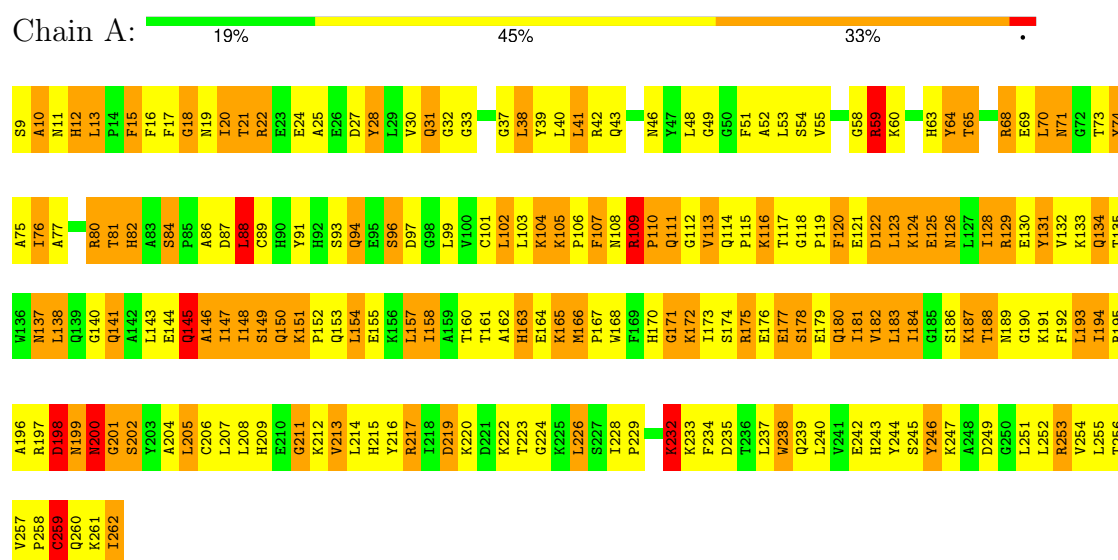
Chain	Residue	Modelled	Actual	Comment	Reference
B	181	PTR	TYR	conflict	UNP P07766
D	170	PTR	TYR	modified residue	UNP P07766
D	181	PTR	TYR	modified residue	UNP P07766
F	170	PTR	TYR	modified residue	UNP P07766
F	181	PTR	TYR	modified residue	UNP P07766
H	170	PTR	TYR	modified residue	UNP P07766
H	181	PTR	TYR	modified residue	UNP P07766
J	170	PTR	TYR	modified residue	UNP P07766
J	181	PTR	TYR	modified residue	UNP P07766
L	170	PTR	TYR	modified residue	UNP P07766
L	181	PTR	TYR	modified residue	UNP P07766

3 Residue-property plots

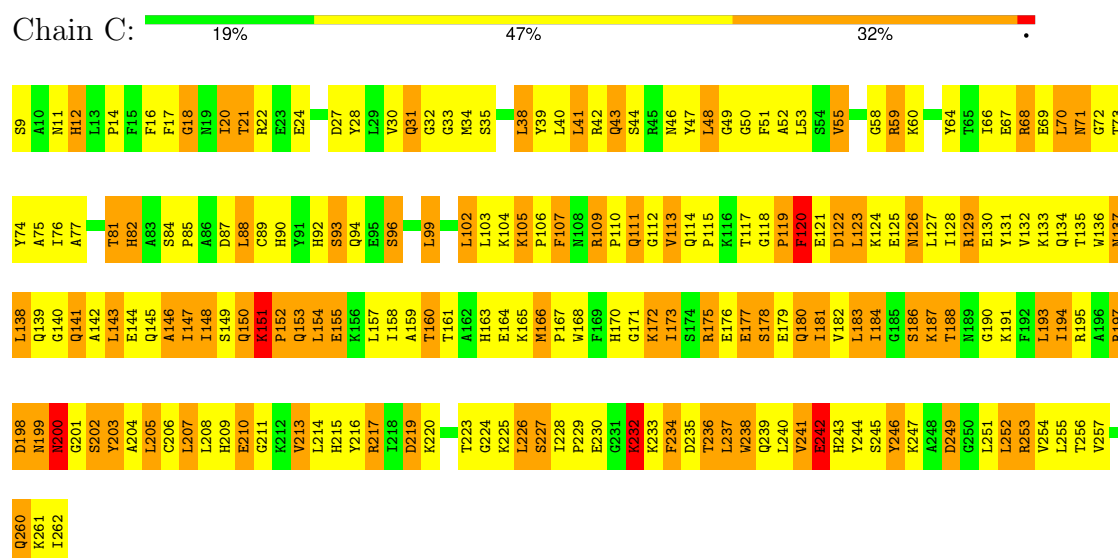
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

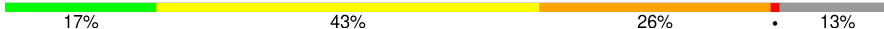
• Molecule 1: SYK KINASE

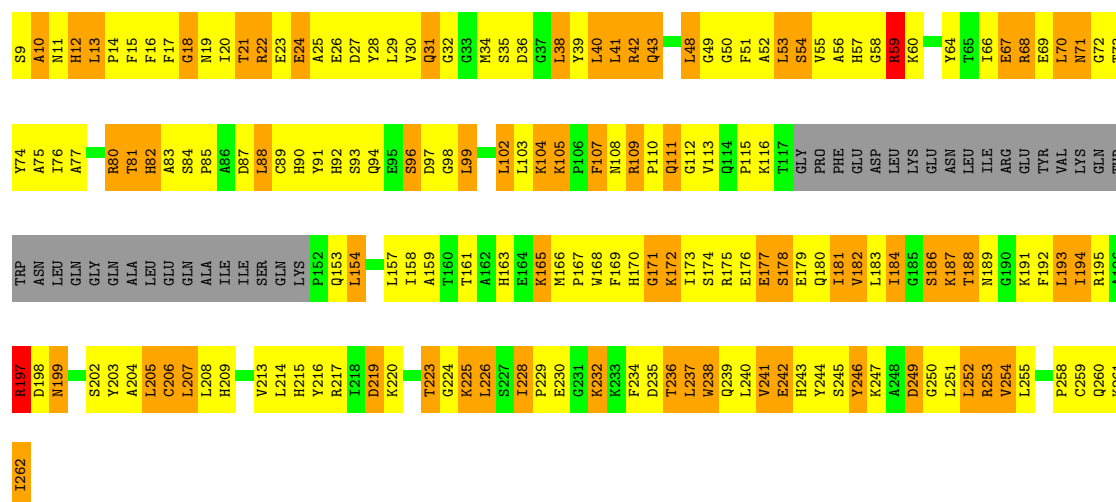


• Molecule 1: SYK KINASE

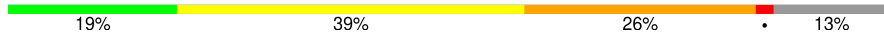


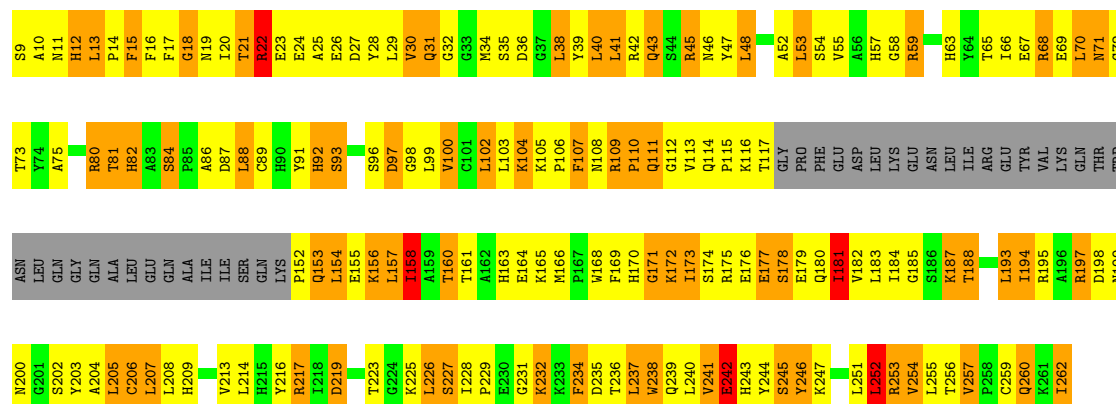
• Molecule 1: SYK KINASE

Chain E: 

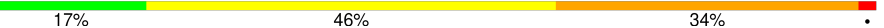


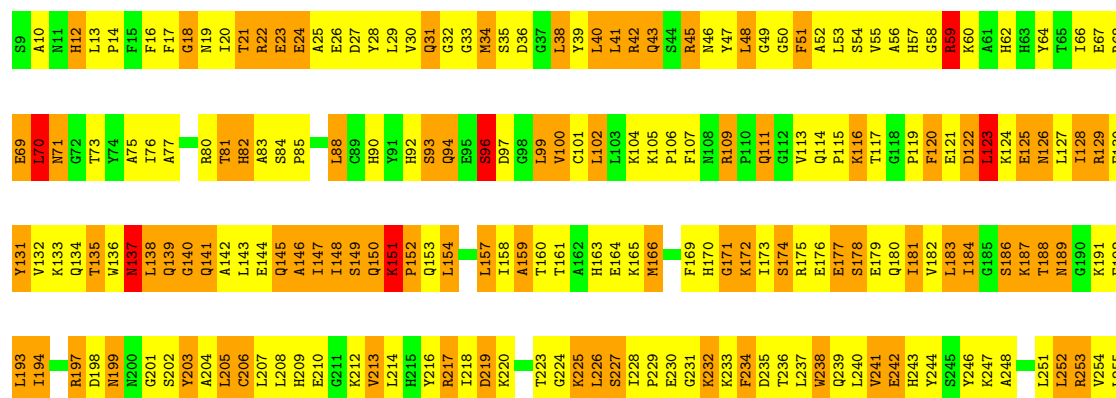
• Molecule 1: SYK KINASE

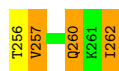
Chain G: 



• Molecule 1: SYK KINASE

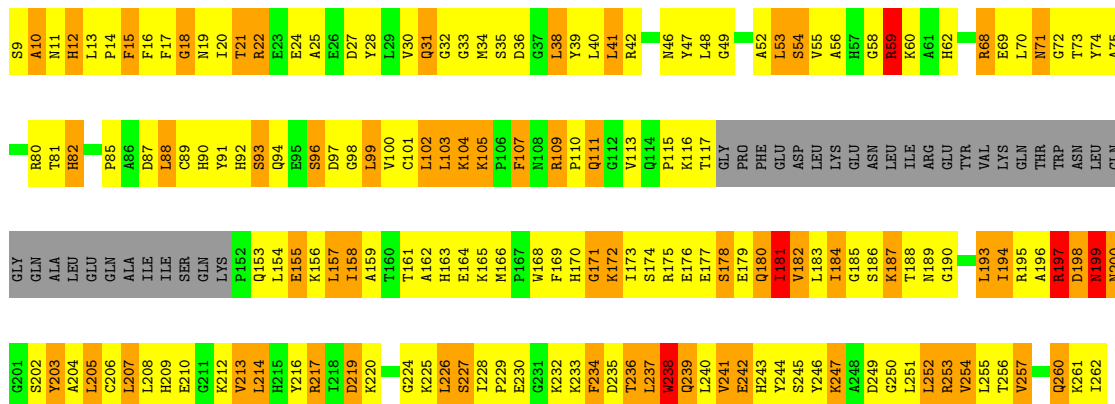
Chain I: 





• Molecule 1: SYK KINASE

Chain K: 17% 44% 24% 13%



• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain B: 22% 33% 33% 11%



• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain D: 17% 50% 28% 6%



• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain F: 11% 50% 39%



• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain H: 17% 33% 50%

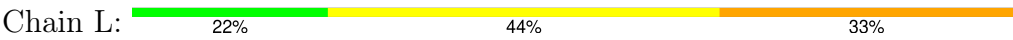


• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain J: 17% 56% 22% 6%

P168	D169	Y170	E171	P172	I173	R174	K175	G176	Q177	R178	D179	L180	Y181	S182	G183	L184	N185
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● Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN



P168	D169	Y170	E171	P172	I173	R174	K175	G176	Q177	R178	D179	L180	Y181	S182	G183	L184	N185
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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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.50Å 146.90Å 91.50Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	89.8 (30.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.226 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12201	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	2/2062 (0.1%)	0.96	2/2787 (0.1%)
1	C	0.80	0/2062	0.93	2/2787 (0.1%)
1	E	0.62	0/1783	0.80	2/2405 (0.1%)
1	G	0.84	0/1779	0.98	3/2401 (0.1%)
1	I	0.74	0/2058	0.87	1/2783 (0.0%)
1	K	0.64	1/1779 (0.1%)	0.79	2/2401 (0.1%)
2	B	0.62	0/124	1.09	0/161
2	D	0.87	0/124	1.04	0/161
2	F	0.58	0/124	0.91	0/161
2	H	0.79	0/124	1.19	1/161 (0.6%)
2	J	0.55	0/124	0.91	0/161
2	L	0.53	0/124	0.98	0/161
All	All	0.75	3/12267 (0.0%)	0.90	13/16530 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	CYS	CB-SG	-5.32	1.73	1.81
1	K	89	CYS	CB-SG	5.20	1.91	1.82
1	A	46	ASN	CG-ND2	-5.05	1.20	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	184	LEU	CA-CB-CG	-6.91	99.41	115.30
1	G	100	VAL	CB-CA-C	-6.28	99.48	111.40
1	K	199	ASN	N-CA-C	-6.14	94.43	111.00
1	G	198	ASP	N-CA-C	5.89	126.89	111.00
1	A	109	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	E	197	ARG	N-CA-C	-5.77	95.43	111.00
1	C	121	GLU	N-CA-C	-5.74	95.51	111.00
1	I	123	LEU	CA-CB-CG	5.70	128.42	115.30
1	G	22	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	K	237	LEU	CA-CB-CG	-5.42	102.84	115.30
1	A	76	ILE	N-CA-C	-5.28	96.75	111.00
1	E	228	ILE	CB-CA-C	-5.15	101.31	111.60
1	C	113	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	TYR	Sidechain
1	A	64	TYR	Sidechain

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	2015	0	1977	387	0
1	C	2015	0	1977	403	0
1	E	1742	0	1718	277	0
1	G	1738	0	1707	293	0
1	I	2011	0	1966	383	0
1	K	1738	0	1707	301	0
2	B	157	0	139	25	0
2	D	157	0	139	30	0
2	F	157	0	139	33	0
2	H	157	0	139	33	0
2	J	157	0	139	30	0
2	L	157	0	139	27	0
All	All	12201	0	11886	2118	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 88.

All (2118) 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:I:21:THR:HG23	1:I:24:GLU:OE1	1.45	1.16
1:I:128:ILE:HG22	1:I:158:ILE:HG12	1.26	1.15
1:C:128:ILE:HG22	1:C:158:ILE:HG12	1.23	1.14
1:E:21:THR:HG23	1:E:24:GLU:HB2	1.22	1.13
1:A:70:LEU:H	1:A:70:LEU:HD12	1.04	1.12
1:A:170:HIS:ND1	1:A:193:LEU:HD12	1.66	1.10
1:C:70:LEU:HD12	1:C:70:LEU:H	0.99	1.10
1:C:197:ARG:HG2	1:C:197:ARG:HH11	1.04	1.10
1:K:226:LEU:H	1:K:226:LEU:HD12	1.17	1.09
1:A:163:HIS:HA	1:A:166:MET:HG3	1.30	1.09
2:L:175:LYS:HD2	2:L:176:GLY:H	1.15	1.08
1:G:226:LEU:HD12	1:G:226:LEU:H	1.06	1.08
2:L:178:ARG:HH11	2:L:178:ARG:CB	1.66	1.08
1:A:194:ILE:HG23	1:A:205:LEU:HD23	1.33	1.08
1:A:150:GLN:HB3	1:A:154:LEU:HD21	1.27	1.08
1:I:39:TYR:HB3	1:I:55:VAL:HG12	1.24	1.08
2:L:178:ARG:HB3	2:L:178:ARG:NH1	1.67	1.07
1:C:154:LEU:HD23	1:C:154:LEU:H	1.20	1.07
2:L:174:ARG:HG2	2:L:174:ARG:HH11	1.16	1.07
1:A:217:ARG:HG2	1:A:217:ARG:HH11	1.20	1.06
1:G:170:HIS:CG	1:G:193:LEU:HD12	1.91	1.05
1:I:128:ILE:HD13	1:I:129:ARG:H	1.21	1.05
1:G:180:GLN:HE22	1:I:59:ARG:HD2	0.95	1.05
1:I:150:GLN:HB3	1:I:154:LEU:HD11	1.38	1.05
1:G:217:ARG:HG2	1:G:217:ARG:HH11	0.91	1.04
1:G:180:GLN:NE2	1:I:59:ARG:HD2	1.73	1.04
2:F:178:ARG:HB3	2:F:178:ARG:HH11	1.21	1.04
1:E:75:ALA:HB2	1:E:81:THR:HA	1.39	1.03
2:H:175:LYS:HD2	2:H:176:GLY:H	1.22	1.02
1:K:68:ARG:HH11	1:K:72:GLY:HA2	1.24	1.02
1:G:70:LEU:H	1:G:70:LEU:HD12	1.24	1.01
1:A:174:SER:OG	1:A:177:GLU:HB2	1.59	1.01
1:C:120:PHE:HB2	1:C:238:TRP:CZ3	1.95	1.00
1:E:154:LEU:HD22	1:E:154:LEU:H	1.21	1.00
1:C:17:PHE:HE1	1:C:109:ARG:HA	1.22	0.99
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.21	0.99
1:C:226:LEU:H	1:C:226:LEU:HD12	1.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ILE:HD13	1:G:158:ILE:H	1.26	0.99
2:L:178:ARG:HH11	2:L:178:ARG:HB3	0.85	0.99
1:I:154:LEU:HD23	1:I:154:LEU:H	1.24	0.99
1:C:39:TYR:HB3	1:C:55:VAL:HG12	1.44	0.99
1:C:17:PHE:CD1	1:C:109:ARG:HD3	1.98	0.98
1:C:177:GLU:O	1:C:181:ILE:HG22	1.62	0.98
1:E:236:THR:HG1	1:E:238:TRP:HD1	1.07	0.98
1:G:217:ARG:HG2	1:G:217:ARG:NH1	1.71	0.98
1:C:207:LEU:HD23	1:C:214:LEU:HB2	1.45	0.98
1:C:154:LEU:H	1:C:154:LEU:CD2	1.77	0.98
1:K:75:ALA:HB2	1:K:81:THR:HA	1.46	0.98
1:A:70:LEU:H	1:A:70:LEU:CD1	1.76	0.97
1:A:123:LEU:HD12	1:A:124:LYS:N	1.79	0.97
1:G:197:ARG:HG2	1:G:197:ARG:HH11	1.29	0.97
1:A:161:THR:HA	1:A:163:HIS:CE1	2.00	0.96
1:C:70:LEU:H	1:C:70:LEU:CD1	1.70	0.96
1:I:88:LEU:HD12	1:I:88:LEU:O	1.66	0.96
2:D:174:ARG:HA	2:D:175:LYS:HE2	1.46	0.95
1:K:197:ARG:HG2	1:K:197:ARG:HH11	1.29	0.95
1:C:138:LEU:HD23	1:C:138:LEU:H	1.31	0.95
1:C:21:THR:HG23	1:C:24:GLU:HB2	1.47	0.95
1:K:17:PHE:HE1	1:K:109:ARG:HA	1.29	0.95
1:K:159:ALA:HB1	1:K:236:THR:HG21	1.45	0.95
1:C:41:LEU:HD23	1:C:52:ALA:O	1.66	0.94
1:K:244:TYR:HE1	1:K:249:ASP:HB3	1.30	0.94
1:K:154:LEU:H	1:K:154:LEU:HD22	1.32	0.94
1:C:246:TYR:HE1	1:C:247:LYS:HE3	1.32	0.94
1:E:39:TYR:HB3	1:E:55:VAL:HG12	1.48	0.94
1:C:202:SER:C	1:C:203:TYR:HD1	1.71	0.94
1:C:70:LEU:HD12	1:C:70:LEU:N	1.83	0.93
1:G:173:ILE:HG23	1:G:177:GLU:HB3	1.50	0.93
1:C:191:LYS:HG3	1:C:257:VAL:HG23	1.49	0.93
1:C:17:PHE:HD1	1:C:109:ARG:HD3	1.30	0.93
2:H:175:LYS:O	2:H:178:ARG:HD2	1.68	0.93
1:K:205:LEU:HD22	1:K:206:CYS:N	1.82	0.93
1:A:163:HIS:HA	1:A:166:MET:CG	1.97	0.93
2:F:178:ARG:HB3	2:F:178:ARG:NH1	1.83	0.93
1:E:228:ILE:HG21	2:F:173:ILE:HD11	1.49	0.93
1:G:58:GLY:O	1:G:59:ARG:HG3	1.67	0.93
1:G:59:ARG:HD2	1:K:180:GLN:NE2	1.84	0.93
1:A:132:VAL:HG12	1:A:138:LEU:HD21	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:ASN:ND2	1:K:199:ASN:H	1.65	0.92
1:C:226:LEU:HD13	1:C:234:PHE:O	1.70	0.92
1:G:154:LEU:HD23	1:G:154:LEU:H	1.35	0.92
1:A:138:LEU:HD23	1:A:138:LEU:H	1.33	0.92
1:K:39:TYR:HB3	1:K:55:VAL:HG12	1.52	0.92
1:C:170:HIS:HB3	1:C:173:ILE:HD11	1.50	0.91
1:G:170:HIS:ND1	1:G:193:LEU:HD12	1.86	0.91
1:C:17:PHE:CE1	1:C:109:ARG:HA	2.06	0.91
1:E:209:HIS:ND1	1:E:253:ARG:NH1	2.18	0.91
1:I:27:ASP:O	1:I:30:VAL:HG22	1.70	0.91
1:A:123:LEU:HD12	1:A:124:LYS:H	1.33	0.91
2:L:173:ILE:HG22	2:L:174:ARG:H	1.34	0.90
1:C:240:LEU:HD23	1:C:240:LEU:C	1.91	0.90
1:G:260:GLN:OE1	1:G:260:GLN:HA	1.70	0.90
1:K:48:LEU:HD23	1:K:235:ASP:HB2	1.52	0.90
1:G:240:LEU:C	1:G:240:LEU:HD23	1.92	0.90
1:E:188:THR:O	1:E:208:LEU:HD23	1.70	0.90
1:A:17:PHE:O	1:A:20:ILE:HD13	1.71	0.90
1:G:12:HIS:ND1	1:G:13:LEU:HD23	1.87	0.90
1:I:154:LEU:HD23	1:I:154:LEU:N	1.87	0.90
1:A:70:LEU:HD12	1:A:70:LEU:N	1.87	0.89
1:I:170:HIS:CG	1:I:193:LEU:HD12	2.06	0.89
1:A:82:HIS:HD2	1:A:88:LEU:HA	1.37	0.89
1:C:28:TYR:HA	1:C:31:GLN:HG2	1.54	0.89
1:C:197:ARG:HG2	1:C:197:ARG:NH1	1.78	0.89
1:E:226:LEU:CD1	1:E:226:LEU:H	1.85	0.89
1:K:48:LEU:HD23	1:K:235:ASP:CB	2.03	0.89
1:K:236:THR:HG1	1:K:238:TRP:HD1	0.95	0.89
1:C:187:LYS:HE3	1:C:187:LYS:H	1.36	0.88
1:A:82:HIS:CD2	1:A:88:LEU:HA	2.08	0.88
1:A:172:LYS:O	1:A:173:ILE:HG13	1.72	0.88
1:E:28:TYR:HA	1:E:31:GLN:HG2	1.55	0.88
1:K:158:ILE:CD1	1:K:158:ILE:H	1.87	0.88
1:A:113:VAL:O	1:A:114:GLN:NE2	2.08	0.87
1:C:110:PRO:HD2	1:C:113:VAL:HG21	1.55	0.87
1:E:83:ALA:HB3	1:E:87:ASP:OD2	1.75	0.87
1:I:20:ILE:HD12	1:I:116:LYS:HB2	1.56	0.87
1:K:173:ILE:HG23	1:K:177:GLU:HB2	1.55	0.87
1:G:154:LEU:HD23	1:G:154:LEU:N	1.89	0.87
1:I:39:TYR:CB	1:I:55:VAL:HG12	2.04	0.87
1:K:240:LEU:HD23	1:K:241:VAL:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:CD2	1:A:154:LEU:H	1.88	0.87
1:G:240:LEU:HD23	1:G:240:LEU:O	1.75	0.86
1:I:30:VAL:HA	1:I:34:MET:HG2	1.57	0.86
1:C:216:TYR:CE1	2:D:171:GLU:HB3	2.10	0.86
1:A:253:ARG:HB2	1:A:253:ARG:NH1	1.89	0.86
1:C:260:GLN:OE1	1:C:260:GLN:HA	1.73	0.86
1:E:216:TYR:CE1	2:F:171:GLU:HB3	2.11	0.86
1:K:194:ILE:HG22	1:K:204:ALA:O	1.76	0.86
1:E:236:THR:OG1	1:E:238:TRP:HD1	1.57	0.86
1:I:71:ASN:HB2	1:I:73:THR:HG23	1.57	0.86
1:I:88:LEU:HD12	1:I:88:LEU:C	1.96	0.86
1:I:123:LEU:HD12	1:I:124:LYS:N	1.89	0.86
1:A:217:ARG:HG2	1:A:217:ARG:NH1	1.89	0.86
2:L:174:ARG:HG2	2:L:174:ARG:NH1	1.85	0.85
1:A:170:HIS:ND1	1:A:193:LEU:CD1	2.38	0.85
1:K:199:ASN:H	1:K:199:ASN:HD22	1.22	0.85
1:I:120:PHE:HB2	1:I:238:TRP:CZ3	2.11	0.85
1:A:253:ARG:CB	1:A:253:ARG:HH11	1.90	0.84
1:E:182:VAL:HG23	1:E:259:CYS:SG	2.17	0.84
1:K:21:THR:HG23	1:K:24:GLU:HB2	1.57	0.84
1:K:96:SER:O	1:K:99:LEU:HB2	1.78	0.84
1:C:226:LEU:H	1:C:226:LEU:CD1	1.89	0.84
1:G:217:ARG:HH11	1:G:217:ARG:CG	1.84	0.84
1:A:197:ARG:HB3	1:A:199:ASN:OD1	1.77	0.84
1:A:253:ARG:HB2	1:A:253:ARG:HH11	1.40	0.84
1:E:30:VAL:HG12	1:E:34:MET:SD	2.17	0.84
1:I:21:THR:CG2	1:I:24:GLU:OE1	2.24	0.84
1:I:30:VAL:HG23	1:I:31:GLN:N	1.90	0.84
1:I:69:GLU:HB2	1:I:73:THR:O	1.78	0.83
1:I:70:LEU:H	1:I:70:LEU:HD12	1.43	0.83
1:C:187:LYS:HE3	1:C:187:LYS:N	1.92	0.83
1:I:39:TYR:HB3	1:I:55:VAL:CG1	2.07	0.83
1:E:17:PHE:CD1	1:E:109:ARG:HD3	2.13	0.83
1:A:245:SER:HA	1:A:255:LEU:HB2	1.61	0.83
1:C:207:LEU:HD21	1:C:214:LEU:HD12	1.61	0.83
1:A:129:ARG:HH11	1:A:129:ARG:CG	1.92	0.82
1:E:158:ILE:H	1:E:158:ILE:HD12	1.43	0.82
1:I:32:GLY:HA2	1:I:107:PHE:HE2	1.42	0.82
1:E:154:LEU:H	1:E:154:LEU:CD2	1.91	0.82
1:G:197:ARG:HG2	1:G:197:ARG:NH1	1.88	0.82
1:A:80:ARG:CB	1:A:80:ARG:HH11	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ILE:HG22	2:B:174:ARG:H	1.43	0.82
1:G:246:TYR:HE1	1:G:247:LYS:HE3	1.43	0.82
1:A:128:ILE:HG22	1:A:158:ILE:HG12	1.58	0.82
1:I:240:LEU:HD23	1:I:241:VAL:N	1.94	0.82
1:K:216:TYR:CE1	2:L:171:GLU:HB3	2.14	0.82
1:E:32:GLY:HA3	1:E:107:PHE:CE2	2.14	0.82
1:E:39:TYR:CB	1:E:55:VAL:HG12	2.10	0.82
1:K:236:THR:OG1	1:K:238:TRP:HD1	1.62	0.82
1:C:21:THR:HG22	1:C:24:GLU:OE1	1.80	0.81
1:A:158:ILE:H	1:A:158:ILE:CD1	1.93	0.81
1:G:185:GLY:HA3	1:I:27:ASP:OD1	1.79	0.81
1:K:170:HIS:CG	1:K:193:LEU:HD12	2.16	0.81
1:C:247:LYS:HG2	1:C:249:ASP:HB2	1.60	0.81
1:E:68:ARG:NH1	1:E:72:GLY:HA2	1.95	0.81
1:G:194:ILE:HG22	1:G:204:ALA:O	1.80	0.81
1:E:22:ARG:NH2	2:F:180:LEU:O	2.14	0.81
1:E:226:LEU:N	1:E:226:LEU:HD12	1.94	0.81
1:A:187:LYS:H	1:A:187:LYS:HE2	1.42	0.81
1:A:217:ARG:HH11	1:A:217:ARG:CG	1.93	0.81
1:C:123:LEU:C	1:C:123:LEU:HD12	2.01	0.81
2:B:178:ARG:HB3	2:B:178:ARG:CZ	2.07	0.81
1:K:260:GLN:OE1	1:K:260:GLN:HA	1.80	0.81
1:C:203:TYR:HD1	1:C:203:TYR:N	1.79	0.81
2:L:175:LYS:HD2	2:L:176:GLY:N	1.95	0.81
1:A:182:VAL:HG23	1:A:259:CYS:SG	2.21	0.80
1:E:193:LEU:HD23	1:E:193:LEU:O	1.80	0.80
1:C:226:LEU:HD12	1:C:226:LEU:N	1.95	0.80
1:C:246:TYR:CE1	1:C:247:LYS:HE3	2.17	0.80
1:K:161:THR:HA	1:K:163:HIS:CE1	2.16	0.80
1:G:199:ASN:CG	1:G:200:ASN:H	1.82	0.80
1:A:132:VAL:CG1	1:A:138:LEU:HD21	2.11	0.80
1:A:161:THR:HA	1:A:163:HIS:HE1	1.44	0.80
1:E:206:CYS:HA	1:E:214:LEU:O	1.81	0.80
1:A:71:ASN:HD22	1:A:73:THR:HG23	1.46	0.80
1:C:111:GLN:HE21	1:C:112:GLY:N	1.79	0.80
1:G:92:HIS:CD2	1:G:99:LEU:HG	2.16	0.80
1:K:158:ILE:HD12	1:K:158:ILE:N	1.97	0.80
1:C:170:HIS:CG	1:C:193:LEU:HD12	2.17	0.80
1:E:226:LEU:H	1:E:226:LEU:HD12	1.45	0.80
2:J:178:ARG:HH11	2:J:178:ARG:HG3	1.47	0.80
1:C:241:VAL:HG12	1:C:242:GLU:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD12	1:A:116:LYS:HB2	1.65	0.79
1:A:174:SER:HG	1:A:177:GLU:HB2	1.43	0.79
1:C:110:PRO:O	1:C:113:VAL:HG23	1.83	0.79
1:I:128:ILE:HD13	1:I:129:ARG:N	1.97	0.79
1:K:234:PHE:CE2	1:K:240:LEU:HA	2.17	0.79
1:K:244:TYR:CE1	1:K:249:ASP:HB3	2.17	0.79
1:C:17:PHE:HE1	1:C:109:ARG:CA	1.96	0.79
1:K:92:HIS:CD2	1:K:99:LEU:HG	2.17	0.79
1:K:193:LEU:O	1:K:193:LEU:HD23	1.81	0.79
1:K:234:PHE:HB3	1:K:239:GLN:OE1	1.83	0.79
1:A:226:LEU:HD23	1:A:237:LEU:CD2	2.12	0.79
1:I:145:GLN:N	1:I:145:GLN:HE21	1.80	0.79
1:I:238:TRP:CD1	1:I:239:GLN:N	2.51	0.79
1:C:120:PHE:HB2	1:C:238:TRP:CH2	2.17	0.79
1:A:145:GLN:O	1:A:148:ILE:HD13	1.82	0.79
1:G:226:LEU:HD12	1:G:226:LEU:N	1.91	0.78
1:I:48:LEU:HD23	1:I:235:ASP:OD2	1.82	0.78
1:K:240:LEU:HD23	1:K:240:LEU:C	2.02	0.78
1:C:88:LEU:C	1:C:88:LEU:HD12	2.04	0.78
1:I:20:ILE:HG23	1:I:24:GLU:HB3	1.66	0.78
1:I:238:TRP:HD1	1:I:239:GLN:N	1.79	0.78
1:G:188:THR:O	1:G:208:LEU:HD23	1.84	0.78
1:I:40:LEU:C	1:I:40:LEU:HD12	2.04	0.78
1:K:158:ILE:H	1:K:158:ILE:HD12	1.46	0.78
1:A:187:LYS:H	1:A:187:LYS:CE	1.96	0.78
1:E:170:HIS:O	1:E:173:ILE:HD12	1.84	0.78
1:E:240:LEU:HD23	1:E:240:LEU:C	2.04	0.78
1:A:145:GLN:HA	1:A:145:GLN:HE21	1.47	0.78
1:A:176:GLU:OE1	1:A:176:GLU:N	2.17	0.78
1:A:68:ARG:HG3	1:A:68:ARG:O	1.83	0.78
1:A:172:LYS:HE2	1:A:173:ILE:N	1.99	0.78
1:C:238:TRP:CD1	1:C:239:GLN:HG3	2.19	0.78
1:I:209:HIS:ND1	1:I:253:ARG:NH1	2.32	0.78
1:I:40:LEU:HD12	1:I:41:LEU:N	1.99	0.77
1:A:38:LEU:HD23	1:A:105:LYS:O	1.84	0.77
1:G:241:VAL:HG12	1:G:242:GLU:N	1.98	0.77
1:I:36:ASP:OD1	1:I:58:GLY:N	2.18	0.77
1:I:240:LEU:HD23	1:I:240:LEU:C	2.05	0.77
1:A:82:HIS:ND1	1:A:82:HIS:N	2.32	0.77
1:K:217:ARG:CG	1:K:217:ARG:HH11	1.96	0.77
1:A:226:LEU:HD23	1:A:237:LEU:HD21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:TYR:N	1:C:203:TYR:CD1	2.48	0.77
1:E:158:ILE:H	1:E:158:ILE:CD1	1.97	0.77
1:A:21:THR:CG2	1:A:24:GLU:HG3	2.15	0.77
1:C:128:ILE:HD12	1:C:129:ARG:N	1.99	0.77
1:E:108:ASN:O	1:E:110:PRO:HD3	1.84	0.77
1:C:227:SER:HB2	1:C:232:LYS:O	1.84	0.77
1:A:238:TRP:HD1	1:A:239:GLN:N	1.82	0.76
1:A:194:ILE:HG22	1:A:204:ALA:O	1.84	0.76
1:G:253:ARG:HG3	1:G:254:VAL:N	1.98	0.76
1:K:226:LEU:HD12	1:K:226:LEU:N	1.97	0.76
1:C:151:LYS:HG2	1:C:152:PRO:HD3	1.66	0.76
1:C:187:LYS:H	1:C:187:LYS:CE	1.97	0.76
1:E:99:LEU:CD1	1:E:103:LEU:HD21	2.15	0.76
1:E:241:VAL:HG12	1:E:242:GLU:N	2.00	0.76
1:I:146:ALA:O	1:I:150:GLN:HB2	1.86	0.76
1:A:195:ARG:NH2	1:A:215:HIS:ND1	2.33	0.76
1:C:39:TYR:HB3	1:C:55:VAL:CG1	2.15	0.76
1:I:18:GLY:H	1:I:115:PRO:HB3	1.50	0.76
1:A:80:ARG:HH11	1:A:80:ARG:HB3	1.50	0.76
1:A:174:SER:OG	1:A:177:GLU:N	2.18	0.76
1:A:163:HIS:HD2	1:A:237:LEU:HD12	1.48	0.76
2:H:175:LYS:HD2	2:H:176:GLY:N	1.98	0.76
1:A:163:HIS:CD2	1:A:237:LEU:HD12	2.20	0.76
1:G:69:GLU:OE1	1:G:69:GLU:HA	1.85	0.76
1:K:172:LYS:HZ3	1:K:173:ILE:N	1.83	0.76
1:K:217:ARG:HH11	1:K:217:ARG:HG2	1.51	0.76
1:G:163:HIS:CG	1:G:237:LEU:HD13	2.21	0.76
1:K:154:LEU:H	1:K:154:LEU:CD2	1.99	0.76
1:K:182:VAL:HG12	1:K:183:LEU:HD22	1.66	0.76
1:I:69:GLU:OE1	1:I:69:GLU:HA	1.83	0.75
1:A:48:LEU:HD23	1:A:235:ASP:HB3	1.68	0.75
1:C:138:LEU:HD12	1:C:142:ALA:O	1.87	0.75
1:E:32:GLY:HA3	1:E:107:PHE:HE2	1.49	0.75
1:A:128:ILE:CG2	1:A:158:ILE:HG12	2.17	0.75
1:E:82:HIS:CD2	1:E:88:LEU:HA	2.22	0.75
1:G:58:GLY:C	1:G:59:ARG:HG3	2.06	0.75
1:C:17:PHE:CE2	1:C:40:LEU:HD22	2.22	0.75
1:C:207:LEU:CD2	1:C:214:LEU:HB2	2.17	0.75
1:E:228:ILE:CG2	2:F:173:ILE:HD11	2.16	0.75
1:I:21:THR:HG23	1:I:24:GLU:HB2	1.69	0.75
1:C:253:ARG:NH1	1:C:253:ARG:HB3	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ILE:HD13	1:G:184:ILE:N	2.01	0.75
1:K:237:LEU:O	1:K:239:GLN:N	2.20	0.74
1:G:48:LEU:HD22	1:G:235:ASP:CB	2.16	0.74
2:D:184:LEU:O	2:D:185:ASN:HB3	1.86	0.74
1:K:157:LEU:HB3	1:K:158:ILE:HD12	1.70	0.74
1:K:193:LEU:CD2	1:K:206:CYS:HB2	2.17	0.74
1:K:226:LEU:H	1:K:226:LEU:CD1	1.98	0.74
1:A:110:PRO:HB2	1:A:113:VAL:HG21	1.68	0.74
1:I:70:LEU:HD12	1:I:70:LEU:N	2.01	0.74
1:I:136:TRP:O	1:I:138:LEU:HD23	1.85	0.74
1:K:205:LEU:HD22	1:K:206:CYS:H	1.50	0.74
1:A:260:GLN:HA	1:A:260:GLN:OE1	1.86	0.74
1:C:17:PHE:O	1:C:18:GLY:O	2.04	0.74
1:K:197:ARG:HG2	1:K:197:ARG:NH1	1.89	0.74
1:C:132:VAL:HG12	1:C:143:LEU:HD11	1.70	0.74
1:C:173:ILE:HG22	1:C:177:GLU:HB3	1.69	0.74
1:G:187:LYS:HE3	1:G:187:LYS:H	1.53	0.74
1:C:150:GLN:HB3	1:C:154:LEU:HD21	1.69	0.74
1:C:170:HIS:ND1	1:C:193:LEU:HD12	2.01	0.74
1:I:38:LEU:HD22	1:I:39:TYR:N	2.03	0.74
1:C:17:PHE:HE2	1:C:40:LEU:HD22	1.53	0.74
1:G:17:PHE:CD1	1:G:109:ARG:HD3	2.23	0.74
1:I:22:ARG:NH1	2:J:181:PTR:O3P	2.21	0.74
1:K:38:LEU:HD23	1:K:105:LYS:O	1.88	0.74
2:B:174:ARG:HA	2:B:175:LYS:HE2	1.69	0.74
1:K:47:TYR:CE1	1:K:225:LYS:NZ	2.56	0.74
1:A:120:PHE:HB2	1:A:238:TRP:CZ3	2.23	0.73
1:C:138:LEU:HG	1:C:143:LEU:HD13	1.70	0.73
1:I:58:GLY:C	1:I:59:ARG:HG3	2.08	0.73
1:I:80:ARG:CB	1:I:80:ARG:HH11	2.02	0.73
2:L:173:ILE:HG22	2:L:174:ARG:N	2.02	0.73
1:K:68:ARG:NH1	1:K:72:GLY:HA2	2.02	0.73
1:A:190:GLY:HA3	1:A:256:THR:HG23	1.71	0.73
1:G:17:PHE:HD1	1:G:109:ARG:HD3	1.52	0.73
1:E:99:LEU:HD11	1:E:103:LEU:HD21	1.71	0.73
1:A:17:PHE:HB3	1:A:20:ILE:HD13	1.70	0.73
1:G:178:SER:O	1:G:181:ILE:HG22	1.87	0.73
1:I:48:LEU:HB2	1:I:235:ASP:OD2	1.87	0.73
2:L:184:LEU:O	2:L:185:ASN:HB3	1.89	0.73
1:A:244:TYR:O	1:A:254:VAL:HG23	1.89	0.72
1:E:20:ILE:HG23	1:E:24:GLU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:LEU:H	1:G:226:LEU:CD1	1.89	0.72
1:K:48:LEU:CD2	1:K:235:ASP:HB2	2.19	0.72
1:K:166:MET:HB3	1:K:168:TRP:NE1	2.03	0.72
1:C:154:LEU:HD23	1:C:154:LEU:N	2.00	0.72
1:G:29:LEU:HD22	1:G:38:LEU:HD13	1.70	0.72
1:A:173:ILE:HG23	1:A:177:GLU:HB3	1.69	0.72
1:E:216:TYR:CD1	2:F:171:GLU:HB3	2.23	0.72
1:G:39:TYR:HB3	1:G:55:VAL:HG12	1.70	0.72
1:G:70:LEU:H	1:G:70:LEU:CD1	1.98	0.72
1:A:80:ARG:HG2	1:A:81:THR:N	2.05	0.72
1:I:177:GLU:O	1:I:181:ILE:HG22	1.89	0.72
1:I:188:THR:O	1:I:208:LEU:HD23	1.90	0.72
1:A:20:ILE:HG23	1:A:24:GLU:HB2	1.71	0.72
1:A:58:GLY:C	1:A:59:ARG:HG3	2.09	0.72
1:K:250:GLY:O	2:L:174:ARG:HG3	1.89	0.72
1:G:39:TYR:CB	1:G:55:VAL:HG12	2.19	0.72
1:E:226:LEU:CD1	1:E:226:LEU:N	2.52	0.72
1:K:172:LYS:O	1:K:173:ILE:HG13	1.89	0.72
2:D:175:LYS:O	2:D:178:ARG:HD3	1.90	0.72
1:A:28:TYR:O	1:A:107:PHE:HE2	1.72	0.72
1:I:123:LEU:HD11	1:I:127:LEU:HD22	1.71	0.72
1:A:129:ARG:HH11	1:A:129:ARG:HG3	1.55	0.71
1:E:18:GLY:H	1:E:115:PRO:HB3	1.54	0.71
1:A:150:GLN:HB3	1:A:154:LEU:CD2	2.16	0.71
1:K:228:ILE:CG2	2:L:173:ILE:HD11	2.20	0.71
1:A:128:ILE:HG22	1:A:158:ILE:CG1	2.20	0.71
1:E:172:LYS:O	1:E:173:ILE:HG13	1.89	0.71
1:G:16:PHE:HA	1:G:41:LEU:O	1.89	0.71
1:G:172:LYS:NZ	1:G:173:ILE:N	2.37	0.71
1:G:246:TYR:CE1	1:G:247:LYS:HE3	2.24	0.71
1:E:158:ILE:HD12	1:E:158:ILE:N	2.05	0.71
1:I:144:GLU:O	1:I:148:ILE:HG23	1.91	0.71
1:K:10:ALA:HA	1:K:12:HIS:HE1	1.56	0.71
1:A:93:SER:HA	1:A:103:LEU:HB2	1.72	0.71
1:G:42:ARG:NH2	1:G:63:HIS:ND1	2.38	0.71
1:A:176:GLU:O	1:A:178:SER:N	2.22	0.71
1:A:199:ASN:C	1:A:201:GLY:H	1.94	0.71
1:I:20:ILE:CD1	1:I:116:LYS:HB2	2.21	0.71
1:K:39:TYR:CE2	1:K:103:LEU:HB3	2.25	0.71
1:A:154:LEU:H	1:A:154:LEU:HD22	1.55	0.71
1:E:98:GLY:HA2	2:F:185:ASN:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HG23	1:A:24:GLU:HG3	1.72	0.70
1:G:234:PHE:N	1:G:234:PHE:CD1	2.57	0.70
1:I:241:VAL:HG12	1:I:242:GLU:N	2.05	0.70
1:A:134:GLN:NE2	1:A:135:THR:HG23	2.05	0.70
1:A:158:ILE:CD1	1:A:158:ILE:N	2.53	0.70
2:D:175:LYS:HD2	2:D:176:GLY:H	1.57	0.70
1:E:172:LYS:HD3	1:E:198:ASP:OD2	1.90	0.70
1:K:28:TYR:HA	1:K:31:GLN:HG2	1.73	0.70
1:C:82:HIS:CD2	1:C:88:LEU:HA	2.25	0.70
1:C:207:LEU:CD2	1:C:214:LEU:HD12	2.20	0.70
1:C:228:ILE:HG22	1:C:229:PRO:HD2	1.73	0.70
1:I:216:TYR:CE1	2:J:171:GLU:HB3	2.26	0.70
1:C:138:LEU:CD2	1:C:143:LEU:HD13	2.21	0.70
1:G:154:LEU:N	1:G:154:LEU:CD2	2.55	0.70
1:K:10:ALA:HA	1:K:12:HIS:CE1	2.26	0.70
1:A:120:PHE:HA	1:A:123:LEU:HG	1.74	0.70
1:C:193:LEU:O	1:C:193:LEU:HD23	1.91	0.70
1:G:163:HIS:CD2	1:G:237:LEU:HD13	2.27	0.70
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.00	0.70
1:I:226:LEU:H	1:I:226:LEU:HD13	1.55	0.70
1:A:74:TYR:CD1	1:A:74:TYR:N	2.57	0.69
1:A:12:HIS:N	1:A:12:HIS:ND1	2.34	0.69
1:A:16:PHE:HA	1:A:41:LEU:O	1.91	0.69
1:E:193:LEU:CD2	1:E:206:CYS:SG	2.80	0.69
1:G:109:ARG:HG2	1:G:109:ARG:HH11	1.57	0.69
2:D:179:ASP:N	2:D:179:ASP:OD1	2.23	0.69
1:I:219:ASP:N	1:I:219:ASP:OD1	2.25	0.69
1:K:39:TYR:CB	1:K:55:VAL:HG12	2.22	0.69
1:K:187:LYS:HD2	1:K:187:LYS:N	2.07	0.69
1:I:180:GLN:O	1:I:184:ILE:HD13	1.92	0.69
1:A:133:LYS:O	1:A:137:ASN:HA	1.91	0.69
1:A:253:ARG:HG2	1:A:254:VAL:N	2.07	0.69
1:C:138:LEU:HD23	1:C:138:LEU:N	2.06	0.69
1:C:240:LEU:C	1:C:240:LEU:CD2	2.61	0.69
1:C:253:ARG:NH1	1:C:253:ARG:CB	2.56	0.69
1:G:244:TYR:HB3	1:G:251:LEU:HD11	1.74	0.69
1:I:80:ARG:NH1	1:I:80:ARG:HB2	2.08	0.69
1:I:253:ARG:HG3	1:I:254:VAL:N	2.08	0.69
1:K:154:LEU:HD22	1:K:154:LEU:N	2.07	0.69
1:G:172:LYS:HZ1	1:G:173:ILE:N	1.90	0.69
1:I:29:LEU:HD22	1:I:38:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:LEU:HD23	1:I:235:ASP:HB3	1.74	0.69
1:I:207:LEU:CD2	1:I:214:LEU:HB2	2.23	0.69
1:C:161:THR:HA	1:C:163:HIS:CE1	2.27	0.69
1:I:123:LEU:HD12	1:I:123:LEU:C	2.13	0.69
1:C:68:ARG:HG3	1:C:68:ARG:O	1.91	0.68
1:E:243:HIS:HE1	1:E:249:ASP:OD2	1.75	0.68
1:E:58:GLY:C	1:E:59:ARG:HG3	2.12	0.68
1:E:82:HIS:HD2	1:E:88:LEU:HA	1.56	0.68
1:C:46:ASN:O	1:C:234:PHE:HA	1.94	0.68
1:C:163:HIS:CE1	1:C:164:GLU:HG2	2.27	0.68
1:G:174:SER:OG	1:G:177:GLU:HB2	1.93	0.68
1:G:68:ARG:HG3	1:G:68:ARG:O	1.93	0.68
1:G:209:HIS:ND1	1:G:253:ARG:NH1	2.29	0.68
1:I:82:HIS:CD2	1:I:88:LEU:HA	2.29	0.68
1:C:123:LEU:CD1	1:C:127:LEU:HB2	2.22	0.68
1:G:107:PHE:CD1	1:G:107:PHE:C	2.67	0.68
1:I:243:HIS:O	1:I:246:TYR:HB3	1.94	0.68
1:E:98:GLY:HA3	2:F:184:LEU:CD2	2.24	0.68
1:A:163:HIS:CE1	1:A:164:GLU:HG2	2.29	0.68
1:C:12:HIS:ND1	1:C:12:HIS:N	2.40	0.68
1:A:40:LEU:C	1:A:40:LEU:HD12	2.15	0.68
1:C:141:GLN:NE2	1:C:141:GLN:H	1.91	0.68
1:G:262:ILE:HG22	1:I:33:GLY:HA2	1.74	0.68
1:I:48:LEU:HD23	1:I:235:ASP:CB	2.23	0.68
1:I:57:HIS:HB3	1:I:62:HIS:NE2	2.09	0.68
1:I:194:ILE:HG22	1:I:204:ALA:O	1.93	0.68
1:K:237:LEU:C	1:K:239:GLN:N	2.46	0.68
1:C:88:LEU:C	1:C:88:LEU:CD1	2.62	0.68
1:C:119:PRO:HD2	1:C:120:PHE:CE1	2.28	0.68
1:G:48:LEU:CD2	1:G:235:ASP:HB3	2.24	0.68
1:A:128:ILE:HG22	1:A:158:ILE:HG21	1.74	0.68
1:C:123:LEU:HD12	1:C:123:LEU:O	1.94	0.68
1:E:191:LYS:O	1:E:207:LEU:HA	1.94	0.68
1:G:28:TYR:HA	1:G:31:GLN:HG2	1.76	0.68
1:I:197:ARG:HG2	1:I:197:ARG:HH11	1.59	0.68
1:I:17:PHE:O	1:I:18:GLY:O	2.12	0.67
1:I:17:PHE:HE1	1:I:109:ARG:HA	1.59	0.67
1:I:32:GLY:HA2	1:I:107:PHE:CE2	2.27	0.67
1:A:158:ILE:H	1:A:158:ILE:HD13	1.58	0.67
1:I:22:ARG:NH1	2:J:181:PTR:P	2.68	0.67
1:I:229:PRO:O	2:J:173:ILE:HD11	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:256:THR:OG1	1:I:257:VAL:N	2.20	0.67
1:C:138:LEU:HD11	1:C:146:ALA:HB2	1.76	0.67
1:A:28:TYR:HA	1:A:31:GLN:HG2	1.75	0.67
1:A:172:LYS:HD2	1:A:198:ASP:HA	1.76	0.67
1:E:10:ALA:HB1	1:E:13:LEU:HG	1.77	0.67
1:G:14:PRO:HB2	1:G:108:ASN:HD22	1.60	0.67
1:G:175:ARG:HG3	2:H:170:PTR:O3P	1.95	0.67
1:E:181:ILE:HD11	1:E:260:GLN:O	1.94	0.67
1:I:75:ALA:HB2	1:I:81:THR:HA	1.77	0.67
1:K:17:PHE:CE1	1:K:109:ARG:HA	2.21	0.67
1:K:20:ILE:HD12	1:K:116:LYS:HB2	1.75	0.67
1:E:199:ASN:ND2	1:E:199:ASN:H	1.92	0.67
1:A:180:GLN:OE1	1:C:59:ARG:CZ	2.43	0.67
1:G:71:ASN:OD1	1:G:71:ASN:N	2.26	0.67
1:G:153:GLN:O	1:G:156:LYS:HB3	1.95	0.67
1:G:158:ILE:H	1:G:158:ILE:CD1	1.99	0.67
1:G:245:SER:HA	1:G:255:LEU:HB2	1.75	0.67
1:I:260:GLN:HA	1:I:260:GLN:OE1	1.94	0.67
1:C:111:GLN:HE21	1:C:112:GLY:H	1.41	0.67
1:C:229:PRO:O	2:D:173:ILE:HG13	1.95	0.67
1:I:172:LYS:O	1:I:173:ILE:HG13	1.95	0.67
1:K:161:THR:HA	1:K:163:HIS:HE1	1.58	0.67
1:K:173:ILE:CG2	1:K:177:GLU:HB2	2.25	0.67
1:A:154:LEU:O	1:A:157:LEU:N	2.27	0.66
1:A:80:ARG:CB	1:A:80:ARG:NH1	2.57	0.66
1:C:133:LYS:CB	1:C:143:LEU:HD21	2.25	0.66
1:C:209:HIS:ND1	1:C:253:ARG:NH1	2.30	0.66
1:C:253:ARG:HG3	1:C:254:VAL:N	2.09	0.66
1:G:109:ARG:HH11	1:G:109:ARG:CG	2.08	0.66
1:A:170:HIS:CG	1:A:193:LEU:HD12	2.30	0.66
1:C:226:LEU:HD11	1:C:235:ASP:O	1.93	0.66
1:I:23:GLU:HG2	1:I:246:TYR:OH	1.95	0.66
1:A:22:ARG:NH1	2:B:181:PTR:O3P	2.28	0.66
1:A:172:LYS:HE2	1:A:173:ILE:H	1.60	0.66
1:C:252:LEU:HD13	2:D:174:ARG:HD2	1.75	0.66
2:F:178:ARG:HH11	2:F:178:ARG:CB	2.03	0.66
1:I:22:ARG:HH12	2:J:181:PTR:CZ	2.08	0.66
1:E:74:TYR:CE2	1:E:85:PRO:HD3	2.30	0.66
1:G:172:LYS:O	1:G:173:ILE:HG13	1.95	0.66
1:G:216:TYR:CE1	2:H:171:GLU:HB3	2.31	0.66
1:K:41:LEU:HD22	1:K:52:ALA:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:ARG:HB2	2:H:181:PTR:O3P	1.95	0.66
1:K:241:VAL:O	1:K:243:HIS:N	2.29	0.66
1:I:30:VAL:CG2	1:I:31:GLN:N	2.58	0.66
1:I:96:SER:OG	1:I:97:ASP:N	2.24	0.66
1:A:17:PHE:CD1	1:A:109:ARG:HD3	2.31	0.66
1:A:131:TYR:C	1:A:131:TYR:CD1	2.69	0.66
1:A:180:GLN:O	1:A:182:VAL:N	2.29	0.66
1:G:182:VAL:HG23	1:G:259:CYS:SG	2.35	0.66
1:G:253:ARG:NH1	1:G:253:ARG:HB3	2.11	0.66
1:E:253:ARG:HH11	1:E:253:ARG:CG	2.09	0.66
1:C:241:VAL:CG1	1:C:242:GLU:N	2.59	0.66
1:E:189:ASN:ND2	1:E:253:ARG:NH2	2.44	0.66
1:G:9:SER:O	1:G:11:ASN:N	2.29	0.66
2:J:184:LEU:O	2:J:185:ASN:CG	2.34	0.66
1:K:170:HIS:CD2	1:K:193:LEU:HD12	2.30	0.66
1:K:178:SER:O	1:K:181:ILE:HG22	1.95	0.66
1:G:41:LEU:CD2	1:G:52:ALA:O	2.44	0.65
1:G:98:GLY:HA3	2:H:184:LEU:HD22	1.78	0.65
1:G:226:LEU:O	1:G:227:SER:HB3	1.96	0.65
1:I:170:HIS:ND1	1:I:193:LEU:HD12	2.09	0.65
1:A:170:HIS:O	1:A:171:GLY:O	2.13	0.65
1:A:238:TRP:CD1	1:A:239:GLN:N	2.63	0.65
1:C:217:ARG:HH11	1:C:217:ARG:CG	2.04	0.65
1:E:9:SER:C	1:E:11:ASN:H	2.00	0.65
1:E:22:ARG:O	1:E:26:GLU:HG3	1.96	0.65
1:G:80:ARG:HB3	1:G:80:ARG:HH11	1.61	0.65
1:A:30:VAL:C	1:A:32:GLY:N	2.49	0.65
1:C:178:SER:O	1:C:179:GLU:C	2.35	0.65
1:K:243:HIS:O	1:K:246:TYR:HB3	1.96	0.65
1:A:107:PHE:HD1	1:A:107:PHE:C	1.99	0.65
1:A:111:GLN:HE21	1:A:112:GLY:N	1.95	0.65
1:C:30:VAL:CG2	1:C:31:GLN:N	2.60	0.65
1:E:30:VAL:HA	1:E:34:MET:HB2	1.79	0.65
1:G:46:ASN:O	1:G:47:TYR:HD1	1.79	0.65
1:I:209:HIS:CG	1:I:253:ARG:HH12	2.14	0.65
1:K:209:HIS:ND1	1:K:253:ARG:NH1	2.44	0.65
1:A:154:LEU:HD22	1:A:154:LEU:N	2.10	0.65
1:C:113:VAL:HG12	1:C:114:GLN:N	2.12	0.65
1:K:197:ARG:HH11	1:K:197:ARG:CG	2.04	0.65
1:A:190:GLY:HA3	1:A:256:THR:CG2	2.25	0.65
1:A:216:TYR:CE2	1:A:251:LEU:HD22	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:OG1	1:A:257:VAL:N	2.30	0.65
1:C:179:GLU:O	1:C:182:VAL:HG12	1.96	0.65
1:E:38:LEU:HD23	1:E:105:LYS:HB3	1.79	0.65
1:K:250:GLY:HA3	2:L:173:ILE:CG2	2.26	0.65
1:A:110:PRO:HB2	1:A:113:VAL:CG2	2.26	0.65
1:C:175:ARG:NH2	1:C:215:HIS:HD2	1.93	0.65
1:G:107:PHE:HE1	1:G:110:PRO:HD3	1.61	0.65
1:G:170:HIS:ND1	1:G:193:LEU:CD1	2.58	0.65
1:A:87:ASP:O	1:A:88:LEU:C	2.33	0.65
1:A:117:THR:HG22	1:A:118:GLY:O	1.96	0.65
1:C:148:ILE:HG12	1:C:149:SER:N	2.09	0.65
1:C:188:THR:O	1:C:208:LEU:HD23	1.97	0.65
1:I:134:GLN:HG2	1:I:135:THR:N	2.11	0.65
1:I:194:ILE:HG23	1:I:205:LEU:HD23	1.78	0.65
1:C:172:LYS:HE3	1:C:198:ASP:OD1	1.96	0.65
1:C:208:LEU:HD11	1:C:211:GLY:HA2	1.79	0.65
1:E:82:HIS:ND1	1:E:82:HIS:N	2.44	0.65
2:J:174:ARG:HA	2:J:175:LYS:HE3	1.77	0.65
1:C:69:GLU:OE1	1:C:69:GLU:HA	1.95	0.64
1:C:123:LEU:HD12	1:C:127:LEU:HB2	1.79	0.64
1:I:58:GLY:O	1:I:59:ARG:HG3	1.97	0.64
1:I:203:TYR:N	1:I:203:TYR:HD1	1.94	0.64
1:A:80:ARG:NH1	1:A:80:ARG:HB2	2.12	0.64
1:A:144:GLU:O	1:A:148:ILE:HG23	1.96	0.64
1:I:173:ILE:HG23	1:I:177:GLU:HB3	1.79	0.64
1:I:179:GLU:CD	1:I:213:VAL:HG11	2.18	0.64
1:E:69:GLU:HB2	1:E:73:THR:O	1.97	0.64
1:A:128:ILE:HG13	1:A:129:ARG:N	2.11	0.64
1:C:27:ASP:O	1:C:30:VAL:HG22	1.97	0.64
2:D:174:ARG:CA	2:D:175:LYS:HE2	2.25	0.64
1:E:253:ARG:HH11	1:E:253:ARG:HG2	1.62	0.64
1:I:30:VAL:HG23	1:I:31:GLN:H	1.62	0.64
1:I:163:HIS:O	1:I:169:PHE:HD2	1.81	0.64
1:A:148:ILE:HD13	1:A:149:SER:H	1.62	0.64
1:C:168:TRP:HE3	1:C:194:ILE:HG13	1.63	0.64
1:E:159:ALA:HB1	1:E:236:THR:HG21	1.80	0.64
1:K:41:LEU:CD2	1:K:52:ALA:O	2.44	0.64
1:K:58:GLY:C	1:K:59:ARG:HG3	2.16	0.64
1:C:109:ARG:HG2	1:C:109:ARG:HH11	1.62	0.64
1:A:107:PHE:C	1:A:107:PHE:CD1	2.70	0.64
1:A:138:LEU:HD23	1:A:138:LEU:N	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:H	1:A:154:LEU:HD23	1.63	0.64
1:A:207:LEU:CD2	1:A:214:LEU:HB2	2.28	0.64
1:K:99:LEU:CD1	1:K:103:LEU:HD21	2.28	0.64
1:A:184:ILE:HD13	1:A:184:ILE:N	2.12	0.64
1:C:50:GLY:C	1:C:51:PHE:CD1	2.71	0.64
1:C:200:ASN:N	1:C:200:ASN:OD1	2.31	0.64
1:K:199:ASN:O	1:K:202:SER:N	2.30	0.64
1:A:207:LEU:HD21	1:A:214:LEU:HB2	1.79	0.64
1:C:186:SER:HB3	1:C:188:THR:HG22	1.80	0.64
1:I:132:VAL:HG12	1:I:143:LEU:HD11	1.80	0.64
1:K:207:LEU:HD21	1:K:214:LEU:HB2	1.80	0.64
1:G:173:ILE:CG2	1:G:177:GLU:HB3	2.26	0.64
1:K:71:ASN:HB2	1:K:73:THR:HG23	1.79	0.64
1:C:238:TRP:CD1	1:C:239:GLN:N	2.66	0.63
1:G:253:ARG:NH1	1:G:253:ARG:CB	2.61	0.63
1:I:144:GLU:HB2	1:I:145:GLN:NE2	2.13	0.63
1:K:22:ARG:O	1:K:25:ALA:HB3	1.98	0.63
1:A:15:PHE:N	1:A:15:PHE:CD1	2.64	0.63
1:G:107:PHE:C	1:G:107:PHE:HD1	2.00	0.63
1:G:199:ASN:ND2	1:G:200:ASN:H	1.96	0.63
1:A:208:LEU:HD11	1:A:211:GLY:HA2	1.80	0.63
1:C:197:ARG:HD3	1:C:202:SER:OG	1.97	0.63
1:G:202:SER:O	1:G:203:TYR:HD1	1.82	0.63
1:G:237:LEU:C	1:G:239:GLN:N	2.49	0.63
1:I:203:TYR:N	1:I:203:TYR:CD1	2.66	0.63
1:I:21:THR:HG1	1:I:24:GLU:H	1.46	0.63
1:K:180:GLN:O	1:K:182:VAL:N	2.31	0.63
1:A:260:GLN:OE1	1:A:260:GLN:CA	2.45	0.63
1:E:17:PHE:CE1	1:E:109:ARG:HA	2.33	0.63
1:E:193:LEU:HD23	1:E:193:LEU:C	2.18	0.63
1:G:84:SER:OG	1:G:86:ALA:HB3	1.98	0.63
1:A:122:ASP:OD1	1:A:122:ASP:N	2.27	0.63
2:B:178:ARG:HB3	2:B:178:ARG:NH1	2.13	0.63
1:C:138:LEU:CG	1:C:143:LEU:HD13	2.29	0.63
1:C:234:PHE:CE2	1:C:240:LEU:HA	2.33	0.63
1:G:158:ILE:HD13	1:G:158:ILE:N	2.06	0.63
1:E:17:PHE:HD1	1:E:109:ARG:HD3	1.62	0.63
1:E:29:LEU:HD21	1:E:40:LEU:HD23	1.80	0.63
1:G:17:PHE:CE1	1:G:109:ARG:HA	2.34	0.63
1:I:179:GLU:O	1:I:182:VAL:HG12	1.99	0.63
1:K:199:ASN:ND2	1:K:199:ASN:N	2.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG12	1:A:149:SER:N	2.14	0.63
1:C:20:ILE:CG2	1:C:21:THR:N	2.62	0.63
1:C:150:GLN:O	1:C:151:LYS:C	2.36	0.63
1:C:240:LEU:HD23	1:C:240:LEU:O	1.97	0.63
1:I:205:LEU:HD22	1:I:206:CYS:N	2.13	0.63
1:K:168:TRP:CZ3	1:K:194:ILE:HD11	2.34	0.63
1:I:189:ASN:OD1	1:I:209:HIS:HA	1.99	0.63
1:A:37:GLY:HA3	1:A:104:LYS:HG3	1.81	0.62
1:A:151:LYS:O	1:A:152:PRO:C	2.36	0.62
1:E:241:VAL:O	1:E:243:HIS:N	2.32	0.62
1:I:128:ILE:CG2	1:I:158:ILE:HG12	2.16	0.62
1:A:240:LEU:HD23	1:A:244:TYR:HD2	1.63	0.62
1:C:30:VAL:HG23	1:C:31:GLN:N	2.14	0.62
1:E:58:GLY:C	1:E:60:LYS:H	2.02	0.62
1:K:227:SER:HB2	1:K:232:LYS:O	1.99	0.62
2:D:184:LEU:O	2:D:185:ASN:CB	2.47	0.62
1:G:170:HIS:O	1:G:173:ILE:HD12	1.98	0.62
1:A:120:PHE:C	1:A:122:ASP:H	2.03	0.62
2:F:173:ILE:HG22	2:F:174:ARG:N	2.15	0.62
1:C:138:LEU:HD12	1:C:142:ALA:C	2.20	0.62
1:I:138:LEU:O	1:I:139:GLN:HG3	1.98	0.62
1:C:238:TRP:HD1	1:C:239:GLN:N	1.97	0.62
1:C:48:LEU:O	1:C:50:GLY:N	2.33	0.62
1:C:234:PHE:CD2	1:C:240:LEU:HA	2.34	0.62
1:I:128:ILE:CD1	1:I:129:ARG:H	2.04	0.62
1:A:21:THR:HG22	1:A:24:GLU:OE1	1.99	0.62
1:A:189:ASN:HA	1:A:208:LEU:HD23	1.80	0.62
1:C:153:GLN:NE2	1:C:153:GLN:C	2.53	0.62
1:E:154:LEU:O	1:E:158:ILE:HD13	1.99	0.62
1:A:24:GLU:O	1:A:27:ASP:HB2	2.00	0.62
1:A:193:LEU:O	1:A:193:LEU:HD23	2.00	0.62
1:C:241:VAL:HG12	1:C:242:GLU:H	1.63	0.62
1:A:158:ILE:N	1:A:158:ILE:HD12	2.12	0.61
1:I:39:TYR:CZ	1:I:106:PRO:HB3	2.35	0.61
2:L:173:ILE:CG2	2:L:174:ARG:H	2.11	0.61
1:C:154:LEU:CD2	1:C:154:LEU:N	2.52	0.61
1:E:70:LEU:H	1:E:70:LEU:HD12	1.65	0.61
1:I:202:SER:C	1:I:203:TYR:HD1	2.02	0.61
1:I:207:LEU:HD21	1:I:214:LEU:HB2	1.82	0.61
1:G:216:TYR:CD1	2:H:171:GLU:HB3	2.35	0.61
1:I:21:THR:OG1	1:I:24:GLU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:GLU:HB2	1:G:73:THR:O	2.00	0.61
1:I:16:PHE:HA	1:I:41:LEU:O	2.01	0.61
1:I:120:PHE:HB2	1:I:238:TRP:HZ3	1.66	0.61
1:K:217:ARG:HG2	1:K:217:ARG:NH1	2.12	0.61
1:A:180:GLN:NE2	1:C:59:ARG:CB	2.63	0.61
1:I:120:PHE:CG	1:I:238:TRP:CZ3	2.89	0.61
1:K:16:PHE:HA	1:K:41:LEU:O	2.00	0.61
1:K:178:SER:O	1:K:179:GLU:C	2.39	0.61
1:K:187:LYS:HD2	1:K:187:LYS:H	1.65	0.61
1:G:178:SER:O	1:G:179:GLU:C	2.38	0.61
1:C:228:ILE:CG2	1:C:229:PRO:HD2	2.30	0.61
1:G:197:ARG:HH11	1:G:197:ARG:CG	2.07	0.61
1:A:30:VAL:HG22	1:A:31:GLN:N	2.15	0.61
1:A:197:ARG:O	1:A:199:ASN:N	2.33	0.61
1:G:181:ILE:O	1:G:181:ILE:HD13	2.00	0.61
1:C:161:THR:HB	1:C:164:GLU:HG3	1.83	0.61
2:H:174:ARG:HA	2:H:175:LYS:HE2	1.82	0.61
1:I:202:SER:HB2	1:I:218:ILE:O	2.00	0.61
1:A:21:THR:CG2	1:A:24:GLU:CG	2.79	0.60
1:A:22:ARG:NH2	2:B:180:LEU:O	2.34	0.60
1:A:120:PHE:CB	1:A:123:LEU:HD11	2.31	0.60
1:E:21:THR:HG23	1:E:24:GLU:CB	2.15	0.60
1:K:38:LEU:HA	1:K:105:LYS:O	2.00	0.60
1:A:163:HIS:N	1:A:163:HIS:ND1	2.49	0.60
1:E:53:LEU:HD22	1:E:54:SER:N	2.16	0.60
1:G:80:ARG:HG2	1:G:81:THR:N	2.16	0.60
1:G:170:HIS:O	1:G:171:GLY:O	2.18	0.60
1:G:238:TRP:O	1:G:242:GLU:HB2	2.01	0.60
1:I:36:ASP:HA	1:I:56:ALA:O	2.01	0.60
1:I:151:LYS:HB3	1:I:152:PRO:HD2	1.84	0.60
1:A:58:GLY:O	1:A:59:ARG:HG3	2.01	0.60
1:A:182:VAL:HG23	1:A:259:CYS:CB	2.31	0.60
1:G:180:GLN:HG2	1:G:181:ILE:H	1.66	0.60
1:G:219:ASP:OD1	1:G:219:ASP:N	2.35	0.60
1:I:48:LEU:CD2	1:I:235:ASP:CB	2.80	0.60
1:I:138:LEU:C	1:I:139:GLN:HE21	2.04	0.60
1:K:181:ILE:CD1	1:K:181:ILE:O	2.50	0.60
1:K:253:ARG:HG2	1:K:253:ARG:HH11	1.65	0.60
1:G:260:GLN:OE1	1:G:260:GLN:CA	2.46	0.60
1:A:260:GLN:OE1	1:A:261:LYS:N	2.31	0.60
1:E:202:SER:C	1:E:203:TYR:CD1	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:LYS:CD	2:F:175:LYS:N	2.65	0.60
1:I:197:ARG:O	1:I:198:ASP:OD1	2.19	0.60
1:I:238:TRP:CD1	1:I:238:TRP:C	2.75	0.60
1:K:237:LEU:C	1:K:239:GLN:H	2.05	0.60
1:A:30:VAL:O	1:A:33:GLY:N	2.33	0.60
1:A:176:GLU:C	1:A:178:SER:N	2.53	0.60
1:C:46:ASN:N	1:C:46:ASN:OD1	2.32	0.60
1:C:246:TYR:CD1	1:C:247:LYS:HB3	2.37	0.60
1:I:120:PHE:HA	1:I:123:LEU:HB3	1.83	0.60
1:I:137:ASN:N	1:I:137:ASN:OD1	2.34	0.60
1:C:210:GLU:HA	1:C:210:GLU:OE1	2.02	0.60
2:F:173:ILE:HG22	2:F:174:ARG:H	1.66	0.60
1:G:12:HIS:CE1	1:G:13:LEU:HD23	2.36	0.60
1:I:30:VAL:C	1:I:32:GLY:N	2.54	0.60
1:A:174:SER:OG	1:A:177:GLU:CB	2.42	0.60
1:A:197:ARG:C	1:A:199:ASN:H	2.04	0.60
1:C:125:GLU:O	1:C:128:ILE:HG13	2.02	0.60
1:E:181:ILE:HD12	1:E:262:ILE:HD13	1.84	0.60
1:G:246:TYR:C	1:G:246:TYR:CD1	2.75	0.60
1:I:226:LEU:H	1:I:226:LEU:CD1	2.15	0.60
1:K:253:ARG:HG3	1:K:254:VAL:N	2.17	0.60
1:A:21:THR:HG23	1:A:24:GLU:CG	2.31	0.59
1:C:179:GLU:OE1	1:C:213:VAL:HG11	2.02	0.59
1:C:253:ARG:CB	1:C:253:ARG:CZ	2.79	0.59
1:G:199:ASN:CG	1:G:200:ASN:N	2.50	0.59
1:G:207:LEU:O	1:G:207:LEU:HD23	2.02	0.59
1:I:38:LEU:HD23	1:I:105:LYS:O	2.02	0.59
1:K:88:LEU:C	1:K:88:LEU:HD12	2.23	0.59
1:K:225:LYS:NZ	1:K:235:ASP:OD1	2.32	0.59
1:A:172:LYS:HE3	1:A:196:ALA:O	2.02	0.59
2:B:184:LEU:O	2:B:185:ASN:HB3	2.01	0.59
1:G:109:ARG:HB3	1:G:109:ARG:NH1	2.17	0.59
1:G:172:LYS:HZ1	1:G:173:ILE:CA	2.15	0.59
1:I:80:ARG:HG2	1:I:81:THR:N	2.17	0.59
1:K:199:ASN:HD22	1:K:199:ASN:N	1.96	0.59
1:C:132:VAL:CG1	1:C:143:LEU:HD11	2.32	0.59
1:I:193:LEU:O	1:I:193:LEU:HD23	2.02	0.59
1:I:236:THR:OG1	1:I:238:TRP:CD1	2.56	0.59
1:K:234:PHE:CZ	1:K:240:LEU:HA	2.36	0.59
1:E:181:ILE:HD12	1:E:262:ILE:CD1	2.33	0.59
1:A:209:HIS:ND1	1:A:253:ARG:NH1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PRO:HD2	1:C:120:PHE:CZ	2.37	0.59
1:E:9:SER:O	1:E:11:ASN:N	2.36	0.59
1:I:21:THR:CG2	1:I:24:GLU:HB2	2.32	0.59
1:I:120:PHE:CB	1:I:238:TRP:CZ3	2.84	0.59
1:K:17:PHE:CD2	1:K:40:LEU:HD13	2.37	0.59
1:A:48:LEU:HD23	1:A:235:ASP:CB	2.32	0.59
1:A:232:LYS:HG3	1:A:233:LYS:N	2.15	0.59
1:C:22:ARG:NH2	2:D:180:LEU:O	2.33	0.59
1:C:177:GLU:O	1:C:181:ILE:CG2	2.44	0.59
1:G:93:SER:O	1:G:102:LEU:HD12	2.03	0.59
1:A:145:GLN:HE21	1:A:145:GLN:CA	2.15	0.59
1:A:219:ASP:N	1:A:219:ASP:OD1	2.35	0.59
1:C:16:PHE:HA	1:C:41:LEU:O	2.02	0.59
1:C:158:ILE:HD12	1:C:158:ILE:H	1.66	0.59
1:C:246:TYR:CD1	1:C:246:TYR:C	2.76	0.59
1:G:240:LEU:HD21	1:G:244:TYR:HD2	1.68	0.59
1:I:205:LEU:HD22	1:I:206:CYS:H	1.68	0.59
1:K:17:PHE:O	1:K:18:GLY:O	2.20	0.59
1:K:207:LEU:HD23	1:K:207:LEU:O	2.02	0.59
1:A:120:PHE:C	1:A:122:ASP:N	2.54	0.59
1:A:124:LYS:O	1:A:126:ASN:N	2.35	0.59
1:E:39:TYR:CD1	1:E:103:LEU:HB3	2.38	0.59
1:G:202:SER:C	1:G:203:TYR:HD1	2.06	0.59
1:K:154:LEU:O	1:K:158:ILE:HD13	2.03	0.59
1:K:234:PHE:CD2	1:K:240:LEU:HA	2.37	0.59
1:A:157:LEU:HB3	1:A:158:ILE:HD12	1.84	0.59
1:A:229:PRO:O	2:B:173:ILE:HD11	2.03	0.59
1:C:170:HIS:HB3	1:C:173:ILE:CD1	2.31	0.59
1:I:176:GLU:OE1	1:I:176:GLU:N	2.34	0.59
1:K:39:TYR:CD2	1:K:103:LEU:HD13	2.38	0.59
1:K:253:ARG:HH11	1:K:253:ARG:CG	2.16	0.59
1:C:138:LEU:HG	1:C:143:LEU:HA	1.84	0.58
1:C:198:ASP:HB3	1:C:199:ASN:ND2	2.18	0.58
1:C:236:THR:HG23	1:C:239:GLN:OE1	2.03	0.58
1:E:21:THR:CG2	1:E:24:GLU:OE1	2.51	0.58
1:K:46:ASN:O	1:K:47:TYR:HD1	1.86	0.58
1:K:168:TRP:CE3	1:K:194:ILE:HD11	2.38	0.58
1:E:205:LEU:O	1:E:215:HIS:HA	2.03	0.58
1:E:216:TYR:CE2	1:E:251:LEU:HD22	2.38	0.58
1:G:158:ILE:CD1	1:G:158:ILE:N	2.64	0.58
1:I:70:LEU:H	1:I:70:LEU:CD1	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:250:GLY:HA3	2:L:173:ILE:HG23	1.84	0.58
1:A:173:ILE:HG23	1:A:177:GLU:CB	2.33	0.58
1:C:111:GLN:NE2	1:C:112:GLY:N	2.49	0.58
1:C:144:GLU:HA	1:C:147:ILE:HD11	1.84	0.58
1:I:27:ASP:O	1:I:30:VAL:CG2	2.48	0.58
1:I:130:GLU:O	1:I:131:TYR:C	2.40	0.58
1:A:120:PHE:O	1:A:123:LEU:HD12	2.03	0.58
1:A:129:ARG:HG2	2:H:168:PRO:HA	1.83	0.58
1:A:228:ILE:HG23	1:A:229:PRO:HD2	1.84	0.58
1:C:21:THR:CG2	1:C:24:GLU:HB2	2.27	0.58
1:C:207:LEU:O	1:C:214:LEU:N	2.31	0.58
1:E:10:ALA:HA	1:E:12:HIS:CE1	2.38	0.58
1:E:175:ARG:HH11	2:F:168:PRO:HD2	1.68	0.58
1:G:22:ARG:NH1	2:H:181:PTR:O3P	2.36	0.58
2:H:171:GLU:OE2	2:H:172:PRO:HD2	2.02	0.58
1:I:147:ILE:O	1:I:151:LYS:N	2.34	0.58
1:K:58:GLY:C	1:K:60:LYS:H	2.06	0.58
1:A:129:ARG:CG	1:A:129:ARG:NH1	2.62	0.58
1:C:93:SER:O	1:C:102:LEU:CD1	2.52	0.58
1:C:173:ILE:HG22	1:C:177:GLU:CB	2.33	0.58
1:G:241:VAL:O	1:G:243:HIS:N	2.37	0.58
1:I:38:LEU:CD2	1:I:39:TYR:N	2.66	0.58
1:I:42:ARG:HH12	2:J:181:PTR:P	2.27	0.58
1:I:191:LYS:O	1:I:207:LEU:HA	2.03	0.58
2:J:173:ILE:HG22	2:J:174:ARG:H	1.69	0.58
1:C:18:GLY:H	1:C:115:PRO:HB3	1.69	0.58
1:C:110:PRO:HD2	1:C:113:VAL:CG2	2.31	0.58
1:A:17:PHE:O	1:A:20:ILE:CD1	2.48	0.58
1:C:226:LEU:CD1	1:C:234:PHE:O	2.49	0.58
1:K:71:ASN:OD1	1:K:71:ASN:N	2.36	0.58
1:E:223:THR:HB	1:E:225:LYS:HD3	1.85	0.58
1:G:164:GLU:HA	1:G:169:PHE:CE2	2.38	0.58
1:I:48:LEU:CD2	1:I:235:ASP:HB3	2.33	0.58
1:I:176:GLU:C	1:I:178:SER:N	2.54	0.58
1:I:206:CYS:HA	1:I:214:LEU:O	2.03	0.58
1:I:131:TYR:C	1:I:131:TYR:CD1	2.76	0.58
1:K:109:ARG:HG2	1:K:109:ARG:HH11	1.68	0.58
2:L:184:LEU:O	2:L:185:ASN:CB	2.52	0.58
1:A:28:TYR:O	1:A:107:PHE:CE2	2.53	0.58
1:C:32:GLY:HA3	1:C:107:PHE:CE2	2.39	0.58
1:C:144:GLU:O	1:C:147:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:VAL:C	1:E:32:GLY:H	2.05	0.58
1:C:153:GLN:O	1:C:154:LEU:C	2.40	0.57
1:E:17:PHE:CE1	1:E:109:ARG:HD3	2.38	0.57
1:I:254:VAL:HG22	1:I:255:LEU:O	2.04	0.57
2:J:178:ARG:HH11	2:J:178:ARG:CG	2.14	0.57
1:K:241:VAL:HG12	1:K:242:GLU:N	2.17	0.57
1:A:195:ARG:HH21	1:A:215:HIS:CE1	2.21	0.57
1:A:234:PHE:HD2	1:A:239:GLN:HB3	1.69	0.57
1:E:205:LEU:HD22	1:E:206:CYS:N	2.20	0.57
1:I:251:LEU:HB2	1:I:253:ARG:O	2.04	0.57
1:K:182:VAL:HG11	1:K:213:VAL:HG23	1.86	0.57
1:C:151:LYS:HA	1:C:154:LEU:HG	1.85	0.57
1:C:154:LEU:O	1:C:157:LEU:N	2.36	0.57
1:G:27:ASP:OD1	1:K:185:GLY:HA3	2.03	0.57
1:G:240:LEU:C	1:G:240:LEU:CD2	2.64	0.57
1:I:88:LEU:CD1	1:I:92:HIS:ND1	2.67	0.57
1:I:226:LEU:CD1	1:I:226:LEU:N	2.67	0.57
1:G:163:HIS:CE1	1:G:164:GLU:HG2	2.38	0.57
1:C:118:GLY:O	1:C:122:ASP:OD2	2.22	0.57
1:G:20:ILE:CD1	1:G:116:LYS:HB2	2.35	0.57
2:H:178:ARG:HH11	2:H:178:ARG:CG	2.18	0.57
1:I:150:GLN:OE1	1:I:150:GLN:HA	2.03	0.57
1:A:207:LEU:HD23	1:A:207:LEU:H	1.70	0.57
1:C:120:PHE:N	1:C:122:ASP:OD1	2.38	0.57
1:E:177:GLU:O	1:E:181:ILE:HG22	2.05	0.57
1:E:209:HIS:CE1	1:E:253:ARG:HH22	2.22	0.57
1:I:17:PHE:CE1	1:I:109:ARG:HA	2.37	0.57
1:K:176:GLU:OE1	1:K:176:GLU:N	2.37	0.57
1:C:107:PHE:C	1:C:107:PHE:CD1	2.78	0.57
1:E:193:LEU:HD21	1:E:206:CYS:SG	2.44	0.57
1:G:157:LEU:O	1:G:158:ILE:C	2.42	0.57
1:K:24:GLU:O	1:K:28:TYR:HD2	1.87	0.57
1:E:182:VAL:CG2	1:E:259:CYS:SG	2.90	0.57
1:E:207:LEU:HD23	1:E:214:LEU:HB2	1.87	0.57
1:G:88:LEU:CD1	1:G:88:LEU:C	2.73	0.57
1:I:120:PHE:CD1	1:I:238:TRP:CH2	2.93	0.57
1:K:22:ARG:NH2	2:L:180:LEU:O	2.38	0.57
1:A:151:LYS:O	1:A:155:GLU:OE1	2.22	0.57
1:C:123:LEU:HG	1:C:124:LYS:N	2.19	0.57
2:F:175:LYS:N	2:F:175:LYS:HD2	2.20	0.57
1:G:194:ILE:HG23	1:G:205:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:VAL:O	1:G:242:GLU:C	2.43	0.57
2:H:185:ASN:CG	2:H:185:ASN:O	2.42	0.57
1:C:128:ILE:CD1	1:C:129:ARG:N	2.68	0.57
1:C:178:SER:HA	1:C:181:ILE:CG2	2.34	0.57
1:G:172:LYS:C	1:G:172:LYS:HZ3	2.08	0.57
1:K:28:TYR:O	1:K:107:PHE:CE2	2.58	0.57
1:A:41:LEU:CD2	1:A:52:ALA:O	2.53	0.56
1:A:187:LYS:O	1:A:208:LEU:HD21	2.04	0.56
1:C:205:LEU:HB3	1:C:216:TYR:HB2	1.87	0.56
1:E:88:LEU:HD12	1:E:88:LEU:C	2.25	0.56
1:A:262:ILE:HG22	1:A:262:ILE:O	2.05	0.56
1:C:88:LEU:HD12	1:C:88:LEU:O	2.04	0.56
1:C:161:THR:HA	1:C:163:HIS:ND1	2.19	0.56
1:C:241:VAL:O	1:C:242:GLU:C	2.40	0.56
1:E:15:PHE:HE2	1:E:89:CYS:HG	1.50	0.56
1:G:80:ARG:HH11	1:G:80:ARG:CB	2.18	0.56
1:I:22:ARG:HB2	2:J:181:PTR:O3P	2.05	0.56
1:C:151:LYS:O	1:C:153:GLN:N	2.38	0.56
1:C:252:LEU:CD1	2:D:174:ARG:HD2	2.35	0.56
1:C:253:ARG:CZ	1:C:253:ARG:HB2	2.34	0.56
1:E:207:LEU:HD23	1:E:207:LEU:O	2.05	0.56
1:G:173:ILE:HG23	1:G:177:GLU:CB	2.32	0.56
1:G:179:GLU:O	1:G:183:LEU:HD22	2.05	0.56
1:G:238:TRP:CD1	1:G:239:GLN:N	2.73	0.56
1:I:123:LEU:HD12	1:I:124:LYS:CA	2.35	0.56
2:J:175:LYS:O	2:J:178:ARG:HG2	2.05	0.56
1:K:182:VAL:HG11	1:K:213:VAL:CG2	2.35	0.56
1:A:124:LYS:O	1:A:128:ILE:HG23	2.05	0.56
1:A:154:LEU:CD2	1:A:154:LEU:N	2.58	0.56
1:A:237:LEU:O	1:A:238:TRP:C	2.43	0.56
1:E:88:LEU:HD12	1:E:88:LEU:O	2.06	0.56
1:G:161:THR:HA	1:G:163:HIS:CE1	2.41	0.56
1:I:19:ASN:HD21	1:I:45:ARG:HG2	1.70	0.56
1:I:120:PHE:C	1:I:122:ASP:N	2.54	0.56
1:A:181:ILE:HD12	1:A:262:ILE:CD1	2.36	0.56
1:C:238:TRP:HD1	1:C:239:GLN:HG3	1.70	0.56
1:E:30:VAL:C	1:E:32:GLY:N	2.57	0.56
1:E:168:TRP:HE3	1:E:194:ILE:HG13	1.71	0.56
1:E:193:LEU:HD23	1:E:206:CYS:SG	2.44	0.56
1:E:219:ASP:OD1	1:E:219:ASP:N	2.38	0.56
1:C:12:HIS:O	1:C:14:PRO:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.71	0.56
1:E:179:GLU:CD	1:E:213:VAL:HG11	2.26	0.56
1:G:93:SER:O	1:G:102:LEU:CD1	2.53	0.56
1:A:180:GLN:O	1:A:183:LEU:N	2.39	0.56
1:I:154:LEU:N	1:I:154:LEU:CD2	2.59	0.56
1:A:128:ILE:HG13	1:A:129:ARG:H	1.71	0.56
1:A:192:PHE:CD2	1:A:255:LEU:HD13	2.41	0.56
1:G:48:LEU:HD22	1:G:235:ASP:HB2	1.87	0.56
1:G:109:ARG:CG	1:G:109:ARG:NH1	2.68	0.56
1:I:207:LEU:HD23	1:I:214:LEU:HB2	1.88	0.56
1:K:54:SER:HA	1:K:62:HIS:O	2.06	0.56
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.70	0.56
1:A:165:LYS:HE2	1:A:165:LYS:O	2.06	0.56
1:C:168:TRP:CE3	1:C:194:ILE:HG13	2.41	0.56
1:I:132:VAL:HG12	1:I:143:LEU:CD1	2.35	0.56
1:K:193:LEU:HD23	1:K:206:CYS:HB2	1.87	0.56
1:A:30:VAL:C	1:A:32:GLY:H	2.09	0.56
1:C:194:ILE:HG23	1:C:204:ALA:O	2.06	0.56
1:C:241:VAL:O	1:C:243:HIS:N	2.39	0.56
1:E:166:MET:O	1:E:169:PHE:HB3	2.05	0.56
1:G:241:VAL:CG1	1:G:242:GLU:N	2.67	0.56
1:I:48:LEU:O	1:I:50:GLY:N	2.39	0.56
1:I:128:ILE:CD1	1:I:129:ARG:N	2.67	0.56
1:I:256:THR:HG1	1:I:257:VAL:H	1.53	0.56
1:K:68:ARG:HG3	1:K:68:ARG:O	2.05	0.56
1:K:234:PHE:HB3	1:K:239:GLN:CG	2.36	0.56
1:A:123:LEU:CD1	1:A:124:LYS:N	2.64	0.55
1:C:260:GLN:OE1	1:C:260:GLN:CA	2.50	0.55
2:D:175:LYS:O	2:D:177:GLN:N	2.38	0.55
1:E:22:ARG:HG2	1:E:23:GLU:N	2.22	0.55
1:E:207:LEU:CD2	1:E:214:LEU:HB2	2.36	0.55
1:G:114:GLN:HB3	1:G:115:PRO:CD	2.36	0.55
1:I:178:SER:O	1:I:179:GLU:C	2.42	0.55
1:K:166:MET:HE2	1:K:166:MET:HA	1.87	0.55
1:K:227:SER:HB2	1:K:233:LYS:HA	1.87	0.55
1:A:20:ILE:CD1	1:A:116:LYS:HB2	2.34	0.55
1:A:199:ASN:OD1	1:A:199:ASN:N	2.38	0.55
1:G:9:SER:C	1:G:11:ASN:H	2.08	0.55
1:K:175:ARG:CZ	2:L:168:PRO:HD2	2.36	0.55
1:A:48:LEU:CD2	1:A:235:ASP:HB3	2.35	0.55
1:C:154:LEU:O	1:C:155:GLU:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLN:O	1:C:184:ILE:HD13	2.06	0.55
1:C:194:ILE:CG2	1:C:204:ALA:O	2.53	0.55
1:G:30:VAL:CG2	1:G:31:GLN:N	2.69	0.55
1:A:22:ARG:O	1:A:25:ALA:HB3	2.06	0.55
1:C:161:THR:HG22	1:C:163:HIS:HE1	1.72	0.55
1:E:96:SER:O	1:E:99:LEU:HB2	2.05	0.55
1:E:170:HIS:HE1	1:E:260:GLN:O	1.89	0.55
1:I:58:GLY:O	1:I:60:LYS:N	2.40	0.55
1:I:234:PHE:CD2	1:I:240:LEU:HA	2.41	0.55
1:A:17:PHE:O	1:A:18:GLY:O	2.24	0.55
1:C:206:CYS:HA	1:C:214:LEU:O	2.07	0.55
1:G:161:THR:HB	1:G:164:GLU:HG3	1.89	0.55
1:G:240:LEU:CD2	1:G:244:TYR:HD2	2.18	0.55
1:I:36:ASP:OD1	1:I:57:HIS:HA	2.06	0.55
1:I:136:TRP:HB3	1:I:138:LEU:CD2	2.36	0.55
1:I:163:HIS:HA	1:I:166:MET:HG3	1.89	0.55
1:A:168:TRP:HE3	1:A:194:ILE:HG13	1.72	0.55
1:A:253:ARG:CG	1:A:254:VAL:N	2.69	0.55
1:G:15:PHE:N	1:G:15:PHE:CD1	2.75	0.55
1:G:17:PHE:O	1:G:18:GLY:O	2.25	0.55
2:J:179:ASP:N	2:J:179:ASP:OD1	2.40	0.55
1:K:237:LEU:O	1:K:238:TRP:C	2.43	0.55
1:C:50:GLY:C	1:C:51:PHE:HD1	2.08	0.55
1:C:173:ILE:HG21	1:C:177:GLU:HG2	1.88	0.55
1:I:128:ILE:HG22	1:I:158:ILE:CG1	2.18	0.55
1:K:30:VAL:HG12	1:K:34:MET:SD	2.46	0.55
1:K:205:LEU:HB3	1:K:216:TYR:HB2	1.89	0.55
1:C:228:ILE:HG22	1:C:229:PRO:CD	2.37	0.55
1:E:20:ILE:HD12	1:E:116:LYS:HB2	1.87	0.55
1:E:229:PRO:O	1:E:230:GLU:HB2	2.06	0.55
1:E:232:LYS:HZ1	2:F:181:PTR:HE1	1.72	0.55
1:G:30:VAL:HG22	1:G:31:GLN:N	2.22	0.55
1:G:109:ARG:NH1	1:G:109:ARG:CB	2.69	0.55
1:G:168:TRP:CZ3	1:G:194:ILE:HD11	2.42	0.55
1:K:53:LEU:HD22	1:K:54:SER:N	2.21	0.55
1:K:88:LEU:HD12	1:K:88:LEU:O	2.06	0.55
1:K:234:PHE:HB3	1:K:239:GLN:CD	2.27	0.55
1:A:148:ILE:CG1	1:A:149:SER:N	2.69	0.55
1:A:173:ILE:CG2	1:A:177:GLU:HB3	2.37	0.55
1:G:46:ASN:C	1:G:47:TYR:HD1	2.10	0.55
1:G:170:HIS:CE1	1:G:193:LEU:HD12	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:ILE:HG23	1:K:24:GLU:HB3	1.88	0.55
1:C:175:ARG:CZ	1:C:215:HIS:CD2	2.90	0.55
1:E:75:ALA:CB	1:E:81:THR:HA	2.27	0.55
1:A:234:PHE:CE2	1:A:240:LEU:HA	2.43	0.54
1:I:30:VAL:CG2	1:I:31:GLN:H	2.19	0.54
2:B:173:ILE:HG22	2:B:174:ARG:N	2.18	0.54
1:C:191:LYS:HA	1:C:257:VAL:O	2.07	0.54
1:I:151:LYS:CB	1:I:152:PRO:CD	2.85	0.54
1:K:30:VAL:C	1:K:32:GLY:H	2.11	0.54
1:A:246:TYR:CD1	1:A:246:TYR:C	2.80	0.54
1:C:210:GLU:OE1	1:C:210:GLU:CA	2.56	0.54
1:G:41:LEU:HD23	1:G:52:ALA:O	2.07	0.54
1:K:207:LEU:CD2	1:K:214:LEU:HB2	2.37	0.54
1:K:228:ILE:HG21	2:L:173:ILE:HD11	1.87	0.54
1:A:145:GLN:HA	1:A:148:ILE:HD12	1.88	0.54
1:C:129:ARG:HH11	1:C:129:ARG:HG3	1.72	0.54
1:C:202:SER:C	1:C:203:TYR:CD1	2.64	0.54
1:I:161:THR:HA	1:I:163:HIS:CE1	2.43	0.54
1:I:164:GLU:HA	1:I:169:PHE:CE2	2.42	0.54
1:K:30:VAL:CG2	1:K:31:GLN:N	2.69	0.54
1:A:150:GLN:C	1:A:154:LEU:HD23	2.27	0.54
1:A:193:LEU:HG	1:A:194:ILE:N	2.21	0.54
1:A:216:TYR:CE1	2:B:171:GLU:HB3	2.42	0.54
1:C:244:TYR:CG	1:C:251:LEU:HD11	2.42	0.54
1:E:240:LEU:C	1:E:240:LEU:CD2	2.76	0.54
1:G:87:ASP:O	1:G:88:LEU:C	2.45	0.54
1:G:180:GLN:O	1:G:182:VAL:N	2.40	0.54
1:G:262:ILE:CG2	1:I:33:GLY:HA2	2.37	0.54
1:I:71:ASN:HB2	1:I:73:THR:CG2	2.34	0.54
1:K:187:LYS:H	1:K:187:LYS:CD	2.19	0.54
1:A:18:GLY:HA3	1:A:116:LYS:O	2.08	0.54
1:C:140:GLY:C	1:C:142:ALA:H	2.08	0.54
1:E:99:LEU:CD1	1:E:103:LEU:CD2	2.85	0.54
1:G:16:PHE:HD1	1:G:41:LEU:O	1.89	0.54
1:G:70:LEU:HD12	1:G:70:LEU:N	2.08	0.54
1:K:93:SER:O	1:K:102:LEU:HD13	2.08	0.54
1:A:243:HIS:O	1:A:246:TYR:N	2.39	0.54
1:C:96:SER:O	1:C:99:LEU:HB2	2.07	0.54
1:C:180:GLN:HE22	1:E:59:ARG:NH2	2.05	0.54
1:G:68:ARG:HH11	1:G:72:GLY:HA2	1.73	0.54
1:G:108:ASN:O	1:G:110:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:ARG:HH11	1:G:253:ARG:CG	2.21	0.54
1:I:230:GLU:HB2	2:J:173:ILE:HD12	1.89	0.54
2:B:174:ARG:HG2	2:B:174:ARG:HH11	1.73	0.54
1:C:193:LEU:HD23	1:C:206:CYS:HB2	1.90	0.54
1:G:187:LYS:H	1:G:187:LYS:CE	2.19	0.54
1:I:39:TYR:HA	1:I:54:SER:O	2.07	0.54
1:I:237:LEU:C	1:I:239:GLN:N	2.59	0.54
2:J:185:ASN:C	2:J:185:ASN:HD22	2.11	0.54
1:K:18:GLY:HA3	1:K:116:LYS:O	2.08	0.54
1:C:141:GLN:H	1:C:141:GLN:HE21	1.55	0.54
1:A:209:HIS:CE1	1:A:253:ARG:HH12	2.26	0.54
2:B:184:LEU:O	2:B:185:ASN:CB	2.56	0.54
1:C:138:LEU:HB2	1:C:142:ALA:HB3	1.90	0.54
1:C:147:ILE:O	1:C:151:LYS:N	2.33	0.54
1:E:19:ASN:HA	1:E:43:GLN:HG2	1.89	0.54
1:E:181:ILE:O	1:E:181:ILE:HG13	2.08	0.54
2:H:171:GLU:CD	2:H:172:PRO:HD2	2.28	0.54
1:A:172:LYS:HE2	1:A:172:LYS:CA	2.37	0.53
1:G:57:HIS:CD2	1:G:57:HIS:C	2.81	0.53
1:I:22:ARG:NH1	2:J:181:PTR:O1P	2.41	0.53
1:K:17:PHE:HD2	1:K:40:LEU:HD13	1.74	0.53
1:C:113:VAL:HG12	1:C:114:GLN:H	1.73	0.53
1:G:228:ILE:CG2	1:G:229:PRO:HD2	2.39	0.53
1:K:99:LEU:O	1:K:101:CYS:N	2.41	0.53
1:C:151:LYS:N	1:C:152:PRO:HD2	2.22	0.53
1:G:157:LEU:O	1:G:160:THR:OG1	2.22	0.53
1:I:144:GLU:HA	1:I:147:ILE:HD11	1.90	0.53
1:K:58:GLY:O	1:K:59:ARG:HG3	2.07	0.53
1:K:176:GLU:C	1:K:178:SER:N	2.60	0.53
1:K:237:LEU:O	1:K:240:LEU:N	2.42	0.53
1:C:245:SER:CB	1:C:255:LEU:HB2	2.38	0.53
1:G:237:LEU:O	1:G:238:TRP:C	2.47	0.53
1:I:23:GLU:H	1:I:23:GLU:CD	2.12	0.53
1:I:193:LEU:CD2	1:I:206:CYS:SG	2.97	0.53
1:I:209:HIS:HB3	1:I:214:LEU:HD12	1.90	0.53
1:I:244:TYR:O	1:I:254:VAL:HG23	2.08	0.53
1:C:21:THR:CG2	1:C:24:GLU:OE1	2.56	0.53
1:G:39:TYR:HB2	1:G:55:VAL:HG12	1.91	0.53
2:J:175:LYS:CD	2:J:175:LYS:N	2.72	0.53
1:K:22:ARG:HD2	2:L:179:ASP:OD2	2.09	0.53
1:K:41:LEU:HD22	1:K:42:ARG:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:GLY:HA2	2:L:185:ASN:C	2.28	0.53
1:E:176:GLU:O	1:E:177:GLU:C	2.47	0.53
1:E:237:LEU:C	1:E:239:GLN:N	2.62	0.53
1:G:15:PHE:CE2	1:G:39:TYR:HE1	2.27	0.53
1:G:182:VAL:CG2	1:G:259:CYS:SG	2.96	0.53
1:G:184:ILE:N	1:G:184:ILE:CD1	2.69	0.53
1:G:197:ARG:NH1	2:H:170:PTR:O2P	2.35	0.53
1:G:244:TYR:CG	1:G:251:LEU:HD11	2.44	0.53
1:I:176:GLU:C	1:I:178:SER:H	2.12	0.53
1:A:208:LEU:HD11	1:A:211:GLY:CA	2.38	0.53
1:G:240:LEU:HD21	1:G:244:TYR:CD2	2.44	0.53
1:I:38:LEU:CD2	1:I:39:TYR:H	2.22	0.53
1:A:28:TYR:O	1:A:32:GLY:N	2.42	0.53
1:A:182:VAL:CG2	1:A:259:CYS:HB2	2.38	0.53
1:C:172:LYS:HD2	1:C:198:ASP:HA	1.89	0.53
1:G:17:PHE:CD2	1:G:40:LEU:HD13	2.44	0.53
1:I:17:PHE:HD1	1:I:109:ARG:HD3	1.73	0.53
1:A:220:LYS:HG3	1:A:224:GLY:HA2	1.90	0.53
1:E:36:ASP:HA	1:E:56:ALA:O	2.08	0.53
1:G:30:VAL:C	1:G:32:GLY:H	2.12	0.53
1:I:120:PHE:CD1	1:I:120:PHE:N	2.77	0.53
1:I:133:LYS:O	1:I:137:ASN:HA	2.09	0.53
1:K:240:LEU:HD23	1:K:241:VAL:CA	2.38	0.53
1:I:84:SER:HB2	1:I:85:PRO:HD2	1.91	0.53
1:K:193:LEU:HD23	1:K:193:LEU:C	2.29	0.53
2:D:175:LYS:HA	2:D:178:ARG:HH11	1.73	0.52
1:E:43:GLN:HG3	1:E:43:GLN:O	2.05	0.52
1:I:19:ASN:O	1:I:116:LYS:HB3	2.09	0.52
1:I:20:ILE:CG2	1:I:21:THR:N	2.71	0.52
1:I:48:LEU:CD2	1:I:235:ASP:OD2	2.55	0.52
1:A:129:ARG:HG3	1:A:129:ARG:O	2.08	0.52
1:C:173:ILE:CG2	1:C:177:GLU:HG2	2.38	0.52
1:K:230:GLU:OE1	1:K:230:GLU:HA	2.08	0.52
1:A:76:ILE:HG22	1:A:77:ALA:N	2.23	0.52
1:I:174:SER:OG	1:I:177:GLU:HB2	2.09	0.52
1:I:175:ARG:HH11	2:J:168:PRO:HD2	1.74	0.52
1:K:12:HIS:ND1	1:K:12:HIS:N	2.57	0.52
1:K:117:THR:O	1:K:117:THR:HG22	2.10	0.52
1:A:20:ILE:HG22	1:A:21:THR:O	2.10	0.52
1:A:202:SER:OG	1:A:217:ARG:NH1	2.41	0.52
1:C:158:ILE:HD12	1:C:158:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:GLU:HB2	1:I:145:GLN:HE21	1.72	0.52
1:A:40:LEU:HD12	1:A:41:LEU:N	2.24	0.52
1:A:88:LEU:C	1:A:88:LEU:HD12	2.30	0.52
1:A:184:ILE:HD13	1:A:184:ILE:H	1.71	0.52
1:C:48:LEU:N	1:C:235:ASP:OD2	2.34	0.52
1:C:58:GLY:C	1:C:60:LYS:H	2.12	0.52
1:C:197:ARG:NH1	2:D:170:PTR:OH	2.43	0.52
1:G:17:PHE:O	1:G:20:ILE:HD13	2.09	0.52
1:G:253:ARG:HB3	1:G:253:ARG:HH11	1.75	0.52
1:I:150:GLN:HB3	1:I:154:LEU:CD1	2.26	0.52
1:I:209:HIS:CE1	1:I:253:ARG:HH22	2.28	0.52
1:I:238:TRP:CD1	1:I:239:GLN:HG3	2.45	0.52
1:A:91:TYR:OH	1:A:97:ASP:OD2	2.25	0.52
1:A:144:GLU:O	1:A:147:ILE:HG13	2.09	0.52
1:A:176:GLU:N	1:A:176:GLU:CD	2.63	0.52
1:C:244:TYR:HE1	1:C:249:ASP:HB3	1.75	0.52
1:G:30:VAL:C	1:G:32:GLY:N	2.63	0.52
1:I:38:LEU:HD22	1:I:39:TYR:H	1.75	0.52
1:A:38:LEU:HD21	1:A:107:PHE:HB2	1.91	0.52
1:A:238:TRP:HD1	1:A:239:GLN:H	1.57	0.52
1:E:17:PHE:O	1:E:18:GLY:O	2.28	0.52
1:E:170:HIS:O	1:E:171:GLY:O	2.26	0.52
1:G:197:ARG:HH12	2:H:170:PTR:P	2.32	0.52
1:G:237:LEU:O	1:G:240:LEU:N	2.41	0.52
1:I:251:LEU:N	1:I:251:LEU:HD23	2.24	0.52
1:K:80:ARG:HG2	1:K:81:THR:N	2.25	0.52
1:K:96:SER:OG	1:K:97:ASP:N	2.43	0.52
1:K:168:TRP:O	1:K:193:LEU:HA	2.09	0.52
1:K:216:TYR:CD1	2:L:171:GLU:HB3	2.44	0.52
1:K:228:ILE:HG23	1:K:229:PRO:HD2	1.92	0.52
1:A:180:GLN:O	1:A:181:ILE:C	2.48	0.52
1:C:17:PHE:O	1:C:18:GLY:C	2.48	0.52
1:C:20:ILE:HG23	1:C:21:THR:N	2.25	0.52
1:E:12:HIS:ND1	1:E:13:LEU:HD23	2.25	0.52
1:G:244:TYR:CD1	1:G:251:LEU:HD11	2.45	0.52
1:I:170:HIS:O	1:I:173:ILE:HD12	2.09	0.52
1:I:209:HIS:O	1:I:212:LYS:HB3	2.09	0.52
1:K:107:PHE:C	1:K:107:PHE:CD1	2.82	0.52
1:K:180:GLN:O	1:K:183:LEU:N	2.42	0.52
1:A:111:GLN:HE21	1:A:111:GLN:CA	2.23	0.52
1:C:128:ILE:HG13	1:C:129:ARG:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:HIS:O	1:C:173:ILE:HD11	2.08	0.52
1:C:256:THR:OG1	1:C:257:VAL:N	2.42	0.52
1:E:154:LEU:CD2	1:E:154:LEU:N	2.69	0.52
1:K:245:SER:CB	1:K:255:LEU:HB2	2.40	0.52
1:A:39:TYR:HB2	1:A:55:VAL:HG12	1.90	0.52
1:C:30:VAL:C	1:C:32:GLY:N	2.63	0.52
1:C:238:TRP:CD1	1:C:239:GLN:CG	2.91	0.52
1:G:17:PHE:HE1	1:G:109:ARG:HA	1.72	0.52
1:G:217:ARG:NH2	1:G:219:ASP:OD2	2.43	0.52
1:I:176:GLU:O	1:I:178:SER:N	2.43	0.52
2:L:174:ARG:HH11	2:L:174:ARG:CG	2.02	0.52
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.71	0.51
1:C:120:PHE:HE2	1:C:242:GLU:HG3	1.75	0.51
1:C:151:LYS:HG2	1:C:152:PRO:CD	2.39	0.51
1:C:206:CYS:HG	1:C:215:HIS:CE1	2.23	0.51
1:E:67:GLU:OE2	1:E:77:ALA:HB2	2.09	0.51
1:E:217:ARG:HG3	1:E:217:ARG:HH11	1.75	0.51
1:I:234:PHE:N	1:I:234:PHE:CD1	2.76	0.51
1:K:216:TYR:CE2	1:K:251:LEU:HD22	2.45	0.51
1:A:178:SER:O	1:A:179:GLU:C	2.47	0.51
1:C:32:GLY:CA	1:C:107:PHE:HE2	2.24	0.51
1:E:52:ALA:HA	1:E:64:TYR:O	2.10	0.51
1:E:172:LYS:C	1:E:173:ILE:HG13	2.30	0.51
1:E:199:ASN:ND2	1:E:199:ASN:N	2.58	0.51
1:K:35:SER:O	1:K:38:LEU:HB2	2.10	0.51
1:K:87:ASP:O	1:K:88:LEU:C	2.47	0.51
1:A:76:ILE:CG2	1:A:77:ALA:N	2.73	0.51
1:C:68:ARG:HB2	1:C:74:TYR:CE1	2.46	0.51
1:C:199:ASN:C	1:C:201:GLY:H	2.12	0.51
1:E:176:GLU:O	1:E:178:SER:N	2.43	0.51
1:E:178:SER:O	1:E:179:GLU:C	2.48	0.51
1:I:23:GLU:O	1:I:25:ALA:N	2.43	0.51
1:I:123:LEU:CD1	1:I:127:LEU:HD22	2.38	0.51
1:I:145:GLN:O	1:I:148:ILE:HD13	2.10	0.51
1:K:30:VAL:HG23	1:K:31:GLN:N	2.24	0.51
1:K:184:ILE:HD13	1:K:184:ILE:N	2.25	0.51
1:A:17:PHE:CE1	1:A:109:ARG:HA	2.46	0.51
1:C:197:ARG:NH1	1:C:197:ARG:CG	2.60	0.51
1:C:225:LYS:NZ	1:C:235:ASP:OD1	2.44	0.51
2:D:175:LYS:HA	2:D:178:ARG:HD3	1.92	0.51
1:K:176:GLU:N	1:K:176:GLU:CD	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HG22	1:A:24:GLU:CD	2.31	0.51
1:C:153:GLN:HE21	1:C:154:LEU:N	2.08	0.51
1:C:172:LYS:CE	1:C:198:ASP:OD1	2.59	0.51
1:I:58:GLY:C	1:I:60:LYS:H	2.13	0.51
1:I:189:ASN:HD21	1:I:210:GLU:H	1.58	0.51
1:K:21:THR:HG22	1:K:24:GLU:OE1	2.10	0.51
1:K:47:TYR:CE1	1:K:225:LYS:HE3	2.45	0.51
1:C:158:ILE:H	1:C:158:ILE:CD1	2.22	0.51
1:E:18:GLY:O	1:E:43:GLN:HB3	2.11	0.51
1:I:31:GLN:O	1:I:31:GLN:HG3	2.10	0.51
1:I:124:LYS:O	1:I:126:ASN:N	2.44	0.51
1:I:174:SER:CB	1:I:177:GLU:HB2	2.41	0.51
1:I:231:GLY:O	1:I:232:LYS:O	2.28	0.51
1:C:32:GLY:HA3	1:C:107:PHE:HE2	1.76	0.51
1:C:87:ASP:O	1:C:90:HIS:HB2	2.10	0.51
1:E:165:LYS:HE2	1:E:166:MET:HE2	1.92	0.51
1:E:189:ASN:HD21	1:E:253:ARG:NH2	2.09	0.51
1:G:86:ALA:O	1:G:89:CYS:HB2	2.11	0.51
1:I:64:TYR:CE2	1:I:99:LEU:HD22	2.46	0.51
1:K:189:ASN:HA	1:K:208:LEU:HD23	1.93	0.51
1:E:260:GLN:OE1	1:E:260:GLN:HA	2.09	0.51
1:I:17:PHE:O	1:I:18:GLY:C	2.49	0.51
1:I:66:ILE:O	1:I:66:ILE:HG22	2.11	0.51
1:E:168:TRP:HB3	1:E:258:PRO:HB3	1.93	0.51
1:E:187:LYS:HD2	1:E:187:LYS:C	2.32	0.51
1:I:17:PHE:CE2	1:I:40:LEU:HD22	2.46	0.51
1:I:30:VAL:C	1:I:32:GLY:H	2.13	0.51
1:I:71:ASN:N	1:I:71:ASN:OD1	2.43	0.51
1:K:27:ASP:O	1:K:30:VAL:HG22	2.11	0.51
1:K:47:TYR:HA	1:K:235:ASP:OD2	2.11	0.51
1:K:181:ILE:O	1:K:181:ILE:HD13	2.10	0.51
1:A:30:VAL:CG2	1:A:31:GLN:N	2.73	0.50
1:A:76:ILE:HG22	1:A:77:ALA:O	2.11	0.50
1:I:184:ILE:N	1:I:184:ILE:CD1	2.73	0.50
1:I:192:PHE:HA	1:I:206:CYS:O	2.10	0.50
1:I:241:VAL:O	1:I:243:HIS:N	2.44	0.50
1:A:145:GLN:O	1:A:146:ALA:C	2.50	0.50
1:A:197:ARG:C	1:A:199:ASN:N	2.64	0.50
1:C:190:GLY:C	1:C:256:THR:HG1	2.15	0.50
1:C:217:ARG:O	1:C:228:ILE:HG23	2.11	0.50
1:G:53:LEU:HD13	1:G:55:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:ASN:O	2:H:185:ASN:ND2	2.44	0.50
1:I:131:TYR:CD1	1:I:132:VAL:N	2.80	0.50
1:K:210:GLU:HA	1:K:210:GLU:OE1	2.11	0.50
1:A:120:PHE:HA	1:A:123:LEU:CG	2.40	0.50
1:A:157:LEU:HB3	1:A:158:ILE:CD1	2.40	0.50
1:A:172:LYS:HD2	1:A:198:ASP:CA	2.42	0.50
1:A:176:GLU:O	1:A:179:GLU:N	2.45	0.50
1:A:187:LYS:CE	1:A:187:LYS:N	2.71	0.50
1:A:206:CYS:HA	1:A:214:LEU:O	2.11	0.50
1:C:110:PRO:CD	1:C:113:VAL:HG21	2.34	0.50
2:D:175:LYS:CA	2:D:178:ARG:HH11	2.23	0.50
1:E:194:ILE:HG22	1:E:204:ALA:O	2.11	0.50
1:G:48:LEU:CD2	1:G:235:ASP:CB	2.83	0.50
1:I:225:LYS:NZ	1:I:235:ASP:OD1	2.40	0.50
1:I:226:LEU:HD23	1:I:237:LEU:HD23	1.92	0.50
2:J:184:LEU:O	2:J:185:ASN:OD1	2.29	0.50
1:A:59:ARG:NE	1:E:180:GLN:NE2	2.59	0.50
1:E:13:LEU:HD23	1:E:13:LEU:H	1.77	0.50
1:I:126:ASN:CG	1:I:127:LEU:N	2.65	0.50
1:K:225:LYS:HZ3	1:K:235:ASP:CG	2.14	0.50
1:C:120:PHE:C	1:C:122:ASP:N	2.64	0.50
1:C:220:LYS:CG	1:C:224:GLY:HA2	2.41	0.50
1:E:17:PHE:CD2	1:E:40:LEU:HD13	2.47	0.50
1:K:28:TYR:HE1	1:K:110:PRO:HG2	1.77	0.50
1:K:69:GLU:N	1:K:73:THR:O	2.44	0.50
1:A:145:GLN:O	1:A:147:ILE:N	2.45	0.50
1:A:176:GLU:C	1:A:178:SER:H	2.13	0.50
1:C:120:PHE:HA	1:C:123:LEU:HB3	1.93	0.50
1:C:175:ARG:O	1:C:178:SER:OG	2.28	0.50
1:C:175:ARG:O	1:C:179:GLU:HG2	2.12	0.50
1:C:238:TRP:CD1	1:C:238:TRP:C	2.84	0.50
1:E:161:THR:HA	1:E:163:HIS:CE1	2.46	0.50
1:G:75:ALA:HB2	1:G:81:THR:HA	1.92	0.50
1:G:179:GLU:O	1:G:183:LEU:CD2	2.59	0.50
1:I:18:GLY:HA3	1:I:116:LYS:O	2.11	0.50
1:I:39:TYR:CB	1:I:55:VAL:CG1	2.79	0.50
1:I:237:LEU:O	1:I:238:TRP:C	2.49	0.50
1:K:226:LEU:HD11	1:K:235:ASP:O	2.11	0.50
1:A:199:ASN:C	1:A:201:GLY:N	2.64	0.50
1:A:226:LEU:CD1	1:A:226:LEU:N	2.74	0.50
1:A:243:HIS:O	1:A:246:TYR:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LYS:HG2	1:E:249:ASP:H	1.75	0.50
1:G:164:GLU:HA	1:G:169:PHE:CD2	2.46	0.50
1:I:32:GLY:CA	1:I:107:PHE:CE2	2.94	0.50
2:J:184:LEU:O	2:J:185:ASN:CB	2.59	0.50
1:A:111:GLN:HE21	1:A:111:GLN:C	2.14	0.50
1:A:237:LEU:HA	1:A:240:LEU:HB2	1.94	0.50
1:C:141:GLN:O	1:C:145:GLN:HG2	2.12	0.50
1:E:74:TYR:CD2	1:E:85:PRO:HD3	2.47	0.50
1:E:176:GLU:CD	1:E:176:GLU:H	2.14	0.50
1:G:105:LYS:HG2	1:G:106:PRO:HD2	1.93	0.50
1:A:120:PHE:O	1:A:122:ASP:N	2.44	0.50
1:A:131:TYR:CE1	1:A:135:THR:OG1	2.65	0.50
1:C:111:GLN:HE21	1:C:111:GLN:CA	2.24	0.50
1:C:240:LEU:HD21	1:C:244:TYR:HD2	1.76	0.50
1:G:82:HIS:N	1:G:82:HIS:ND1	2.59	0.50
1:I:17:PHE:O	1:I:20:ILE:HD13	2.12	0.50
1:I:69:GLU:N	1:I:73:THR:O	2.43	0.50
1:I:80:ARG:HH11	1:I:80:ARG:HB2	1.66	0.50
1:A:18:GLY:H	1:A:115:PRO:HB3	1.77	0.49
1:A:105:LYS:HG2	1:A:106:PRO:HD2	1.94	0.49
1:A:216:TYR:CD2	1:A:251:LEU:HD22	2.46	0.49
1:C:132:VAL:HG12	1:C:133:LYS:N	2.27	0.49
1:C:170:HIS:CE1	1:C:261:LYS:HA	2.47	0.49
1:I:237:LEU:HA	1:I:240:LEU:HB3	1.93	0.49
1:C:245:SER:HB3	1:C:255:LEU:HD12	1.93	0.49
1:E:70:LEU:HD12	1:E:70:LEU:N	2.26	0.49
1:E:174:SER:OG	1:E:176:GLU:OE1	2.22	0.49
1:E:245:SER:OG	1:E:255:LEU:HD12	2.12	0.49
1:I:123:LEU:C	1:I:123:LEU:CD1	2.80	0.49
1:A:16:PHE:HD1	1:A:41:LEU:O	1.94	0.49
1:C:35:SER:O	1:C:38:LEU:HB2	2.12	0.49
1:C:168:TRP:O	1:C:194:ILE:N	2.40	0.49
1:G:91:TYR:OH	1:G:97:ASP:OD2	2.24	0.49
1:I:182:VAL:HG11	1:I:213:VAL:CG2	2.42	0.49
1:K:219:ASP:O	1:K:226:LEU:HA	2.13	0.49
1:A:91:TYR:C	1:A:91:TYR:CD1	2.85	0.49
1:A:93:SER:O	1:A:102:LEU:HD13	2.11	0.49
1:C:138:LEU:HD11	1:C:146:ALA:CB	2.41	0.49
1:C:153:GLN:NE2	1:C:154:LEU:N	2.60	0.49
1:E:170:HIS:O	1:E:171:GLY:C	2.50	0.49
1:E:175:ARG:O	1:E:178:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:LEU:O	1:G:239:GLN:N	2.45	0.49
1:G:253:ARG:CB	1:G:253:ARG:HH11	2.23	0.49
1:K:179:GLU:O	1:K:182:VAL:HG12	2.12	0.49
1:K:194:ILE:HG23	1:K:205:LEU:HD23	1.93	0.49
1:C:30:VAL:C	1:C:32:GLY:H	2.16	0.49
1:C:123:LEU:HD11	1:C:127:LEU:HD22	1.93	0.49
1:E:168:TRP:CE3	1:E:194:ILE:HG13	2.47	0.49
1:E:243:HIS:CE1	1:E:249:ASP:OD2	2.62	0.49
1:G:17:PHE:HE1	1:G:109:ARG:CA	2.26	0.49
1:G:89:CYS:O	1:G:103:LEU:HD12	2.12	0.49
1:G:109:ARG:CB	1:G:109:ARG:CZ	2.87	0.49
1:I:126:ASN:OD1	1:I:126:ASN:C	2.50	0.49
2:J:178:ARG:CG	2:J:178:ARG:NH1	2.75	0.49
1:K:173:ILE:HG22	1:K:174:SER:O	2.12	0.49
1:C:131:TYR:CD1	1:C:131:TYR:C	2.86	0.49
1:E:18:GLY:HA3	1:E:116:LYS:O	2.13	0.49
1:G:152:PRO:C	1:G:155:GLU:OE1	2.51	0.49
1:G:168:TRP:O	1:G:193:LEU:HA	2.12	0.49
1:K:93:SER:O	1:K:102:LEU:CD1	2.59	0.49
1:K:228:ILE:O	1:K:229:PRO:C	2.50	0.49
1:K:256:THR:OG1	1:K:257:VAL:N	2.44	0.49
1:A:187:LYS:O	1:A:208:LEU:CD2	2.61	0.49
1:C:50:GLY:O	1:C:51:PHE:CD1	2.65	0.49
1:C:138:LEU:H	1:C:138:LEU:CD2	2.15	0.49
1:E:39:TYR:CE1	1:E:103:LEU:HB3	2.48	0.49
1:G:39:TYR:CE2	1:G:103:LEU:HB3	2.48	0.49
1:I:17:PHE:HE2	1:I:40:LEU:HD22	1.78	0.49
1:I:82:HIS:ND1	1:I:82:HIS:N	2.60	0.49
1:K:176:GLU:O	1:K:178:SER:N	2.45	0.49
1:K:187:LYS:O	1:K:208:LEU:CD2	2.61	0.49
1:K:203:TYR:N	1:K:203:TYR:CD1	2.81	0.49
1:A:17:PHE:O	1:A:18:GLY:C	2.50	0.49
1:A:199:ASN:O	1:A:201:GLY:N	2.43	0.49
1:A:243:HIS:HE1	1:A:249:ASP:OD2	1.96	0.49
1:C:39:TYR:CZ	1:C:106:PRO:HB3	2.48	0.49
1:C:71:ASN:N	1:C:71:ASN:OD1	2.46	0.49
1:C:128:ILE:CG1	1:C:129:ARG:N	2.75	0.49
1:I:123:LEU:HD12	1:I:124:LYS:HA	1.93	0.49
1:K:69:GLU:HB2	1:K:73:THR:O	2.13	0.49
1:K:169:PHE:HD1	1:K:194:ILE:O	1.96	0.49
1:K:207:LEU:HD21	1:K:214:LEU:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:236:THR:OG1	1:K:237:LEU:N	2.44	0.49
1:A:93:SER:O	1:A:102:LEU:CD1	2.60	0.49
1:A:202:SER:HG	1:A:217:ARG:HH12	1.58	0.49
1:C:109:ARG:HH11	1:C:109:ARG:CG	2.24	0.49
1:E:53:LEU:N	1:E:64:TYR:O	2.34	0.49
1:I:38:LEU:O	1:I:55:VAL:HA	2.12	0.49
1:I:48:LEU:HD23	1:I:235:ASP:CG	2.33	0.49
1:I:128:ILE:O	1:I:129:ARG:C	2.51	0.49
1:K:22:ARG:HB2	1:K:22:ARG:HH11	1.76	0.49
1:E:16:PHE:HA	1:E:41:LEU:O	2.13	0.49
1:G:194:ILE:HG22	1:G:205:LEU:HA	1.95	0.49
1:I:234:PHE:CE2	1:I:240:LEU:HA	2.48	0.49
1:I:244:TYR:C	1:I:246:TYR:H	2.15	0.49
1:K:173:ILE:HG23	1:K:177:GLU:CB	2.36	0.49
1:A:55:VAL:HG23	1:A:55:VAL:O	2.12	0.48
1:A:207:LEU:HD23	1:A:207:LEU:N	2.28	0.48
1:C:38:LEU:HD23	1:C:105:LYS:HB3	1.95	0.48
1:C:203:TYR:CE2	1:C:237:LEU:HD11	2.48	0.48
1:C:226:LEU:CD2	1:C:237:LEU:HG	2.42	0.48
1:G:46:ASN:OD1	1:G:46:ASN:N	2.46	0.48
1:I:136:TRP:N	1:I:136:TRP:CD1	2.81	0.48
1:K:9:SER:C	1:K:11:ASN:H	2.17	0.48
1:K:175:ARG:NH1	2:L:168:PRO:HD2	2.28	0.48
1:C:239:GLN:O	1:C:240:LEU:C	2.51	0.48
1:E:10:ALA:HA	1:E:12:HIS:HE1	1.78	0.48
1:E:23:GLU:O	1:E:25:ALA:N	2.46	0.48
1:E:154:LEU:HD22	1:E:154:LEU:N	2.06	0.48
1:E:197:ARG:CZ	2:F:170:PTR:OH	2.61	0.48
1:E:237:LEU:C	1:E:239:GLN:H	2.16	0.48
1:G:39:TYR:CD2	1:G:103:LEU:HB3	2.48	0.48
1:I:147:ILE:O	1:I:151:LYS:CB	2.61	0.48
1:K:46:ASN:N	1:K:46:ASN:OD1	2.45	0.48
1:K:234:PHE:N	1:K:234:PHE:CD1	2.80	0.48
1:C:28:TYR:O	1:C:32:GLY:N	2.46	0.48
1:C:88:LEU:CD1	1:C:88:LEU:O	2.59	0.48
1:C:126:ASN:O	1:C:129:ARG:N	2.47	0.48
1:C:128:ILE:HD12	1:C:128:ILE:C	2.34	0.48
1:C:199:ASN:ND2	1:C:199:ASN:N	2.60	0.48
1:C:246:TYR:HD1	1:C:247:LYS:HB3	1.77	0.48
1:E:178:SER:O	1:E:181:ILE:HG22	2.13	0.48
1:E:180:GLN:O	1:E:184:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:GLN:HA	1:I:144:GLU:HG3	1.95	0.48
1:C:141:GLN:HE21	1:C:141:GLN:N	2.10	0.48
1:E:182:VAL:HA	1:E:259:CYS:SG	2.53	0.48
1:G:21:THR:HG23	1:G:24:GLU:HB2	1.95	0.48
1:I:24:GLU:O	1:I:28:TYR:HD2	1.95	0.48
1:I:64:TYR:CE2	1:I:99:LEU:CD2	2.96	0.48
1:I:105:LYS:HG2	1:I:106:PRO:HD2	1.95	0.48
1:I:120:PHE:HD1	1:I:121:GLU:N	2.11	0.48
1:I:219:ASP:O	1:I:226:LEU:HA	2.13	0.48
1:K:179:GLU:O	1:K:180:GLN:O	2.32	0.48
1:K:181:ILE:CG2	1:K:182:VAL:N	2.76	0.48
1:A:13:LEU:H	1:A:13:LEU:HD23	1.79	0.48
1:C:124:LYS:O	1:C:128:ILE:HG23	2.13	0.48
1:C:151:LYS:CG	1:C:152:PRO:HD3	2.42	0.48
1:C:205:LEU:O	1:C:216:TYR:N	2.39	0.48
2:D:171:GLU:HA	2:D:171:GLU:OE1	2.13	0.48
1:G:228:ILE:HG22	1:G:229:PRO:HD2	1.95	0.48
1:K:47:TYR:CE1	1:K:225:LYS:CE	2.95	0.48
1:A:191:LYS:O	1:A:207:LEU:HA	2.14	0.48
1:C:234:PHE:N	1:C:234:PHE:CD1	2.82	0.48
1:E:51:PHE:HB2	1:E:66:ILE:HB	1.96	0.48
1:G:14:PRO:O	1:G:109:ARG:N	2.36	0.48
1:I:93:SER:O	1:I:102:LEU:HD12	2.13	0.48
1:I:128:ILE:C	1:I:130:GLU:N	2.61	0.48
1:I:138:LEU:HD13	1:I:142:ALA:HB1	1.94	0.48
1:K:181:ILE:O	1:K:181:ILE:HD12	2.13	0.48
1:A:161:THR:HB	1:A:164:GLU:HG3	1.95	0.48
2:B:171:GLU:HG3	2:B:172:PRO:HD2	1.94	0.48
1:C:193:LEU:CD2	1:C:206:CYS:HB2	2.43	0.48
1:E:64:TYR:CZ	2:F:182:SER:HB2	2.48	0.48
1:G:180:GLN:CG	1:G:181:ILE:N	2.77	0.48
2:H:185:ASN:ND2	2:H:185:ASN:C	2.67	0.48
1:I:51:PHE:N	1:I:51:PHE:CD1	2.81	0.48
1:A:39:TYR:CB	1:A:55:VAL:HG12	2.44	0.48
1:A:217:ARG:NH1	1:A:217:ARG:CG	2.62	0.48
1:A:226:LEU:HD23	1:A:237:LEU:HD23	1.94	0.48
1:C:40:LEU:C	1:C:40:LEU:HD12	2.34	0.48
1:G:38:LEU:HD23	1:G:105:LYS:O	2.13	0.48
1:I:80:ARG:HH11	1:I:80:ARG:HB3	1.79	0.48
1:I:90:HIS:O	1:I:93:SER:HB3	2.13	0.48
1:I:119:PRO:HD2	1:I:120:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:PHE:CD1	1:K:194:ILE:O	2.67	0.48
1:C:138:LEU:HG	1:C:143:LEU:CA	2.44	0.48
1:C:246:TYR:CE1	1:C:247:LYS:CE	2.95	0.48
1:E:102:LEU:HB3	1:E:104:LYS:HE3	1.96	0.48
1:E:228:ILE:O	1:E:229:PRO:C	2.49	0.48
1:G:226:LEU:HD11	1:G:235:ASP:O	2.14	0.48
1:I:12:HIS:ND1	1:I:12:HIS:N	2.57	0.48
1:I:220:LYS:CG	1:I:224:GLY:HA2	2.43	0.48
1:K:15:PHE:N	1:K:15:PHE:CD1	2.81	0.48
1:K:21:THR:CG2	1:K:24:GLU:HB2	2.36	0.48
1:A:87:ASP:O	1:A:89:CYS:N	2.47	0.48
1:A:186:SER:HB3	1:A:188:THR:HG22	1.94	0.48
1:A:197:ARG:NH1	2:B:170:PTR:OH	2.47	0.48
2:B:174:ARG:HG2	2:B:174:ARG:NH1	2.28	0.48
1:C:253:ARG:HG3	1:C:254:VAL:O	2.14	0.48
1:E:58:GLY:C	1:E:60:LYS:N	2.67	0.48
1:E:178:SER:HA	1:E:181:ILE:HG22	1.96	0.48
1:E:186:SER:OG	1:E:188:THR:HG22	2.13	0.48
1:G:114:GLN:HA	1:G:114:GLN:NE2	2.29	0.48
1:I:144:GLU:O	1:I:148:ILE:CG2	2.61	0.48
1:I:175:ARG:O	1:I:178:SER:OG	2.32	0.48
1:K:187:LYS:O	1:K:208:LEU:HD21	2.13	0.48
1:A:41:LEU:HD22	1:A:52:ALA:O	2.14	0.47
1:A:180:GLN:CD	1:C:59:ARG:NE	2.68	0.47
1:C:21:THR:O	1:C:22:ARG:C	2.49	0.47
1:C:151:LYS:CG	1:C:152:PRO:CD	2.92	0.47
1:C:175:ARG:CZ	1:C:215:HIS:HD2	2.27	0.47
1:C:245:SER:HB3	1:C:255:LEU:HB2	1.95	0.47
1:C:253:ARG:CG	1:C:253:ARG:HH11	2.27	0.47
1:E:20:ILE:HG22	1:E:42:ARG:HD3	1.96	0.47
1:E:178:SER:HA	1:E:181:ILE:CG2	2.44	0.47
1:G:180:GLN:O	1:G:181:ILE:C	2.52	0.47
2:H:175:LYS:CD	2:H:175:LYS:N	2.77	0.47
1:I:202:SER:C	1:I:203:TYR:CD1	2.85	0.47
1:K:41:LEU:HD22	1:K:42:ARG:N	2.29	0.47
1:K:107:PHE:C	1:K:107:PHE:HD1	2.17	0.47
1:K:196:ALA:HA	1:K:203:TYR:HA	1.95	0.47
1:K:198:ASP:O	1:K:200:ASN:N	2.47	0.47
1:C:173:ILE:CG2	1:C:177:GLU:HB3	2.40	0.47
1:E:35:SER:O	1:E:36:ASP:C	2.52	0.47
1:E:157:LEU:HB3	1:E:158:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ARG:CB	1:G:80:ARG:NH1	2.76	0.47
1:I:42:ARG:HG2	1:I:52:ALA:HB3	1.96	0.47
1:I:130:GLU:O	1:I:132:VAL:N	2.47	0.47
1:I:254:VAL:CG2	1:I:255:LEU:N	2.77	0.47
1:K:30:VAL:C	1:K:32:GLY:N	2.67	0.47
1:G:111:GLN:HE21	1:G:112:GLY:N	2.13	0.47
1:G:173:ILE:HG22	1:G:174:SER:O	2.14	0.47
1:G:176:GLU:C	1:G:178:SER:N	2.67	0.47
1:I:151:LYS:CB	1:I:152:PRO:HD2	2.43	0.47
1:I:262:ILE:H	1:I:262:ILE:HG12	1.39	0.47
1:A:17:PHE:HD1	1:A:109:ARG:HD3	1.77	0.47
1:G:19:ASN:O	1:G:20:ILE:HD12	2.14	0.47
1:G:93:SER:C	1:G:102:LEU:CD1	2.83	0.47
1:G:160:THR:HA	1:G:236:THR:HG22	1.96	0.47
1:A:154:LEU:O	1:A:158:ILE:HD13	2.13	0.47
1:C:216:TYR:CD1	2:D:171:GLU:HB3	2.47	0.47
1:E:26:GLU:O	1:E:29:LEU:HB2	2.14	0.47
1:E:43:GLN:O	1:E:43:GLN:CG	2.61	0.47
1:E:173:ILE:HG23	1:E:177:GLU:HB3	1.96	0.47
1:G:14:PRO:HB2	1:G:108:ASN:ND2	2.26	0.47
1:G:22:ARG:CZ	2:H:179:ASP:HB3	2.44	0.47
1:G:22:ARG:NE	2:H:179:ASP:HB3	2.29	0.47
1:G:46:ASN:O	1:G:234:PHE:HA	2.13	0.47
1:G:202:SER:C	1:G:203:TYR:CD1	2.88	0.47
1:I:174:SER:HB3	1:I:177:GLU:OE1	2.14	0.47
1:C:99:LEU:HD11	1:C:103:LEU:HD21	1.96	0.47
1:C:176:GLU:C	1:C:178:SER:N	2.67	0.47
1:C:205:LEU:CD2	1:C:206:CYS:N	2.77	0.47
1:E:13:LEU:HD23	1:E:13:LEU:N	2.28	0.47
1:E:17:PHE:HE1	1:E:109:ARG:CB	2.28	0.47
1:E:236:THR:O	1:E:239:GLN:HB2	2.14	0.47
1:I:151:LYS:HB3	1:I:152:PRO:CD	2.44	0.47
1:A:27:ASP:OD2	1:E:186:SER:HB3	2.14	0.47
1:A:170:HIS:O	1:A:171:GLY:C	2.53	0.47
1:A:226:LEU:CD1	1:A:226:LEU:H	2.28	0.47
1:A:226:LEU:N	1:A:226:LEU:HD12	2.30	0.47
1:A:244:TYR:C	1:A:246:TYR:H	2.17	0.47
2:F:171:GLU:HA	2:F:172:PRO:HD3	1.80	0.47
2:F:173:ILE:CG2	2:F:174:ARG:H	2.28	0.47
1:G:66:ILE:O	1:G:66:ILE:HG22	2.13	0.47
1:G:237:LEU:C	1:G:239:GLN:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:ARG:HH11	2:H:178:ARG:CB	2.28	0.47
2:H:184:LEU:O	2:H:185:ASN:HB3	2.14	0.47
1:K:97:ASP:C	1:K:99:LEU:H	2.18	0.47
1:K:237:LEU:HA	1:K:240:LEU:HB3	1.96	0.47
1:K:247:LYS:HG2	1:K:249:ASP:N	2.29	0.47
1:C:88:LEU:HD13	1:C:92:HIS:ND1	2.30	0.47
1:G:12:HIS:CE1	1:G:13:LEU:CD2	2.98	0.47
1:I:18:GLY:H	1:I:115:PRO:CB	2.23	0.47
1:I:123:LEU:CD1	1:I:127:LEU:HB2	2.45	0.47
1:K:19:ASN:O	1:K:116:LYS:HB3	2.15	0.47
1:C:228:ILE:CG2	2:D:173:ILE:HD11	2.45	0.47
1:G:244:TYR:CB	1:G:251:LEU:HD11	2.42	0.47
1:I:213:VAL:O	1:I:213:VAL:HG12	2.15	0.47
1:K:18:GLY:H	1:K:115:PRO:CB	2.26	0.47
1:K:235:ASP:N	1:K:239:GLN:OE1	2.43	0.47
1:A:10:ALA:O	1:A:16:PHE:CD2	2.68	0.47
1:A:75:ALA:HB2	1:A:81:THR:HA	1.97	0.47
1:A:167:PRO:HB2	1:A:258:PRO:HB2	1.95	0.47
1:C:197:ARG:HH11	1:C:197:ARG:CG	1.94	0.47
1:E:21:THR:HG23	1:E:24:GLU:OE1	2.15	0.47
1:E:89:CYS:O	1:E:93:SER:N	2.48	0.47
1:E:176:GLU:C	1:E:178:SER:N	2.65	0.47
1:E:203:TYR:CD1	1:E:203:TYR:N	2.82	0.47
1:I:181:ILE:HG13	1:I:181:ILE:O	2.15	0.47
1:K:82:HIS:CD2	1:K:88:LEU:HA	2.50	0.47
1:A:107:PHE:CD1	1:A:108:ASN:O	2.68	0.46
1:C:41:LEU:HD22	1:C:42:ARG:N	2.30	0.46
1:E:246:TYR:CD1	1:E:246:TYR:C	2.89	0.46
1:I:16:PHE:HE1	1:I:43:GLN:N	2.14	0.46
1:K:32:GLY:HA3	1:K:107:PHE:CE2	2.50	0.46
1:K:180:GLN:C	1:K:184:ILE:HD11	2.35	0.46
1:C:38:LEU:CD2	1:C:105:LYS:O	2.63	0.46
1:C:253:ARG:CB	1:C:253:ARG:HH11	2.27	0.46
1:E:69:GLU:N	1:E:73:THR:O	2.46	0.46
1:G:16:PHE:HE1	1:G:43:GLN:N	2.13	0.46
1:G:91:TYR:CD1	1:G:91:TYR:C	2.89	0.46
1:K:166:MET:HA	1:K:166:MET:CE	2.45	0.46
1:A:22:ARG:HB2	2:B:181:PTR:O3P	2.16	0.46
1:A:55:VAL:O	1:A:55:VAL:CG2	2.63	0.46
1:A:70:LEU:CD1	1:A:70:LEU:N	2.57	0.46
1:A:124:LYS:C	1:A:126:ASN:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:LYS:HA	2:D:178:ARG:CD	2.45	0.46
2:D:185:ASN:C	2:D:185:ASN:ND2	2.68	0.46
1:E:178:SER:O	1:E:181:ILE:CG2	2.63	0.46
1:I:19:ASN:N	1:I:116:LYS:O	2.41	0.46
1:I:136:TRP:CZ3	1:I:146:ALA:HB1	2.50	0.46
1:A:174:SER:HG	1:A:177:GLU:N	2.12	0.46
1:A:191:LYS:HG2	1:A:259:CYS:HB2	1.97	0.46
1:C:89:CYS:O	1:C:90:HIS:C	2.54	0.46
1:E:111:GLN:HE21	1:E:111:GLN:C	2.19	0.46
1:E:241:VAL:C	1:E:243:HIS:N	2.69	0.46
1:G:88:LEU:O	1:G:88:LEU:HD13	2.15	0.46
1:I:150:GLN:O	1:I:151:LYS:C	2.54	0.46
1:A:172:LYS:HE2	1:A:172:LYS:C	2.36	0.46
1:C:195:ARG:HH21	1:C:215:HIS:CE1	2.33	0.46
1:G:21:THR:HG23	1:G:24:GLU:HG3	1.97	0.46
1:G:58:GLY:C	1:G:59:ARG:CG	2.80	0.46
1:G:237:LEU:H	1:G:237:LEU:HD12	1.80	0.46
1:I:88:LEU:C	1:I:88:LEU:CD1	2.72	0.46
1:K:109:ARG:HH11	1:K:109:ARG:CG	2.28	0.46
1:K:246:TYR:CD2	1:K:247:LYS:HB3	2.51	0.46
1:C:64:TYR:CE2	1:C:99:LEU:HD22	2.51	0.46
1:C:124:LYS:O	1:C:125:GLU:C	2.54	0.46
1:E:209:HIS:CE1	1:E:253:ARG:NH2	2.84	0.46
1:I:58:GLY:C	1:I:60:LYS:N	2.69	0.46
1:I:128:ILE:CG1	1:I:129:ARG:N	2.78	0.46
1:I:136:TRP:HB3	1:I:138:LEU:HD21	1.98	0.46
1:I:237:LEU:O	1:I:239:GLN:N	2.49	0.46
1:A:17:PHE:CB	1:A:20:ILE:HD13	2.44	0.46
1:A:58:GLY:C	1:A:60:LYS:H	2.19	0.46
1:A:154:LEU:O	1:A:157:LEU:HB2	2.15	0.46
1:A:176:GLU:O	1:A:177:GLU:C	2.52	0.46
1:E:30:VAL:CG2	1:E:31:GLN:N	2.79	0.46
1:E:170:HIS:HB3	1:E:173:ILE:CD1	2.45	0.46
1:G:107:PHE:CD1	1:G:108:ASN:O	2.68	0.46
1:I:39:TYR:OH	1:I:106:PRO:HB3	2.15	0.46
1:A:54:SER:OG	1:A:63:HIS:ND1	2.49	0.46
1:A:186:SER:CB	1:A:188:THR:HG22	2.46	0.46
2:B:171:GLU:HA	2:B:172:PRO:HD3	1.79	0.46
1:C:39:TYR:CB	1:C:55:VAL:CG1	2.92	0.46
1:G:19:ASN:OD1	1:G:45:ARG:NH2	2.38	0.46
1:G:170:HIS:O	1:G:173:ILE:CD1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ALA:O	1:I:161:THR:N	2.48	0.46
1:I:193:LEU:HD21	1:I:206:CYS:SG	2.56	0.46
1:I:216:TYR:CD1	2:J:171:GLU:O	2.68	0.46
1:I:228:ILE:HG22	2:J:173:ILE:HD11	1.98	0.46
1:K:179:GLU:O	1:K:183:LEU:HD22	2.15	0.46
1:K:234:PHE:CB	1:K:239:GLN:OE1	2.60	0.46
1:A:84:SER:OG	1:A:86:ALA:HB3	2.16	0.46
1:A:170:HIS:HB2	1:A:193:LEU:HD12	1.97	0.46
1:A:184:ILE:N	1:A:184:ILE:CD1	2.76	0.46
1:E:64:TYR:CE1	2:F:182:SER:HB2	2.50	0.46
1:E:247:LYS:HD2	1:E:249:ASP:HB2	1.96	0.46
1:I:173:ILE:CG2	1:I:174:SER:N	2.78	0.46
1:K:38:LEU:HD23	1:K:38:LEU:HA	1.82	0.46
1:K:93:SER:HA	1:K:103:LEU:HB2	1.98	0.46
1:A:69:GLU:HB2	1:A:73:THR:O	2.15	0.46
1:A:150:GLN:O	1:A:154:LEU:HD23	2.16	0.46
1:A:154:LEU:O	1:A:155:GLU:C	2.55	0.46
1:A:184:ILE:H	1:A:184:ILE:CD1	2.26	0.46
1:C:58:GLY:O	1:C:60:LYS:N	2.49	0.46
1:C:172:LYS:CD	1:C:198:ASP:OD1	2.63	0.46
1:E:17:PHE:CZ	1:E:109:ARG:HA	2.51	0.46
2:F:184:LEU:O	2:F:185:ASN:HB3	2.15	0.46
1:I:50:GLY:C	1:I:51:PHE:CD1	2.89	0.46
1:I:93:SER:O	1:I:102:LEU:CD1	2.64	0.46
1:I:100:VAL:CG2	1:I:101:CYS:N	2.78	0.46
1:C:150:GLN:C	1:C:152:PRO:HD2	2.37	0.45
1:C:229:PRO:C	1:C:230:GLU:HG2	2.37	0.45
2:D:185:ASN:ND2	2:D:185:ASN:O	2.50	0.45
1:I:227:SER:CB	1:I:233:LYS:HD3	2.46	0.45
1:A:119:PRO:HD2	1:A:120:PHE:CE2	2.51	0.45
1:A:138:LEU:N	1:A:138:LEU:CD2	2.77	0.45
1:A:189:ASN:O	1:A:256:THR:HG21	2.16	0.45
1:C:46:ASN:HB2	1:C:233:LYS:O	2.16	0.45
1:C:138:LEU:HB2	1:C:142:ALA:CB	2.46	0.45
1:C:151:LYS:O	1:C:155:GLU:HG3	2.16	0.45
1:C:198:ASP:C	1:C:199:ASN:ND2	2.69	0.45
1:K:111:GLN:HE21	1:K:111:GLN:HA	1.80	0.45
1:K:253:ARG:NH1	1:K:253:ARG:HB3	2.31	0.45
1:A:182:VAL:HG23	1:A:259:CYS:HB2	1.97	0.45
1:C:38:LEU:HD23	1:C:105:LYS:O	2.16	0.45
1:C:85:PRO:O	1:C:88:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:LEU:HD23	1:E:241:VAL:N	2.30	0.45
1:G:177:GLU:O	1:G:181:ILE:HB	2.16	0.45
1:I:22:ARG:HH11	2:J:181:PTR:P	2.33	0.45
1:I:175:ARG:NH2	2:J:169:ASP:O	2.40	0.45
1:K:205:LEU:HD22	1:K:205:LEU:C	2.29	0.45
1:C:42:ARG:NH2	2:D:181:PTR:O3P	2.42	0.45
1:G:166:MET:HG3	1:G:168:TRP:CZ2	2.51	0.45
1:I:123:LEU:CD1	1:I:124:LYS:N	2.72	0.45
1:I:157:LEU:HD12	1:I:157:LEU:HA	1.80	0.45
1:I:197:ARG:HH11	1:I:197:ARG:CG	2.24	0.45
1:K:82:HIS:ND1	1:K:82:HIS:N	2.64	0.45
1:K:163:HIS:ND1	1:K:163:HIS:N	2.65	0.45
1:A:200:ASN:OD1	1:A:200:ASN:N	2.44	0.45
1:C:120:PHE:CE2	1:C:242:GLU:HG3	2.51	0.45
1:C:203:TYR:HE2	1:C:237:LEU:HD11	1.81	0.45
1:E:36:ASP:OD1	1:E:57:HIS:HA	2.16	0.45
1:E:109:ARG:HG2	1:E:113:VAL:O	2.15	0.45
1:E:253:ARG:NH1	1:E:253:ARG:CG	2.73	0.45
1:G:180:GLN:O	1:G:184:ILE:HG12	2.15	0.45
2:H:180:LEU:HA	2:H:180:LEU:HD23	1.65	0.45
1:I:42:ARG:NH1	2:J:181:PTR:O2P	2.46	0.45
1:I:100:VAL:HG23	1:I:101:CYS:N	2.31	0.45
2:J:171:GLU:HA	2:J:172:PRO:HD3	1.72	0.45
1:K:170:HIS:O	1:K:173:ILE:HD12	2.16	0.45
1:K:209:HIS:CG	1:K:253:ARG:HH12	2.33	0.45
1:K:241:VAL:C	1:K:243:HIS:N	2.69	0.45
1:A:76:ILE:CD1	1:A:88:LEU:HD21	2.47	0.45
1:A:175:ARG:NH1	2:B:170:PTR:O3P	2.49	0.45
1:A:190:GLY:C	1:A:256:THR:OG1	2.55	0.45
1:E:38:LEU:CD2	1:E:105:LYS:O	2.64	0.45
1:E:48:LEU:O	1:E:50:GLY:N	2.50	0.45
1:E:88:LEU:C	1:E:88:LEU:CD1	2.84	0.45
1:G:35:SER:O	1:G:36:ASP:C	2.54	0.45
1:I:111:GLN:HA	1:I:111:GLN:HE21	1.80	0.45
1:K:163:HIS:O	1:K:169:PHE:HD2	2.00	0.45
1:A:228:ILE:HG22	2:B:173:ILE:HD11	1.98	0.45
1:C:123:LEU:CG	1:C:124:LYS:N	2.78	0.45
1:C:130:GLU:O	1:C:131:TYR:C	2.55	0.45
1:C:166:MET:HA	1:C:167:PRO:HD2	1.66	0.45
1:C:253:ARG:HB3	1:C:253:ARG:HH11	1.75	0.45
1:E:28:TYR:O	1:E:107:PHE:CE2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:LYS:CG	1:K:224:GLY:HA2	2.47	0.45
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.74	0.45
1:C:120:PHE:N	1:C:120:PHE:CD1	2.83	0.45
1:C:126:ASN:OD1	1:C:127:LEU:N	2.50	0.45
1:E:58:GLY:O	1:E:60:LYS:N	2.49	0.45
1:E:84:SER:HB2	1:E:85:PRO:HD2	1.99	0.45
1:E:205:LEU:HB3	1:E:216:TYR:HB2	1.97	0.45
1:E:253:ARG:HG3	1:E:254:VAL:N	2.31	0.45
1:G:93:SER:HA	1:G:103:LEU:HB2	1.98	0.45
1:G:241:VAL:HG22	1:G:255:LEU:CD1	2.47	0.45
1:I:17:PHE:HE1	1:I:109:ARG:CA	2.29	0.45
1:I:105:LYS:CG	1:I:106:PRO:HD2	2.47	0.45
1:I:163:HIS:HA	1:I:166:MET:CG	2.47	0.45
1:C:66:ILE:HG12	1:C:76:ILE:HG13	1.98	0.45
1:C:178:SER:HA	1:C:181:ILE:HG22	1.99	0.45
1:E:76:ILE:CD1	1:E:88:LEU:HD21	2.47	0.45
1:E:111:GLN:HE21	1:E:112:GLY:N	2.15	0.45
1:G:262:ILE:H	1:G:262:ILE:HG12	1.35	0.45
1:K:206:CYS:HA	1:K:214:LEU:O	2.17	0.45
1:A:126:ASN:HB2	2:H:168:PRO:O	2.17	0.45
1:C:111:GLN:NE2	1:C:112:GLY:H	2.12	0.45
1:C:138:LEU:CD2	1:C:138:LEU:N	2.76	0.45
1:C:191:LYS:HG3	1:C:257:VAL:CG2	2.33	0.45
1:C:205:LEU:HA	1:C:205:LEU:HD23	1.68	0.45
1:A:9:SER:C	1:A:11:ASN:H	2.19	0.44
1:A:118:GLY:HA3	1:A:120:PHE:CE1	2.52	0.44
1:A:192:PHE:CE2	1:A:255:LEU:HD13	2.52	0.44
1:E:226:LEU:HD11	1:E:235:ASP:O	2.17	0.44
1:G:246:TYR:CD1	1:G:247:LYS:N	2.85	0.44
1:I:154:LEU:H	1:I:154:LEU:CD2	1.98	0.44
1:K:28:TYR:O	1:K:107:PHE:HE2	1.99	0.44
1:K:91:TYR:CD1	1:K:91:TYR:C	2.90	0.44
1:A:141:GLN:HG3	1:G:202:SER:HB2	1.99	0.44
1:C:38:LEU:O	1:C:55:VAL:HA	2.18	0.44
1:C:232:LYS:HG2	1:C:234:PHE:CZ	2.51	0.44
2:H:178:ARG:CG	2:H:178:ARG:NH1	2.79	0.44
1:A:12:HIS:O	1:A:13:LEU:C	2.54	0.44
1:A:128:ILE:CG1	1:A:129:ARG:N	2.80	0.44
1:A:163:HIS:ND1	1:A:164:GLU:N	2.65	0.44
1:A:180:GLN:HE21	1:C:59:ARG:HB3	1.81	0.44
1:C:126:ASN:OD1	1:C:126:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:CYS:SG	1:C:215:HIS:CE1	3.10	0.44
1:E:17:PHE:HE1	1:E:109:ARG:CA	2.31	0.44
1:E:32:GLY:CA	1:E:107:PHE:HE2	2.25	0.44
1:E:48:LEU:C	1:E:50:GLY:H	2.20	0.44
1:G:166:MET:HB2	1:G:168:TRP:CZ2	2.53	0.44
1:G:170:HIS:CD2	1:G:193:LEU:HD12	2.47	0.44
1:I:57:HIS:HB3	1:I:62:HIS:HE2	1.81	0.44
1:I:138:LEU:CD1	1:I:142:ALA:HB1	2.48	0.44
1:K:58:GLY:O	1:K:60:LYS:N	2.50	0.44
1:K:102:LEU:HD22	1:K:102:LEU:HA	1.88	0.44
1:K:154:LEU:O	1:K:155:GLU:C	2.56	0.44
1:A:30:VAL:O	1:A:32:GLY:N	2.50	0.44
1:A:237:LEU:O	1:A:240:LEU:N	2.51	0.44
1:C:20:ILE:HD12	1:C:20:ILE:HA	1.57	0.44
1:C:75:ALA:HB2	1:C:81:THR:HA	2.00	0.44
1:C:107:PHE:C	1:C:107:PHE:HD1	2.19	0.44
1:C:205:LEU:HD22	1:C:206:CYS:N	2.32	0.44
1:G:217:ARG:CZ	1:G:219:ASP:OD2	2.65	0.44
1:G:253:ARG:CB	1:G:253:ARG:CZ	2.96	0.44
1:I:164:GLU:HA	1:I:169:PHE:CD2	2.52	0.44
1:K:40:LEU:C	1:K:40:LEU:HD12	2.38	0.44
1:K:158:ILE:H	1:K:158:ILE:HD13	1.77	0.44
1:K:217:ARG:CG	1:K:217:ARG:NH1	2.64	0.44
1:A:21:THR:HG23	1:A:24:GLU:H	1.82	0.44
1:C:126:ASN:O	1:C:127:LEU:C	2.54	0.44
2:F:179:ASP:OD1	2:F:179:ASP:N	2.50	0.44
1:G:193:LEU:HD23	1:G:206:CYS:SG	2.58	0.44
1:I:21:THR:OG1	1:I:24:GLU:HB2	2.17	0.44
1:I:147:ILE:O	1:I:151:LYS:HB2	2.18	0.44
1:I:228:ILE:CG2	2:J:173:ILE:HD11	2.47	0.44
1:I:231:GLY:C	1:I:232:LYS:O	2.54	0.44
1:K:166:MET:HB3	1:K:168:TRP:CE2	2.53	0.44
1:C:228:ILE:HB	2:D:173:ILE:HD11	1.99	0.44
1:C:232:LYS:HG3	1:C:233:LYS:N	2.33	0.44
1:E:17:PHE:O	1:E:18:GLY:C	2.56	0.44
1:E:262:ILE:CD1	1:E:262:ILE:H	2.30	0.44
1:G:21:THR:HG22	1:G:24:GLU:OE1	2.17	0.44
1:I:187:LYS:O	1:I:208:LEU:HD21	2.18	0.44
1:K:216:TYR:CD2	1:K:251:LEU:HD22	2.52	0.44
1:A:150:GLN:C	1:A:154:LEU:CD2	2.86	0.44
1:G:23:GLU:CG	1:K:186:SER:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:LEU:C	1:G:184:ILE:HD13	2.38	0.44
1:I:151:LYS:CA	1:I:154:LEU:HG	2.48	0.44
1:A:93:SER:C	1:A:102:LEU:HD13	2.37	0.44
1:A:128:ILE:C	1:A:130:GLU:N	2.68	0.44
1:E:20:ILE:HG23	1:E:21:THR:N	2.33	0.44
1:I:209:HIS:ND1	1:I:253:ARG:NH2	2.66	0.44
1:K:21:THR:OG1	1:K:22:ARG:N	2.51	0.44
1:K:158:ILE:O	1:K:162:ALA:HB2	2.17	0.44
1:A:80:ARG:O	1:A:82:HIS:CE1	2.71	0.44
1:A:172:LYS:CE	1:A:196:ALA:O	2.65	0.44
1:C:170:HIS:O	1:C:171:GLY:C	2.56	0.44
1:C:217:ARG:NH1	1:C:217:ARG:CG	2.69	0.44
1:C:217:ARG:NH1	1:C:219:ASP:OD2	2.51	0.44
1:I:17:PHE:C	1:I:20:ILE:HD13	2.38	0.44
1:I:170:HIS:O	1:I:171:GLY:O	2.35	0.44
1:K:14:PRO:HA	1:K:109:ARG:NH2	2.33	0.44
1:K:199:ASN:HB2	1:K:202:SER:HB3	2.00	0.44
1:A:109:ARG:HH11	1:A:109:ARG:CG	2.30	0.43
2:B:171:GLU:HG3	2:B:172:PRO:CD	2.48	0.43
2:B:173:ILE:C	2:B:174:ARG:HG3	2.37	0.43
1:C:9:SER:C	1:C:11:ASN:H	2.20	0.43
1:C:199:ASN:C	1:C:201:GLY:N	2.71	0.43
1:E:226:LEU:H	1:E:226:LEU:HD13	1.74	0.43
1:E:228:ILE:CD1	1:E:251:LEU:HD21	2.48	0.43
1:G:231:GLY:O	1:G:232:LYS:C	2.56	0.43
1:I:80:ARG:CB	1:I:80:ARG:NH1	2.68	0.43
1:I:193:LEU:HD23	1:I:193:LEU:C	2.38	0.43
1:I:248:ALA:O	1:I:251:LEU:HG	2.16	0.43
1:K:110:PRO:HB2	1:K:113:VAL:HG21	2.00	0.43
1:K:228:ILE:HG22	1:K:229:PRO:N	2.33	0.43
1:K:253:ARG:NH1	1:K:253:ARG:CG	2.77	0.43
2:L:178:ARG:CB	2:L:178:ARG:NH1	2.50	0.43
1:C:16:PHE:O	1:C:109:ARG:NE	2.50	0.43
1:C:237:LEU:C	1:C:239:GLN:N	2.71	0.43
1:E:20:ILE:CG2	1:E:21:THR:N	2.81	0.43
1:E:68:ARG:HH11	1:E:72:GLY:HA2	1.77	0.43
1:E:209:HIS:CE1	1:E:253:ARG:NH1	2.84	0.43
1:G:21:THR:HG23	1:G:24:GLU:CG	2.48	0.43
1:G:38:LEU:HA	1:G:105:LYS:O	2.18	0.43
1:G:241:VAL:C	1:G:243:HIS:N	2.70	0.43
1:I:23:GLU:O	1:I:26:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:GLU:HB2	1:I:73:THR:OG1	2.18	0.43
1:I:138:LEU:HD12	1:I:142:ALA:C	2.38	0.43
1:K:241:VAL:O	1:K:242:GLU:C	2.57	0.43
2:B:179:ASP:N	2:B:179:ASP:OD1	2.50	0.43
1:C:17:PHE:HD1	1:C:109:ARG:CD	2.15	0.43
1:C:111:GLN:HE21	1:C:111:GLN:C	2.22	0.43
1:C:206:CYS:SG	1:C:215:HIS:ND1	2.78	0.43
1:C:226:LEU:HD23	1:C:237:LEU:HG	2.00	0.43
1:E:241:VAL:O	1:E:244:TYR:N	2.51	0.43
1:G:163:HIS:HB2	1:G:168:TRP:CZ3	2.53	0.43
1:G:252:LEU:HD12	1:G:252:LEU:O	2.18	0.43
1:I:23:GLU:O	1:I:24:GLU:C	2.57	0.43
1:I:142:ALA:O	1:I:145:GLN:HG2	2.19	0.43
1:I:240:LEU:HD23	1:I:241:VAL:CA	2.47	0.43
1:A:124:LYS:O	1:A:125:GLU:C	2.56	0.43
1:E:173:ILE:CG2	1:E:177:GLU:HB3	2.49	0.43
1:E:252:LEU:HA	1:E:252:LEU:HD13	1.51	0.43
1:K:170:HIS:O	1:K:171:GLY:C	2.54	0.43
1:E:39:TYR:HB2	1:E:55:VAL:HG12	1.96	0.43
1:E:99:LEU:HD12	1:E:103:LEU:HD21	1.98	0.43
1:E:173:ILE:CG2	1:E:174:SER:N	2.81	0.43
1:G:107:PHE:CE1	1:G:108:ASN:O	2.72	0.43
1:I:120:PHE:O	1:I:121:GLU:C	2.56	0.43
1:I:131:TYR:O	1:I:135:THR:OG1	2.36	0.43
1:E:262:ILE:HD13	1:E:262:ILE:H	1.83	0.43
1:G:17:PHE:O	1:G:18:GLY:C	2.57	0.43
1:G:22:ARG:NH2	2:H:179:ASP:HB3	2.33	0.43
2:H:175:LYS:O	2:H:177:GLN:N	2.51	0.43
1:I:128:ILE:O	1:I:130:GLU:N	2.52	0.43
1:K:170:HIS:CE1	1:K:261:LYS:HA	2.54	0.43
1:A:129:ARG:NH2	2:H:170:PTR:O1P	2.52	0.43
1:A:178:SER:C	1:A:180:GLN:N	2.71	0.43
1:C:126:ASN:O	1:C:128:ILE:N	2.52	0.43
1:E:9:SER:C	1:E:11:ASN:N	2.68	0.43
1:E:80:ARG:HG2	1:E:81:THR:N	2.34	0.43
1:E:108:ASN:O	1:E:110:PRO:CD	2.62	0.43
1:E:244:TYR:CE1	1:E:249:ASP:HB3	2.53	0.43
1:G:69:GLU:N	1:G:73:THR:O	2.48	0.43
1:G:246:TYR:CE1	1:G:247:LYS:CE	3.00	0.43
2:H:178:ARG:NH1	2:H:178:ARG:HG2	2.32	0.43
1:I:217:ARG:HH11	1:I:217:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:GLU:H	1:K:155:GLU:HG3	1.38	0.43
1:A:41:LEU:HD22	1:A:42:ARG:N	2.33	0.43
1:A:65:THR:HG22	2:B:181:PTR:HD2	2.00	0.43
1:A:96:SER:N	1:A:102:LEU:CD2	2.81	0.43
1:E:21:THR:HG1	1:E:23:GLU:HB2	1.84	0.43
1:E:170:HIS:CE1	1:E:261:LYS:HA	2.53	0.43
1:E:209:HIS:CG	1:E:253:ARG:HH12	2.24	0.43
1:G:219:ASP:O	1:G:226:LEU:HA	2.18	0.43
1:I:24:GLU:O	1:I:28:TYR:CD2	2.72	0.43
1:K:92:HIS:CD2	1:K:96:SER:O	2.72	0.43
1:A:128:ILE:HG22	1:A:158:ILE:CG2	2.44	0.43
1:A:181:ILE:HA	1:A:184:ILE:HG12	1.99	0.43
1:C:69:GLU:HB2	1:C:73:THR:O	2.19	0.43
1:G:107:PHE:CE1	1:G:110:PRO:HD3	2.48	0.43
1:G:231:GLY:O	1:G:232:LYS:O	2.36	0.43
1:G:253:ARG:HG3	1:G:254:VAL:O	2.19	0.43
1:K:13:LEU:HD23	1:K:13:LEU:N	2.33	0.43
1:K:190:GLY:C	1:K:256:THR:OG1	2.57	0.43
1:A:207:LEU:HD23	1:A:214:LEU:HB2	2.00	0.43
1:C:128:ILE:C	1:C:130:GLU:N	2.72	0.43
1:E:186:SER:OG	1:E:188:THR:CG2	2.67	0.43
1:G:170:HIS:HB3	1:G:173:ILE:HD13	2.01	0.43
1:G:207:LEU:CD2	1:G:214:LEU:HB2	2.49	0.43
1:I:209:HIS:HA	1:I:253:ARG:NH1	2.34	0.43
1:I:209:HIS:CB	1:I:253:ARG:HH12	2.32	0.43
1:K:110:PRO:HB2	1:K:113:VAL:CG2	2.49	0.43
1:A:38:LEU:HA	1:A:105:LYS:O	2.18	0.42
1:A:93:SER:CA	1:A:103:LEU:HB2	2.47	0.42
1:C:33:GLY:C	1:C:35:SER:N	2.72	0.42
1:E:91:TYR:CD1	1:E:91:TYR:C	2.92	0.42
1:G:21:THR:HG23	1:G:24:GLU:CB	2.48	0.42
1:I:33:GLY:C	1:I:35:SER:N	2.72	0.42
1:I:231:GLY:O	1:I:232:LYS:C	2.56	0.42
1:A:102:LEU:HD22	1:A:102:LEU:HA	1.79	0.42
1:A:180:GLN:HE21	1:C:59:ARG:CB	2.32	0.42
1:C:126:ASN:CG	1:C:127:LEU:N	2.72	0.42
1:C:138:LEU:O	1:C:143:LEU:HB2	2.19	0.42
1:C:150:GLN:O	1:C:152:PRO:N	2.52	0.42
1:C:197:ARG:NH1	2:D:170:PTR:O2P	2.51	0.42
1:G:170:HIS:CG	1:G:193:LEU:CD1	2.83	0.42
1:G:234:PHE:CD2	1:G:240:LEU:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:PHE:HE1	1:I:109:ARG:HG3	1.84	0.42
1:I:19:ASN:O	1:I:116:LYS:CB	2.68	0.42
1:I:80:ARG:CG	1:I:81:THR:N	2.81	0.42
1:I:145:GLN:C	1:I:149:SER:HG	2.22	0.42
1:K:99:LEU:HD11	1:K:103:LEU:HD21	2.01	0.42
1:K:190:GLY:C	1:K:256:THR:HG1	2.22	0.42
2:B:185:ASN:O	2:B:185:ASN:CG	2.58	0.42
1:C:70:LEU:C	1:C:72:GLY:N	2.72	0.42
1:C:228:ILE:CG2	1:C:229:PRO:CD	2.94	0.42
1:C:238:TRP:NE1	1:C:239:GLN:HG3	2.34	0.42
1:E:23:GLU:O	1:E:24:GLU:C	2.57	0.42
1:G:20:ILE:HG23	1:G:24:GLU:HB2	2.00	0.42
1:G:41:LEU:HD22	1:G:42:ARG:N	2.34	0.42
1:G:172:LYS:NZ	1:G:172:LYS:C	2.68	0.42
1:I:17:PHE:CD2	1:I:40:LEU:HD13	2.54	0.42
1:I:76:ILE:O	1:I:77:ALA:C	2.58	0.42
1:K:58:GLY:C	1:K:60:LYS:N	2.73	0.42
1:K:168:TRP:CZ3	1:K:194:ILE:CD1	3.02	0.42
1:A:19:ASN:O	1:A:116:LYS:HB3	2.19	0.42
1:A:51:PHE:CD1	1:A:51:PHE:N	2.88	0.42
1:A:228:ILE:O	1:A:229:PRO:C	2.55	0.42
1:C:48:LEU:C	1:C:50:GLY:H	2.23	0.42
1:C:179:GLU:OE1	1:C:213:VAL:CG1	2.66	0.42
1:G:166:MET:CB	1:G:168:TRP:CZ2	3.01	0.42
1:G:180:GLN:HG2	1:G:181:ILE:N	2.31	0.42
1:I:17:PHE:CD1	1:I:109:ARG:HD3	2.53	0.42
1:I:186:SER:HB3	1:I:188:THR:CG2	2.50	0.42
1:C:260:GLN:HB3	1:E:30:VAL:HG21	2.02	0.42
1:E:14:PRO:O	1:E:109:ARG:N	2.50	0.42
1:E:21:THR:OG1	1:E:23:GLU:HB2	2.19	0.42
1:E:247:LYS:NZ	2:F:179:ASP:OD2	2.53	0.42
1:G:98:GLY:HA2	2:H:185:ASN:C	2.39	0.42
1:G:256:THR:OG1	1:G:257:VAL:N	2.47	0.42
1:I:25:ALA:O	1:I:26:GLU:C	2.58	0.42
1:I:163:HIS:O	1:I:169:PHE:CD2	2.66	0.42
1:K:17:PHE:CD1	1:K:109:ARG:HD3	2.55	0.42
1:A:88:LEU:HD12	1:A:88:LEU:O	2.19	0.42
1:A:111:GLN:NE2	1:A:112:GLY:N	2.66	0.42
1:A:120:PHE:CA	1:A:123:LEU:HD11	2.49	0.42
1:A:180:GLN:NE2	1:C:59:ARG:HB3	2.34	0.42
1:C:27:ASP:O	1:C:28:TYR:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLN:HG3	1:C:44:SER:O	2.19	0.42
1:C:110:PRO:O	1:C:111:GLN:C	2.57	0.42
1:E:68:ARG:O	1:E:68:ARG:HG3	2.18	0.42
1:E:109:ARG:HG3	1:E:113:VAL:HG12	2.01	0.42
1:I:107:PHE:CD1	1:I:107:PHE:C	2.91	0.42
1:I:120:PHE:CG	1:I:238:TRP:CH2	3.08	0.42
1:K:19:ASN:O	1:K:116:LYS:HD2	2.20	0.42
1:K:228:ILE:HG22	2:L:173:ILE:HD11	2.01	0.42
1:A:128:ILE:CB	1:A:158:ILE:HG12	2.50	0.42
1:C:46:ASN:O	1:C:47:TYR:HD1	2.03	0.42
1:E:29:LEU:CD2	1:E:40:LEU:HD23	2.48	0.42
1:E:175:ARG:NH1	2:F:168:PRO:HD2	2.32	0.42
1:E:191:LYS:O	1:E:207:LEU:CA	2.65	0.42
2:F:174:ARG:HA	2:F:175:LYS:HE2	2.01	0.42
2:F:175:LYS:CD	2:F:175:LYS:H	2.30	0.42
2:F:175:LYS:HD2	2:F:176:GLY:H	1.85	0.42
1:K:163:HIS:CE1	1:K:164:GLU:HG2	2.55	0.42
1:K:179:GLU:O	1:K:183:LEU:CD2	2.67	0.42
1:K:260:GLN:OE1	1:K:260:GLN:CA	2.58	0.42
1:A:157:LEU:HD13	1:A:157:LEU:HA	1.82	0.42
1:C:66:ILE:O	1:C:66:ILE:HG22	2.19	0.42
1:C:87:ASP:O	1:C:88:LEU:C	2.56	0.42
1:C:96:SER:N	1:C:102:LEU:CD2	2.83	0.42
1:E:98:GLY:HA2	2:F:185:ASN:C	2.39	0.42
1:E:163:HIS:ND1	1:E:163:HIS:N	2.68	0.42
1:G:163:HIS:HA	1:G:166:MET:HG3	2.01	0.42
1:K:207:LEU:CD2	1:K:214:LEU:CB	2.97	0.42
1:A:162:ALA:C	1:A:164:GLU:N	2.71	0.42
1:A:181:ILE:HD12	1:A:262:ILE:HD11	2.02	0.42
1:A:191:LYS:HD2	1:A:259:CYS:HB2	2.01	0.42
1:C:102:LEU:HD22	1:C:102:LEU:HA	1.92	0.42
1:E:173:ILE:HG22	1:E:174:SER:O	2.19	0.42
1:E:220:LYS:CG	1:E:224:GLY:HA2	2.49	0.42
2:F:173:ILE:CG2	2:F:174:ARG:N	2.81	0.42
1:I:52:ALA:HA	1:I:64:TYR:O	2.20	0.42
1:I:240:LEU:CD2	1:I:241:VAL:N	2.75	0.42
1:C:24:GLU:O	1:C:28:TYR:CD2	2.73	0.42
1:C:58:GLY:C	1:C:60:LYS:N	2.74	0.42
1:C:67:GLU:OE2	1:C:77:ALA:HB2	2.20	0.42
1:E:16:PHE:HE1	1:E:43:GLN:N	2.17	0.42
1:E:21:THR:HG22	1:E:24:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:PHE:HA	1:E:206:CYS:O	2.20	0.42
2:F:184:LEU:CD2	2:F:185:ASN:H	2.33	0.42
1:G:41:LEU:HD22	1:G:52:ALA:O	2.19	0.42
1:G:163:HIS:ND1	1:G:163:HIS:N	2.68	0.42
1:G:175:ARG:O	1:G:178:SER:OG	2.38	0.42
1:I:13:LEU:HA	1:I:14:PRO:HD2	1.89	0.42
1:I:40:LEU:C	1:I:40:LEU:CD1	2.77	0.42
1:I:126:ASN:O	1:I:127:LEU:C	2.57	0.42
1:K:80:ARG:HB2	1:K:80:ARG:HH11	1.85	0.42
1:K:159:ALA:C	1:K:161:THR:N	2.72	0.42
1:A:96:SER:N	1:A:102:LEU:HD21	2.35	0.41
1:C:145:GLN:O	1:C:146:ALA:C	2.58	0.41
1:E:17:PHE:HE1	1:E:109:ARG:HA	1.83	0.41
1:E:214:LEU:HD23	1:E:214:LEU:HA	1.88	0.41
1:E:228:ILE:HD11	1:E:251:LEU:HD21	2.02	0.41
1:E:250:GLY:HA3	2:F:173:ILE:CG2	2.49	0.41
1:E:253:ARG:NH1	1:E:253:ARG:CB	2.83	0.41
1:G:9:SER:C	1:G:11:ASN:N	2.73	0.41
1:G:173:ILE:CG2	1:G:174:SER:N	2.83	0.41
1:K:47:TYR:HE1	1:K:225:LYS:NZ	2.11	0.41
1:K:176:GLU:C	1:K:178:SER:H	2.22	0.41
1:G:25:ALA:O	1:G:26:GLU:C	2.57	0.41
1:I:21:THR:HG23	1:I:24:GLU:CB	2.44	0.41
1:I:164:GLU:HA	1:I:169:PHE:HE2	1.84	0.41
1:I:197:ARG:CG	1:I:197:ARG:NH1	2.82	0.41
1:K:20:ILE:CD1	1:K:116:LYS:HB2	2.47	0.41
1:A:131:TYR:C	1:A:131:TYR:HD1	2.21	0.41
1:A:180:GLN:C	1:A:182:VAL:N	2.73	0.41
1:A:246:TYR:CD1	1:A:247:LYS:HB2	2.54	0.41
1:E:71:ASN:HB2	1:E:73:THR:HG23	2.03	0.41
1:I:174:SER:HB3	1:I:177:GLU:HB2	2.01	0.41
1:I:197:ARG:H	1:I:197:ARG:HG3	1.60	0.41
1:I:252:LEU:HD13	1:I:252:LEU:HA	1.84	0.41
1:K:33:GLY:C	1:K:35:SER:N	2.74	0.41
1:K:156:LYS:O	1:K:156:LYS:HG3	2.21	0.41
1:A:53:LEU:HB3	1:A:64:TYR:HB2	2.02	0.41
1:C:194:ILE:HG22	1:C:204:ALA:O	2.19	0.41
1:E:165:LYS:HG2	1:E:165:LYS:O	2.21	0.41
1:G:21:THR:CG2	1:G:24:GLU:HG3	2.50	0.41
1:I:94:GLN:CA	1:I:102:LEU:HD11	2.50	0.41
1:I:111:GLN:HE21	1:I:111:GLN:CA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:247:LYS:HD2	1:K:249:ASP:HB2	2.03	0.41
1:A:180:GLN:NE2	1:C:59:ARG:CG	2.83	0.41
1:C:20:ILE:HG23	1:C:21:THR:H	1.85	0.41
1:C:136:TRP:N	1:C:136:TRP:CD1	2.87	0.41
1:E:18:GLY:H	1:E:115:PRO:CB	2.28	0.41
1:E:157:LEU:O	1:E:158:ILE:C	2.59	0.41
1:G:168:TRP:CE3	1:G:194:ILE:HD11	2.55	0.41
1:G:252:LEU:HA	1:G:252:LEU:HD13	1.58	0.41
2:H:184:LEU:HA	2:H:184:LEU:HD23	1.28	0.41
1:I:23:GLU:CG	1:I:246:TYR:OH	2.67	0.41
2:J:175:LYS:O	2:J:178:ARG:CG	2.68	0.41
1:K:252:LEU:HD13	1:K:252:LEU:HA	1.65	0.41
1:A:141:GLN:O	1:A:145:GLN:HG2	2.20	0.41
1:A:195:ARG:NH2	1:A:215:HIS:CE1	2.85	0.41
1:C:51:PHE:CD1	1:C:51:PHE:N	2.88	0.41
1:C:199:ASN:O	1:C:201:GLY:N	2.54	0.41
1:C:236:THR:OG1	1:C:238:TRP:CD1	2.70	0.41
1:E:237:LEU:O	1:E:239:GLN:N	2.54	0.41
2:F:184:LEU:O	2:F:185:ASN:CB	2.69	0.41
1:G:241:VAL:HG13	1:G:245:SER:OG	2.21	0.41
1:I:88:LEU:HD13	1:I:92:HIS:CE1	2.56	0.41
1:I:136:TRP:HB3	1:I:138:LEU:HD23	2.02	0.41
1:A:234:PHE:N	1:A:234:PHE:CD1	2.89	0.41
1:C:140:GLY:C	1:C:142:ALA:N	2.71	0.41
1:C:180:GLN:O	1:C:182:VAL:N	2.54	0.41
1:E:260:GLN:OE1	1:E:260:GLN:CA	2.69	0.41
1:G:163:HIS:CB	1:G:168:TRP:CH2	3.04	0.41
1:K:197:ARG:HB3	1:K:198:ASP:H	1.60	0.41
1:K:209:HIS:ND1	1:K:253:ARG:NH2	2.68	0.41
1:A:147:ILE:O	1:A:151:LYS:N	2.40	0.41
1:A:207:LEU:CD2	1:A:207:LEU:N	2.83	0.41
1:C:137:ASN:OD1	1:C:139:GLN:NE2	2.54	0.41
1:C:145:GLN:O	1:C:147:ILE:N	2.53	0.41
2:D:178:ARG:HH21	2:D:180:LEU:HD21	1.85	0.41
1:E:38:LEU:CD1	1:E:107:PHE:HD2	2.33	0.41
1:E:107:PHE:CD1	1:E:107:PHE:C	2.94	0.41
1:I:173:ILE:HG22	1:I:174:SER:O	2.21	0.41
1:I:238:TRP:NE1	1:I:239:GLN:HG3	2.36	0.41
1:K:47:TYR:HD1	1:K:225:LYS:HZ1	1.54	0.41
1:K:180:GLN:O	1:K:181:ILE:C	2.58	0.41
1:K:253:ARG:NH1	1:K:253:ARG:CB	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:CD2	1:A:235:ASP:CB	2.98	0.41
1:A:172:LYS:C	1:A:173:ILE:HG13	2.39	0.41
1:A:213:VAL:HG13	1:A:214:LEU:N	2.36	0.41
1:A:232:LYS:HE2	1:A:232:LYS:HB2	1.58	0.41
1:C:70:LEU:C	1:C:72:GLY:H	2.22	0.41
1:E:226:LEU:HD13	1:E:234:PHE:O	2.21	0.41
1:I:39:TYR:CD1	1:I:105:LYS:O	2.73	0.41
1:I:129:ARG:HD2	1:I:129:ARG:O	2.21	0.41
1:I:132:VAL:O	1:I:133:LYS:C	2.60	0.41
1:I:246:TYR:HE2	1:I:247:LYS:HE3	1.85	0.41
1:K:36:ASP:HA	1:K:56:ALA:O	2.21	0.41
1:K:38:LEU:CD2	1:K:105:LYS:O	2.65	0.41
1:K:229:PRO:O	1:K:230:GLU:HB2	2.20	0.41
1:A:120:PHE:HA	1:A:123:LEU:CD1	2.50	0.41
1:C:172:LYS:HD3	1:C:198:ASP:OD1	2.21	0.41
1:C:216:TYR:CE2	1:C:251:LEU:HD23	2.56	0.41
1:G:32:GLY:CA	1:G:107:PHE:HE2	2.34	0.41
1:I:38:LEU:HD23	1:I:38:LEU:HA	1.75	0.41
1:I:46:ASN:O	1:I:47:TYR:HD1	2.04	0.41
1:I:136:TRP:HZ3	1:I:146:ALA:HB1	1.84	0.41
1:I:174:SER:O	1:I:178:SER:OG	2.34	0.41
1:A:28:TYR:HE1	1:A:110:PRO:HG2	1.86	0.40
1:A:93:SER:HG	1:A:94:GLN:HE21	1.69	0.40
1:A:131:TYR:HD1	1:A:132:VAL:N	2.19	0.40
1:A:193:LEU:HD23	1:A:193:LEU:C	2.41	0.40
1:C:197:ARG:HH12	2:D:170:PTR:P	2.44	0.40
2:D:174:ARG:O	2:D:175:LYS:C	2.60	0.40
1:G:172:LYS:HZ1	1:G:173:ILE:C	2.24	0.40
1:G:251:LEU:O	1:G:253:ARG:N	2.54	0.40
1:I:88:LEU:CD1	1:I:92:HIS:CE1	3.04	0.40
1:K:74:TYR:CE2	1:K:85:PRO:HD3	2.56	0.40
1:K:199:ASN:O	1:K:202:SER:HB3	2.20	0.40
1:A:38:LEU:CD2	1:A:107:PHE:HB2	2.51	0.40
1:A:240:LEU:CD2	1:A:244:TYR:HD2	2.33	0.40
1:C:42:ARG:HH12	2:D:181:PTR:P	2.44	0.40
1:C:128:ILE:HG22	1:C:158:ILE:CG1	2.17	0.40
1:C:205:LEU:CD2	1:C:205:LEU:C	2.89	0.40
1:E:167:PRO:C	1:E:169:PHE:H	2.25	0.40
1:G:170:HIS:O	1:G:171:GLY:C	2.59	0.40
1:I:159:ALA:C	1:I:161:THR:N	2.74	0.40
1:I:183:LEU:HD13	1:I:183:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:LEU:C	1:K:101:CYS:N	2.75	0.40
1:K:214:LEU:HD23	1:K:214:LEU:HA	1.78	0.40
1:K:225:LYS:CE	1:K:235:ASP:OD1	2.70	0.40
1:A:126:ASN:O	1:A:129:ARG:N	2.53	0.40
1:E:25:ALA:O	1:E:26:GLU:C	2.58	0.40
1:E:27:ASP:O	1:E:28:TYR:C	2.60	0.40
1:E:70:LEU:H	1:E:70:LEU:CD1	2.19	0.40
1:E:92:HIS:CD2	1:E:99:LEU:HG	2.55	0.40
1:G:20:ILE:HD12	1:G:116:LYS:HB2	2.03	0.40
1:G:27:ASP:O	1:G:28:TYR:C	2.60	0.40
1:G:109:ARG:HA	1:G:110:PRO:HD2	1.96	0.40
1:I:113:VAL:C	1:I:114:GLN:HE21	2.23	0.40
1:I:120:PHE:N	1:I:122:ASP:OD1	2.53	0.40
1:I:136:TRP:CB	1:I:138:LEU:CD2	3.00	0.40
1:A:22:ARG:NH1	2:B:181:PTR:P	2.94	0.40
1:C:55:VAL:HG11	1:C:103:LEU:HD22	2.03	0.40
1:C:132:VAL:CG1	1:C:143:LEU:CD1	2.98	0.40
1:C:159:ALA:O	1:C:160:THR:C	2.59	0.40
1:C:247:LYS:HG3	1:C:249:ASP:H	1.87	0.40
1:G:227:SER:HB2	1:G:232:LYS:O	2.21	0.40
1:I:27:ASP:O	1:I:28:TYR:C	2.59	0.40
1:I:139:GLN:HB3	1:I:140:GLY:H	1.63	0.40
1:I:202:SER:HB2	1:I:219:ASP:HA	2.04	0.40
1:K:92:HIS:HD2	1:K:96:SER:O	2.05	0.40
1:A:30:VAL:CG2	1:E:260:GLN:HB3	2.52	0.40
1:A:96:SER:OG	1:A:97:ASP:N	2.54	0.40
1:A:232:LYS:HG2	1:A:234:PHE:CE1	2.57	0.40
1:C:183:LEU:HD12	1:C:183:LEU:HA	1.76	0.40
1:I:105:LYS:HA	1:I:106:PRO:HD3	1.87	0.40
1:K:18:GLY:H	1:K:115:PRO:HB3	1.85	0.40
1:K:30:VAL:HA	1:K:34:MET:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/254 (99%)	190 (75%)	39 (16%)	23 (9%)	0	2
1	C	252/254 (99%)	184 (73%)	51 (20%)	17 (7%)	1	5
1	E	216/254 (85%)	164 (76%)	41 (19%)	11 (5%)	1	10
1	G	216/254 (85%)	167 (77%)	36 (17%)	13 (6%)	1	7
1	I	252/254 (99%)	179 (71%)	47 (19%)	26 (10%)	0	2
1	K	216/254 (85%)	158 (73%)	44 (20%)	14 (6%)	1	5
2	B	14/18 (78%)	9 (64%)	3 (21%)	2 (14%)	0	1
2	D	14/18 (78%)	11 (79%)	1 (7%)	2 (14%)	0	1
2	F	14/18 (78%)	8 (57%)	6 (43%)	0	100	100
2	H	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	4
2	J	14/18 (78%)	9 (64%)	4 (29%)	1 (7%)	1	4
2	L	14/18 (78%)	9 (64%)	4 (29%)	1 (7%)	1	4
All	All	1488/1632 (91%)	1098 (74%)	279 (19%)	111 (8%)	1	4

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	A	137	ASN
1	A	140	GLY
1	A	171	GLY
1	A	177	GLU
1	C	18	GLY
1	C	198	ASP
1	E	18	GLY
1	G	10	ALA
1	G	18	GLY
1	G	171	GLY
1	I	10	ALA
1	I	18	GLY
1	I	59	ARG
1	I	151	LYS
1	I	199	ASN
2	J	175	LYS
1	K	18	GLY
1	K	180	GLN

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Mol	Chain	Res	Type
1	K	181	ILE
1	K	197	ARG
1	K	242	GLU
1	A	10	ALA
1	A	49	GLY
1	A	113	VAL
1	A	125	GLU
1	A	146	ALA
1	A	181	ILE
1	A	198	ASP
2	B	175	LYS
1	C	49	GLY
1	C	120	PHE
1	C	137	ASN
1	C	146	ALA
1	C	200	ASN
2	D	176	GLY
1	E	10	ALA
1	E	49	GLY
1	E	97	ASP
1	E	171	GLY
1	E	241	VAL
1	E	242	GLU
1	E	249	ASP
1	G	158	ILE
1	G	181	ILE
1	G	232	LYS
1	I	24	GLU
1	I	49	GLY
1	I	83	ALA
1	I	125	GLU
1	I	137	ASN
1	I	140	GLY
1	I	146	ALA
1	I	152	PRO
1	I	171	GLY
1	I	201	GLY
1	I	232	LYS
1	I	242	GLU
1	K	49	GLY
1	K	100	VAL
1	K	171	GLY

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Mol	Chain	Res	Type
1	K	200	ASN
1	K	238	TRP
2	L	176	GLY
1	C	152	PRO
1	C	180	GLN
1	C	249	ASP
1	E	24	GLU
1	G	104	LYS
1	G	110	PRO
1	G	242	GLU
1	I	34	MET
1	I	70	LEU
1	I	160	THR
1	K	10	ALA
1	A	59	ARG
1	A	88	LEU
1	A	180	GLN
1	A	200	ASN
1	C	155	GLU
1	C	232	LYS
2	D	175	LYS
1	E	59	ARG
1	G	97	ASP
1	G	227	SER
1	G	252	LEU
2	H	176	GLY
1	I	131	TYR
1	K	59	ARG
1	A	145	GLN
1	C	151	LYS
1	E	177	GLU
1	I	96	SER
1	I	177	GLU
1	K	104	LYS
1	A	110	PRO
1	A	124	LYS
1	A	211	GLY
1	A	222	LYS
1	A	232	LYS
1	C	242	GLU
1	I	159	ALA
1	I	241	VAL

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Mol	Chain	Res	Type
1	K	241	VAL
1	C	147	ILE
1	A	201	GLY
1	C	181	ILE
2	B	173	ILE
1	I	100	VAL
1	G	113	VAL
1	C	119	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/216 (98%)	124 (59%)	87 (41%)	0	0
1	C	211/216 (98%)	125 (59%)	86 (41%)	0	0
1	E	183/216 (85%)	118 (64%)	65 (36%)	0	1
1	G	182/216 (84%)	105 (58%)	77 (42%)	0	0
1	I	210/216 (97%)	123 (59%)	87 (41%)	0	0
1	K	182/216 (84%)	116 (64%)	66 (36%)	0	1
2	B	14/14 (100%)	6 (43%)	8 (57%)	0	0
2	D	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	F	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	H	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	J	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	L	14/14 (100%)	8 (57%)	6 (43%)	0	0
All	All	1263/1380 (92%)	757 (60%)	506 (40%)	0	0

All (506) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	15	PHE
1	A	20	ILE
1	A	21	THR
1	A	22	ARG
1	A	31	GLN
1	A	38	LEU
1	A	41	LEU
1	A	43	GLN
1	A	59	ARG
1	A	65	THR
1	A	68	ARG
1	A	70	LEU
1	A	71	ASN
1	A	74	TYR
1	A	80	ARG
1	A	81	THR
1	A	82	HIS
1	A	84	SER
1	A	88	LEU
1	A	94	GLN
1	A	96	SER
1	A	99	LEU
1	A	101	CYS
1	A	102	LEU
1	A	104	LYS
1	A	105	LYS
1	A	107	PHE
1	A	109	ARG
1	A	111	GLN
1	A	116	LYS
1	A	120	PHE
1	A	121	GLU
1	A	122	ASP
1	A	123	LEU
1	A	126	ASN
1	A	128	ILE
1	A	129	ARG
1	A	131	TYR
1	A	134	GLN
1	A	138	LEU
1	A	141	GLN
1	A	143	LEU

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Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	ILE
1	A	148	ILE
1	A	149	SER
1	A	150	GLN
1	A	151	LYS
1	A	153	GLN
1	A	154	LEU
1	A	157	LEU
1	A	158	ILE
1	A	160	THR
1	A	163	HIS
1	A	165	LYS
1	A	166	MET
1	A	172	LYS
1	A	175	ARG
1	A	178	SER
1	A	182	VAL
1	A	183	LEU
1	A	184	ILE
1	A	187	LYS
1	A	188	THR
1	A	193	LEU
1	A	194	ILE
1	A	198	ASP
1	A	199	ASN
1	A	200	ASN
1	A	202	SER
1	A	205	LEU
1	A	212	LYS
1	A	213	VAL
1	A	217	ARG
1	A	219	ASP
1	A	223	THR
1	A	226	LEU
1	A	232	LYS
1	A	238	TRP
1	A	242	GLU
1	A	246	TYR
1	A	252	LEU
1	A	253	ARG
1	A	259	CYS

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Mol	Chain	Res	Type
1	A	262	ILE
2	B	173	ILE
2	B	174	ARG
2	B	175	LYS
2	B	177	GLN
2	B	178	ARG
2	B	179	ASP
2	B	182	SER
2	B	185	ASN
1	C	12	HIS
1	C	20	ILE
1	C	21	THR
1	C	31	GLN
1	C	34	MET
1	C	38	LEU
1	C	41	LEU
1	C	43	GLN
1	C	48	LEU
1	C	53	LEU
1	C	55	VAL
1	C	59	ARG
1	C	68	ARG
1	C	70	LEU
1	C	71	ASN
1	C	81	THR
1	C	82	HIS
1	C	84	SER
1	C	88	LEU
1	C	93	SER
1	C	94	GLN
1	C	96	SER
1	C	99	LEU
1	C	102	LEU
1	C	104	LYS
1	C	105	LYS
1	C	107	PHE
1	C	109	ARG
1	C	111	GLN
1	C	117	THR
1	C	120	PHE
1	C	122	ASP
1	C	123	LEU

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Mol	Chain	Res	Type
1	C	126	ASN
1	C	129	ARG
1	C	134	GLN
1	C	135	THR
1	C	138	LEU
1	C	141	GLN
1	C	143	LEU
1	C	148	ILE
1	C	150	GLN
1	C	151	LYS
1	C	153	GLN
1	C	154	LEU
1	C	160	THR
1	C	165	LYS
1	C	166	MET
1	C	172	LYS
1	C	173	ILE
1	C	175	ARG
1	C	177	GLU
1	C	178	SER
1	C	183	LEU
1	C	184	ILE
1	C	186	SER
1	C	187	LYS
1	C	188	THR
1	C	193	LEU
1	C	194	ILE
1	C	197	ARG
1	C	199	ASN
1	C	200	ASN
1	C	202	SER
1	C	203	TYR
1	C	205	LEU
1	C	207	LEU
1	C	210	GLU
1	C	213	VAL
1	C	217	ARG
1	C	219	ASP
1	C	223	THR
1	C	226	LEU
1	C	227	SER
1	C	232	LYS

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Mol	Chain	Res	Type
1	C	234	PHE
1	C	236	THR
1	C	237	LEU
1	C	238	TRP
1	C	241	VAL
1	C	242	GLU
1	C	246	TYR
1	C	252	LEU
1	C	253	ARG
1	C	260	GLN
1	C	262	ILE
2	D	169	ASP
2	D	173	ILE
2	D	175	LYS
2	D	179	ASP
2	D	182	SER
2	D	185	ASN
1	E	12	HIS
1	E	13	LEU
1	E	21	THR
1	E	22	ARG
1	E	31	GLN
1	E	38	LEU
1	E	40	LEU
1	E	41	LEU
1	E	42	ARG
1	E	43	GLN
1	E	48	LEU
1	E	53	LEU
1	E	54	SER
1	E	59	ARG
1	E	67	GLU
1	E	68	ARG
1	E	70	LEU
1	E	71	ASN
1	E	80	ARG
1	E	81	THR
1	E	82	HIS
1	E	88	LEU
1	E	90	HIS
1	E	94	GLN
1	E	96	SER

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Mol	Chain	Res	Type
1	E	99	LEU
1	E	102	LEU
1	E	104	LYS
1	E	105	LYS
1	E	107	PHE
1	E	109	ARG
1	E	111	GLN
1	E	153	GLN
1	E	154	LEU
1	E	165	LYS
1	E	172	LYS
1	E	178	SER
1	E	181	ILE
1	E	182	VAL
1	E	183	LEU
1	E	184	ILE
1	E	186	SER
1	E	187	LYS
1	E	188	THR
1	E	193	LEU
1	E	194	ILE
1	E	195	ARG
1	E	197	ARG
1	E	199	ASN
1	E	205	LEU
1	E	206	CYS
1	E	207	LEU
1	E	219	ASP
1	E	223	THR
1	E	225	LYS
1	E	226	LEU
1	E	232	LYS
1	E	236	THR
1	E	237	LEU
1	E	238	TRP
1	E	246	TYR
1	E	252	LEU
1	E	253	ARG
1	E	254	VAL
1	E	262	ILE
2	F	173	ILE
2	F	175	LYS

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Mol	Chain	Res	Type
2	F	177	GLN
2	F	178	ARG
2	F	179	ASP
2	F	182	SER
1	G	12	HIS
1	G	13	LEU
1	G	15	PHE
1	G	21	THR
1	G	22	ARG
1	G	30	VAL
1	G	31	GLN
1	G	34	MET
1	G	38	LEU
1	G	40	LEU
1	G	41	LEU
1	G	43	GLN
1	G	45	ARG
1	G	48	LEU
1	G	53	LEU
1	G	54	SER
1	G	59	ARG
1	G	65	THR
1	G	67	GLU
1	G	68	ARG
1	G	70	LEU
1	G	71	ASN
1	G	80	ARG
1	G	81	THR
1	G	82	HIS
1	G	84	SER
1	G	88	LEU
1	G	92	HIS
1	G	93	SER
1	G	96	SER
1	G	100	VAL
1	G	102	LEU
1	G	104	LYS
1	G	107	PHE
1	G	109	ARG
1	G	111	GLN
1	G	117	THR
1	G	153	GLN

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Mol	Chain	Res	Type
1	G	154	LEU
1	G	156	LYS
1	G	157	LEU
1	G	158	ILE
1	G	160	THR
1	G	165	LYS
1	G	172	LYS
1	G	173	ILE
1	G	177	GLU
1	G	178	SER
1	G	181	ILE
1	G	187	LYS
1	G	188	THR
1	G	193	LEU
1	G	194	ILE
1	G	195	ARG
1	G	197	ARG
1	G	205	LEU
1	G	206	CYS
1	G	207	LEU
1	G	213	VAL
1	G	217	ARG
1	G	219	ASP
1	G	223	THR
1	G	225	LYS
1	G	226	LEU
1	G	234	PHE
1	G	237	LEU
1	G	238	TRP
1	G	241	VAL
1	G	242	GLU
1	G	245	SER
1	G	246	TYR
1	G	252	LEU
1	G	253	ARG
1	G	254	VAL
1	G	257	VAL
1	G	260	GLN
1	G	262	ILE
2	H	174	ARG
2	H	175	LYS
2	H	177	GLN

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Mol	Chain	Res	Type
2	H	178	ARG
2	H	182	SER
2	H	185	ASN
1	I	12	HIS
1	I	21	THR
1	I	22	ARG
1	I	23	GLU
1	I	31	GLN
1	I	38	LEU
1	I	40	LEU
1	I	41	LEU
1	I	42	ARG
1	I	43	GLN
1	I	45	ARG
1	I	48	LEU
1	I	51	PHE
1	I	53	LEU
1	I	59	ARG
1	I	67	GLU
1	I	68	ARG
1	I	69	GLU
1	I	70	LEU
1	I	71	ASN
1	I	81	THR
1	I	82	HIS
1	I	88	LEU
1	I	93	SER
1	I	94	GLN
1	I	96	SER
1	I	99	LEU
1	I	102	LEU
1	I	104	LYS
1	I	109	ARG
1	I	111	GLN
1	I	116	LYS
1	I	117	THR
1	I	120	PHE
1	I	122	ASP
1	I	123	LEU
1	I	125	GLU
1	I	126	ASN
1	I	128	ILE

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Mol	Chain	Res	Type
1	I	129	ARG
1	I	135	THR
1	I	137	ASN
1	I	138	LEU
1	I	139	GLN
1	I	141	GLN
1	I	145	GLN
1	I	147	ILE
1	I	148	ILE
1	I	149	SER
1	I	150	GLN
1	I	151	LYS
1	I	153	GLN
1	I	154	LEU
1	I	157	LEU
1	I	165	LYS
1	I	166	MET
1	I	172	LYS
1	I	174	SER
1	I	178	SER
1	I	181	ILE
1	I	183	LEU
1	I	184	ILE
1	I	186	SER
1	I	187	LYS
1	I	188	THR
1	I	189	ASN
1	I	193	LEU
1	I	194	ILE
1	I	197	ARG
1	I	199	ASN
1	I	203	TYR
1	I	205	LEU
1	I	206	CYS
1	I	213	VAL
1	I	217	ARG
1	I	219	ASP
1	I	223	THR
1	I	225	LYS
1	I	226	LEU
1	I	227	SER
1	I	234	PHE

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Mol	Chain	Res	Type
1	I	238	TRP
1	I	252	LEU
1	I	253	ARG
1	I	257	VAL
1	I	260	GLN
1	I	262	ILE
2	J	173	ILE
2	J	175	LYS
2	J	177	GLN
2	J	179	ASP
2	J	182	SER
2	J	185	ASN
1	K	12	HIS
1	K	15	PHE
1	K	21	THR
1	K	22	ARG
1	K	31	GLN
1	K	38	LEU
1	K	41	LEU
1	K	53	LEU
1	K	54	SER
1	K	59	ARG
1	K	68	ARG
1	K	70	LEU
1	K	71	ASN
1	K	82	HIS
1	K	88	LEU
1	K	90	HIS
1	K	93	SER
1	K	94	GLN
1	K	96	SER
1	K	99	LEU
1	K	102	LEU
1	K	103	LEU
1	K	104	LYS
1	K	105	LYS
1	K	107	PHE
1	K	109	ARG
1	K	111	GLN
1	K	153	GLN
1	K	155	GLU
1	K	157	LEU

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Mol	Chain	Res	Type
1	K	158	ILE
1	K	165	LYS
1	K	172	LYS
1	K	178	SER
1	K	181	ILE
1	K	182	VAL
1	K	184	ILE
1	K	187	LYS
1	K	188	THR
1	K	193	LEU
1	K	194	ILE
1	K	195	ARG
1	K	197	ARG
1	K	198	ASP
1	K	199	ASN
1	K	203	TYR
1	K	205	LEU
1	K	207	LEU
1	K	212	LYS
1	K	213	VAL
1	K	214	LEU
1	K	217	ARG
1	K	219	ASP
1	K	226	LEU
1	K	227	SER
1	K	234	PHE
1	K	236	THR
1	K	238	TRP
1	K	239	GLN
1	K	247	LYS
1	K	252	LEU
1	K	253	ARG
1	K	254	VAL
1	K	257	VAL
1	K	260	GLN
1	K	262	ILE
2	L	173	ILE
2	L	174	ARG
2	L	175	LYS
2	L	178	ARG
2	L	182	SER
2	L	185	ASN

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	71	ASN
1	A	111	GLN
1	A	137	ASN
1	A	141	GLN
1	A	145	GLN
1	A	153	GLN
1	A	180	GLN
1	A	243	HIS
2	B	177	GLN
2	B	185	ASN
1	C	43	GLN
1	C	111	GLN
1	C	139	GLN
1	C	141	GLN
1	C	145	GLN
1	C	153	GLN
1	C	180	GLN
1	C	199	ASN
2	D	185	ASN
1	E	111	GLN
1	E	153	GLN
1	E	170	HIS
1	E	180	GLN
1	E	243	HIS
2	F	185	ASN
1	G	43	GLN
1	G	57	HIS
1	G	108	ASN
1	G	111	GLN
1	G	114	GLN
1	G	153	GLN
1	G	180	GLN
1	G	199	ASN
2	H	177	GLN
2	H	185	ASN
1	I	43	GLN
1	I	111	GLN
1	I	139	GLN
1	I	145	GLN
1	I	180	GLN
1	I	200	ASN

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Mol	Chain	Res	Type
2	J	185	ASN
1	K	111	GLN
1	K	153	GLN
1	K	180	GLN
1	K	199	ASN
2	L	185	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PTR	D	181	2	15,16,17	0.94	1 (6%)	17,22,24	1.98	5 (29%)
2	PTR	J	170	2	15,16,17	0.94	0	17,22,24	0.80	1 (5%)
2	PTR	H	181	2	15,16,17	1.20	1 (6%)	17,22,24	1.76	5 (29%)
2	PTR	H	170	2	15,16,17	0.98	2 (13%)	17,22,24	1.20	2 (11%)
2	PTR	F	181	2	15,16,17	0.90	0	17,22,24	1.05	2 (11%)
2	PTR	F	170	2	15,16,17	1.65	1 (6%)	17,22,24	0.84	1 (5%)
2	PTR	J	181	2	15,16,17	1.89	1 (6%)	17,22,24	1.16	3 (17%)
2	PTR	L	181	2	15,16,17	1.03	0	17,22,24	0.96	1 (5%)
2	PTR	B	181	2	15,16,17	1.33	1 (6%)	17,22,24	2.15	3 (17%)
2	PTR	D	170	2	15,16,17	0.85	0	17,22,24	0.62	0
2	PTR	B	170	2	15,16,17	2.37	1 (6%)	17,22,24	1.25	3 (17%)
2	PTR	L	170	2	15,16,17	1.16	2 (13%)	17,22,24	1.07	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	D	181	2	-	1/10/11/13	0/1/1/1
2	PTR	J	170	2	-	1/10/11/13	0/1/1/1
2	PTR	H	181	2	-	3/10/11/13	0/1/1/1
2	PTR	H	170	2	-	0/10/11/13	0/1/1/1
2	PTR	F	181	2	-	2/10/11/13	0/1/1/1
2	PTR	F	170	2	-	0/10/11/13	0/1/1/1
2	PTR	J	181	2	-	1/10/11/13	0/1/1/1
2	PTR	L	181	2	-	0/10/11/13	0/1/1/1
2	PTR	B	181	2	-	2/10/11/13	0/1/1/1
2	PTR	D	170	2	-	1/10/11/13	0/1/1/1
2	PTR	B	170	2	-	0/10/11/13	0/1/1/1
2	PTR	L	170	2	-	0/10/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	170	PTR	P-OH	8.78	1.76	1.59
2	J	181	PTR	P-OH	-6.42	1.47	1.59
2	F	170	PTR	P-OH	5.81	1.70	1.59
2	B	181	PTR	P-OH	-3.59	1.53	1.59
2	H	181	PTR	P-OH	-3.08	1.53	1.59
2	D	181	PTR	OH-CZ	-2.42	1.35	1.40
2	H	170	PTR	CB-CA	-2.28	1.49	1.53
2	L	170	PTR	P-OH	2.22	1.63	1.59
2	H	170	PTR	CB-CG	-2.10	1.46	1.51
2	L	170	PTR	P-O3P	-2.05	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	PTR	O2P-P-OH	-5.65	88.61	105.32
2	D	181	PTR	OH-P-O1P	-5.15	92.30	109.48
2	B	181	PTR	O3P-P-OH	4.82	119.57	105.32
2	D	181	PTR	O3P-P-OH	4.26	117.91	105.32
2	H	181	PTR	O3P-P-OH	4.01	117.16	105.32
2	B	181	PTR	O2P-P-O1P	3.97	126.32	110.83
2	L	170	PTR	P-OH-CZ	3.49	136.30	123.88
2	H	170	PTR	OH-P-O1P	-3.41	98.10	109.48
2	H	181	PTR	O2P-P-OH	-3.26	95.67	105.32
2	B	170	PTR	O3P-P-OH	3.11	114.50	105.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	181	PTR	O3P-P-O2P	2.77	118.19	107.80
2	J	181	PTR	O3P-P-OH	2.72	113.37	105.32
2	J	170	PTR	O3P-P-OH	2.71	113.32	105.32
2	B	170	PTR	OH-P-O1P	-2.65	100.64	109.48
2	H	181	PTR	O3P-P-O2P	2.64	117.71	107.80
2	H	181	PTR	O2P-P-O1P	2.60	120.95	110.83
2	D	181	PTR	O2P-P-OH	2.57	112.92	105.32
2	H	181	PTR	O3P-P-O1P	-2.57	100.83	110.83
2	D	181	PTR	O3P-P-O1P	-2.56	100.87	110.83
2	F	181	PTR	O2P-P-O1P	-2.41	101.46	110.83
2	H	170	PTR	O3P-P-OH	2.40	112.41	105.32
2	F	170	PTR	O3P-P-OH	2.39	112.39	105.32
2	J	181	PTR	O3P-P-O2P	2.39	116.75	107.80
2	B	170	PTR	O2P-P-OH	2.35	112.28	105.32
2	D	181	PTR	O3P-P-O2P	2.34	116.58	107.80
2	J	181	PTR	OH-P-O1P	-2.25	101.96	109.48
2	L	181	PTR	O2P-P-OH	2.22	111.90	105.32

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	181	PTR	C-CA-CB-CG
2	D	170	PTR	O-C-CA-CB
2	D	181	PTR	CZ-OH-P-O1P
2	F	181	PTR	O-C-CA-CB
2	H	181	PTR	O-C-CA-CB
2	H	181	PTR	C-CA-CB-CG
2	J	170	PTR	O-C-CA-CB
2	B	181	PTR	N-CA-CB-CG
2	F	181	PTR	CZ-OH-P-O3P
2	H	181	PTR	N-CA-CB-CG
2	J	181	PTR	CZ-OH-P-O3P

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	181	PTR	2	0
2	H	181	PTR	2	0
2	H	170	PTR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	181	PTR	1	0
2	F	170	PTR	1	0
2	J	181	PTR	8	0
2	B	181	PTR	4	0
2	D	170	PTR	3	0
2	B	170	PTR	2	0

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.