Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 08:13 am GMT

PDB ID	:	2JA6
Title	:	CPD lesion containing RNA Polymerase II elongation complex B
Authors	:	Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on	:	2006-11-23
Resolution	:	4.00 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:

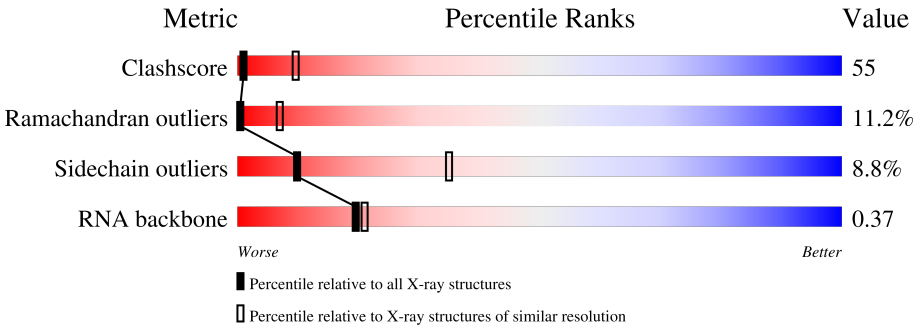
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RNA backbone	3102	1048 (5.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	25% 45% 11% • 18%
2	B	1224	26% 54% 11% • 9%
3	C	318	25% 48% 10% • 16%
4	D	221	27% 40% 12% • 20%
5	E	215	40% 55% 5%
6	F	155	18% 34% • 44%

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Mol	Chain	Length	Quality of chain
7	G	171	34% 57% 9%
8	H	146	26% 56% 10% 8%
9	I	122	34% 46% 13% 5%
10	J	70	16% 49% 26% 7%
11	K	120	36% 44% 14% 5%
12	L	70	17% 31% 16% 34%
13	N	14	50% 7% 43%
14	P	11	9% 73% 9% 9%
15	T	25	52% 24% 24%

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
15	TT	T	17	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32010 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1421	11186	7048	1958	2118	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1115	8866	5614	1553	1644	55	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	267	2101	1320	349	419	13	0	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1427	882	256	287	2	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3 '.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP* TP*TP*TTP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0	0
			403	1	196	62	125	19			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

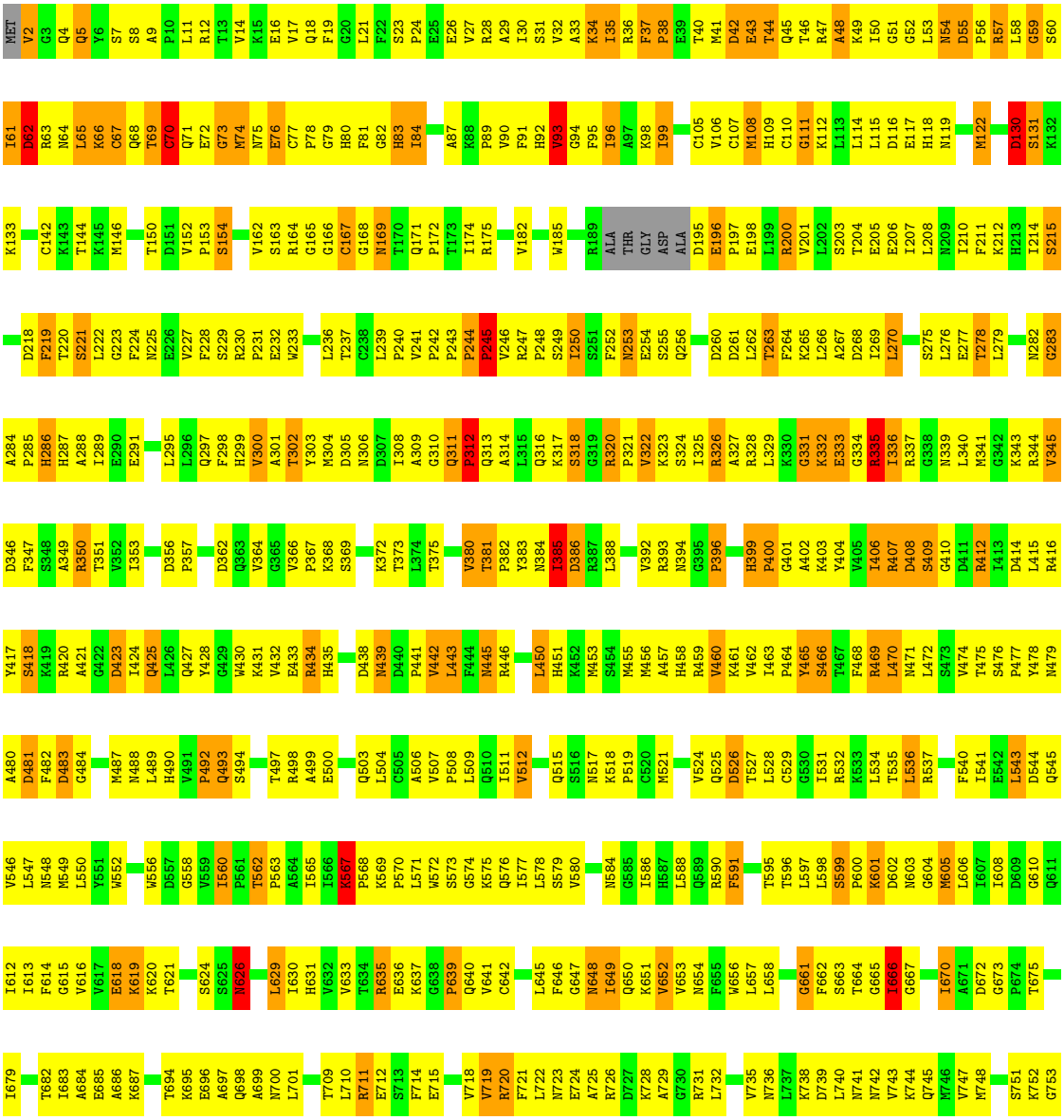
3 Residue-property plots (i)

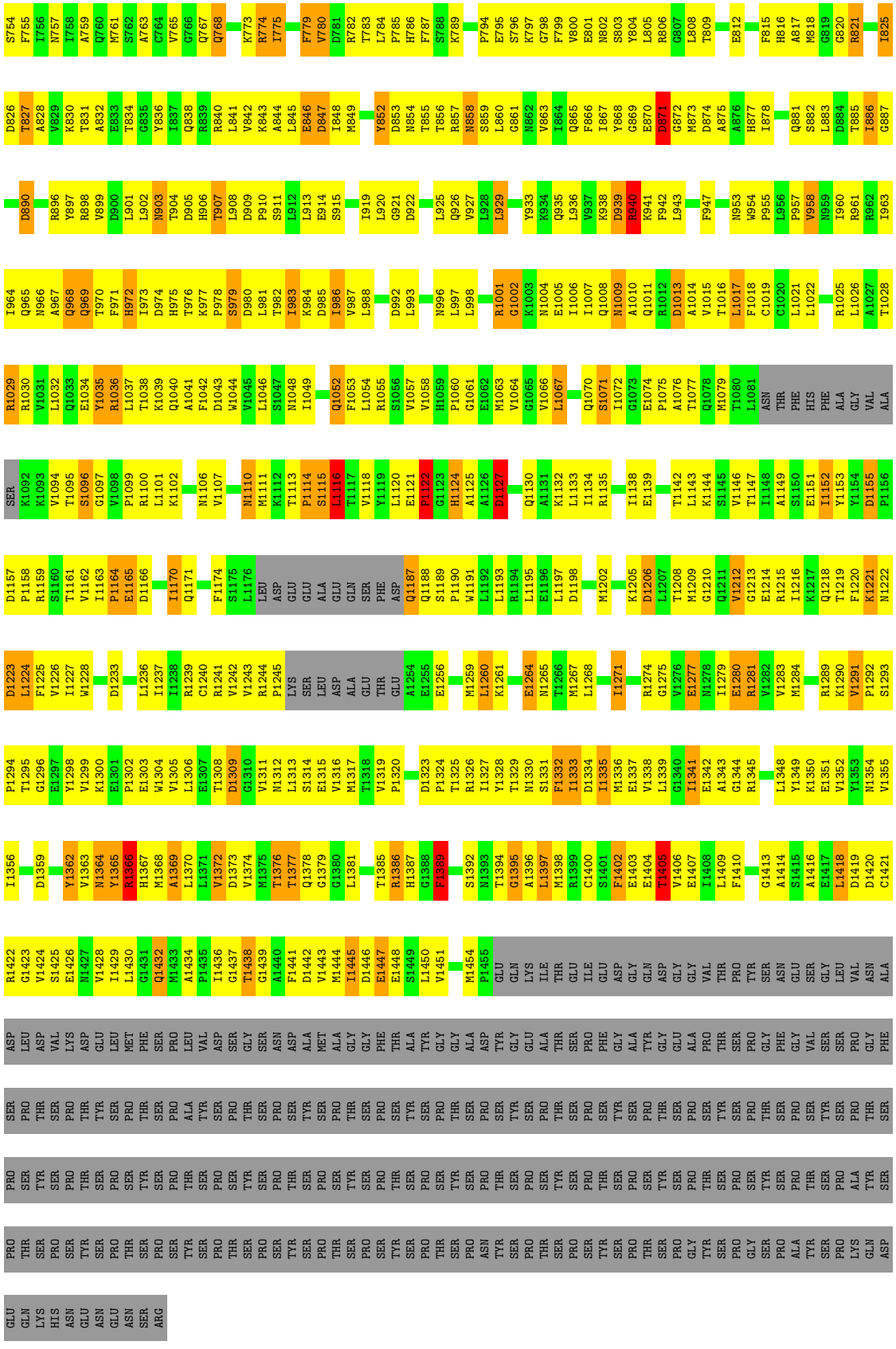
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

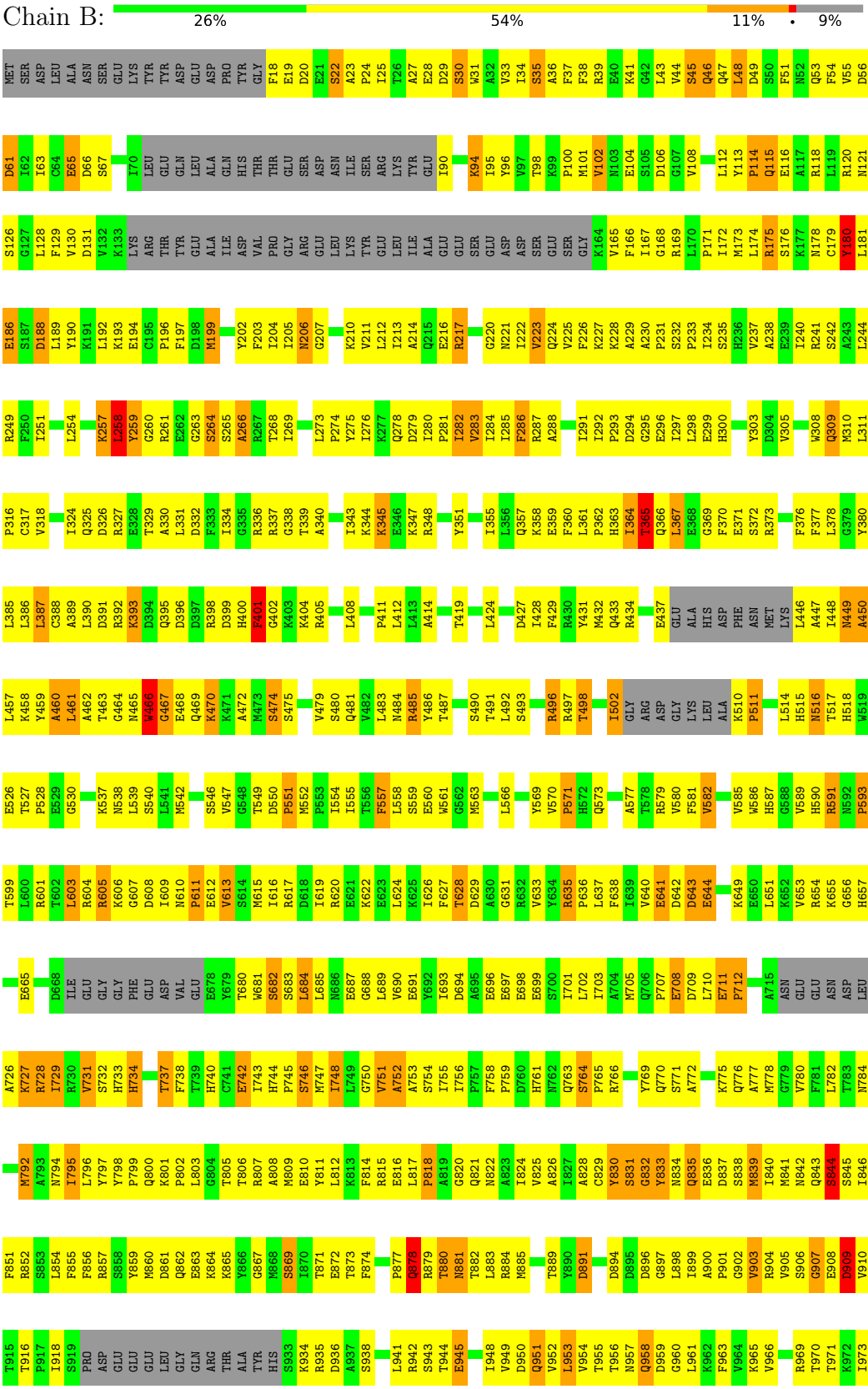
Chain A: 25% 45% 11% 18%

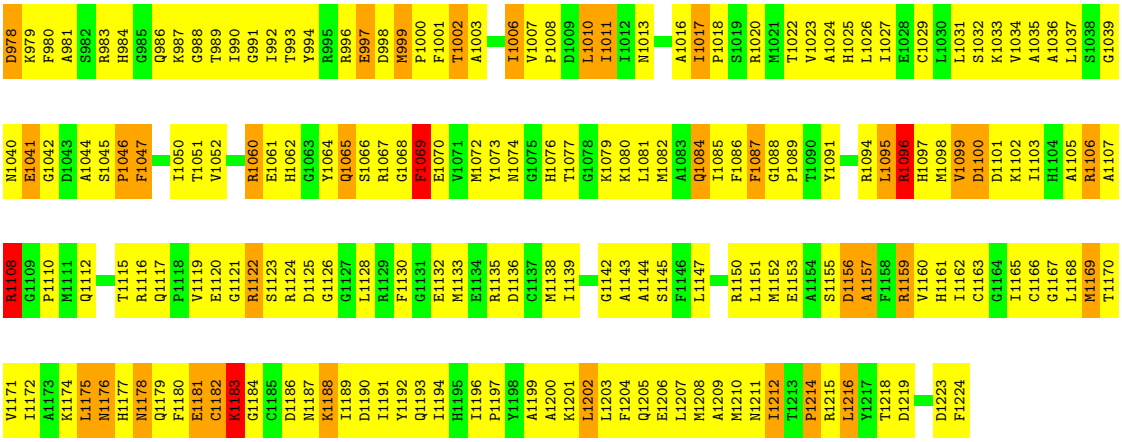




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

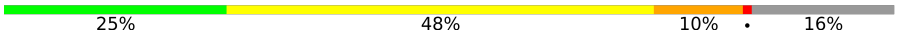
Chain B:

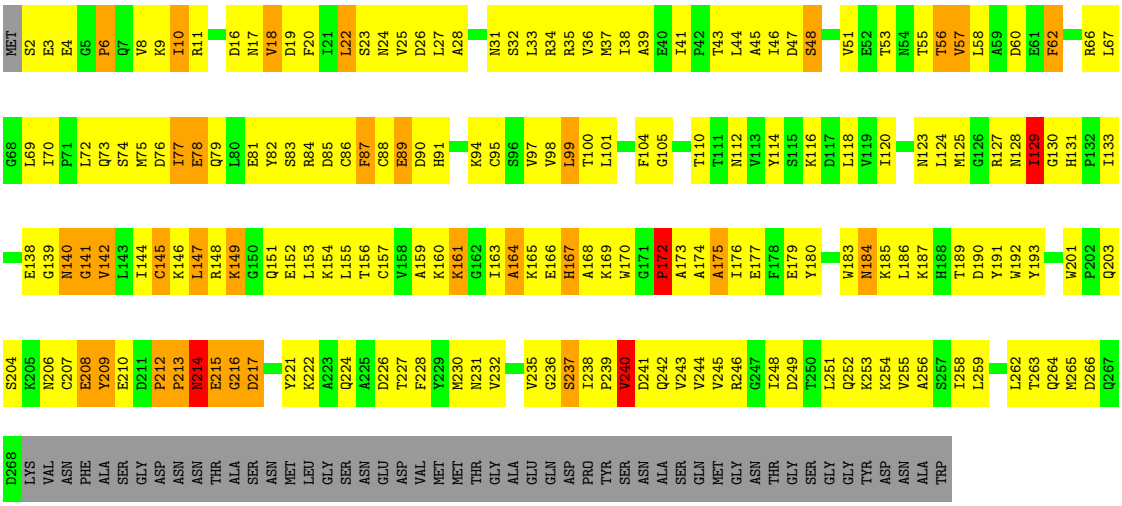




• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

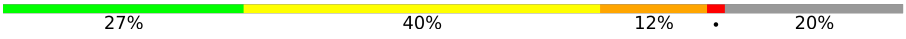
Chain C:

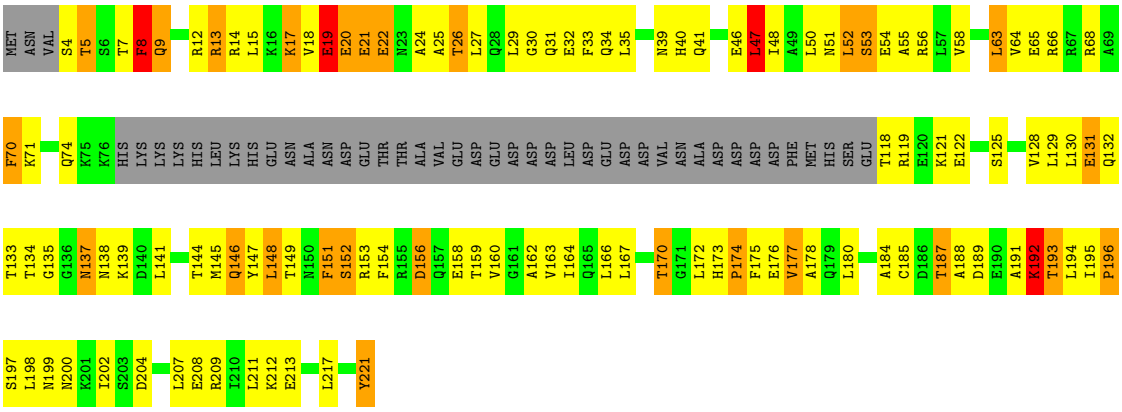




• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE

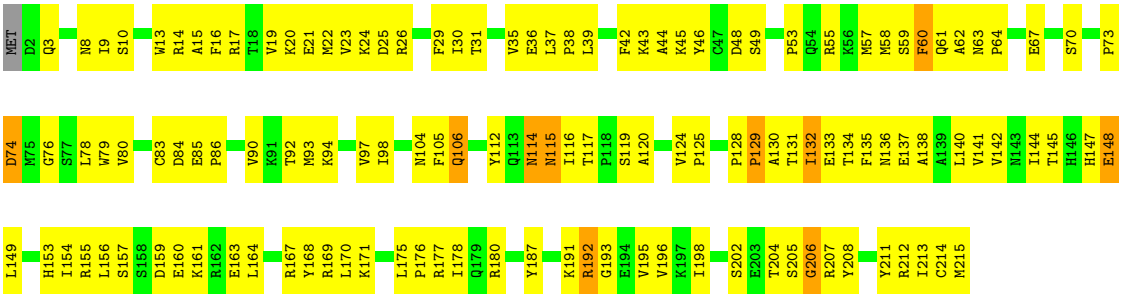
Chain D:





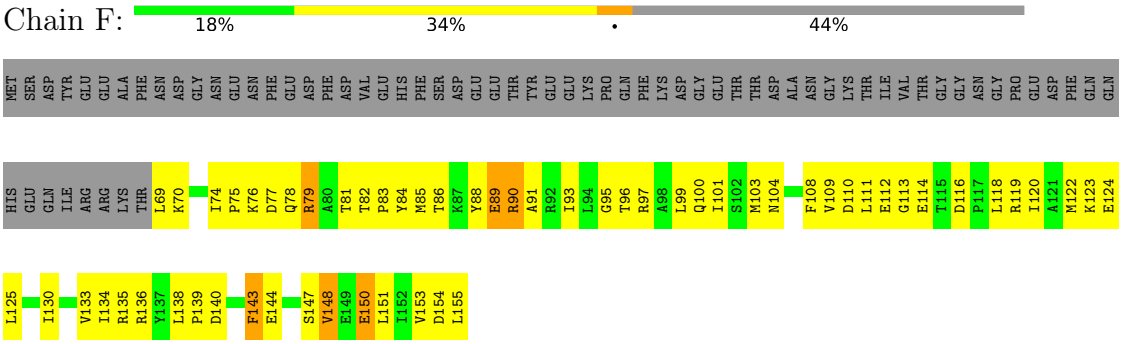
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

Chain E:



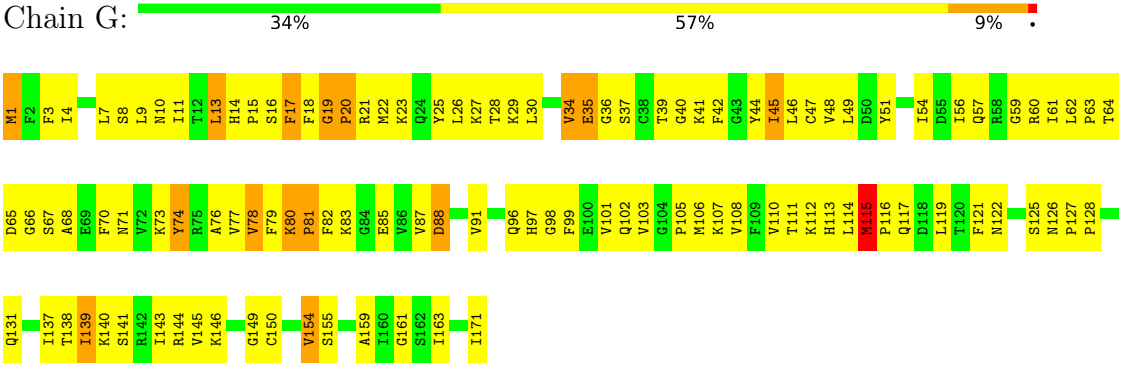
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain F:



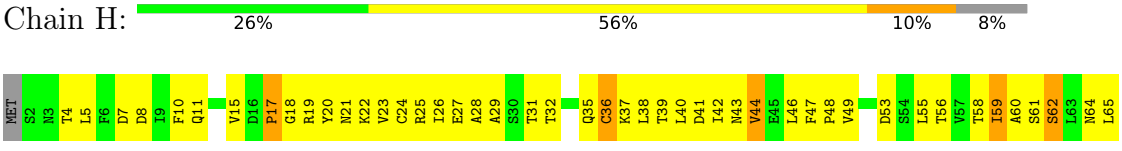
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

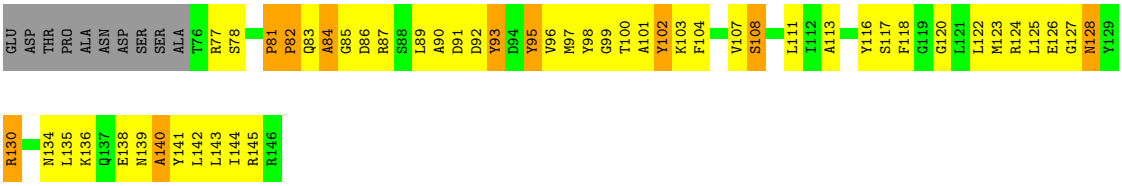
Chain G:



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

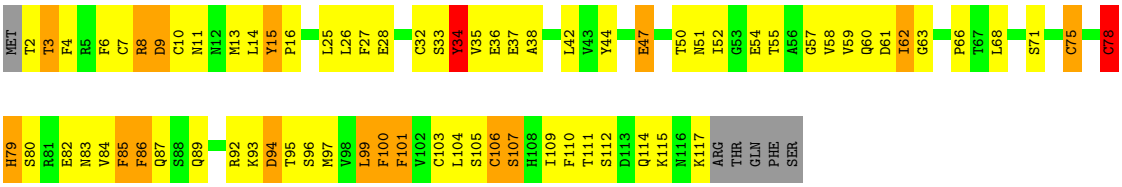
Chain H:





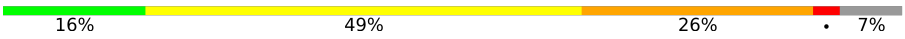
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

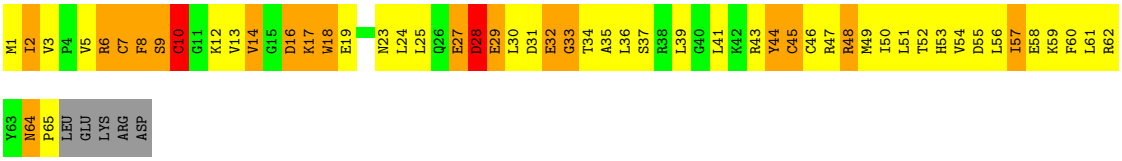
Chain I:



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

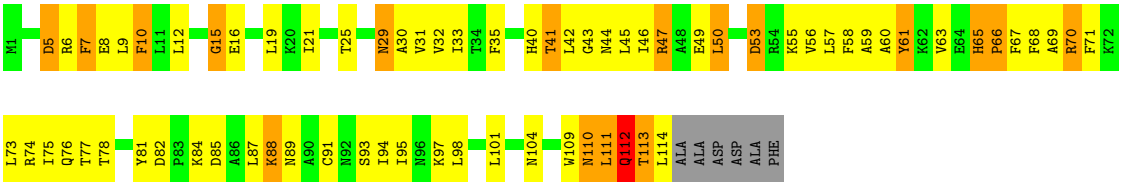
Chain J:





• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K:

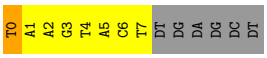


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L:

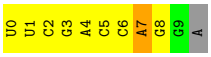
• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain N:



• Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

Chain P:



• Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TTP*TP*CP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain T:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	223.58Å 393.49Å 283.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00	Depositor
% Data completeness (in resolution range)	99.3 (50.00-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.292 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BRU, TT, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	0/11385	0.73	2/15393 (0.0%)
2	B	0.47	0/9037	0.71	2/12181 (0.0%)
3	C	0.47	0/2138	0.72	0/2896
4	D	0.44	0/1437	0.68	1/1925 (0.1%)
5	E	0.43	0/1788	0.63	0/2406
6	F	0.54	0/716	0.76	0/964
7	G	0.50	0/1368	0.73	0/1844
8	H	0.39	0/1102	0.66	0/1492
9	I	0.39	0/962	0.67	0/1295
10	J	0.50	0/541	0.80	1/727 (0.1%)
11	K	0.54	0/937	0.76	1/1265 (0.1%)
12	L	0.45	0/366	0.71	0/485
13	N	1.16	1/184 (0.5%)	1.01	0/280
14	P	0.63	0/237	1.01	0/367
15	T	1.09	1/382 (0.3%)	1.24	3/582 (0.5%)
All	All	0.49	2/32580 (0.0%)	0.73	10/44102 (0.0%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	0	DT	OP3-P	-6.79	1.53	1.61
15	T	21	DC	C3'-O3'	6.37	1.52	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1096	ARG	NE-CZ-NH1	-11.17	114.72	120.30
15	T	24	DG	O4'-C1'-N9	7.13	112.99	108.00
10	J	10	CYS	CA-CB-SG	6.47	125.65	114.00
11	K	113	THR	N-CA-C	6.47	128.47	111.00
15	T	28	DT	O4'-C1'-N1	5.56	111.89	108.00
15	T	19	DT	C5'-C4'-C3'	-5.43	104.33	114.10
1	A	425	GLN	N-CA-C	-5.40	96.42	111.00
2	B	1096	ARG	NE-CZ-NH2	5.32	122.96	120.30
4	D	26	THR	N-CA-C	-5.31	96.65	111.00
1	A	567	LYS	C-N-CD	5.10	139.10	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11186	0	11266	1369	0
2	B	8866	0	8898	1056	0
3	C	2101	0	2055	275	0
4	D	1427	0	1451	150	0
5	E	1752	0	1776	142	0
6	F	705	0	730	77	0
7	G	1340	0	1357	167	0
8	H	1084	0	1057	133	0
9	I	944	0	901	105	0
10	J	532	0	542	101	0
11	K	919	0	929	113	0
12	L	364	0	386	49	0
13	N	165	0	92	14	0
14	P	213	0	109	22	0
15	T	403	0	229	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32010	0	31778	3528	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 55.

All (3528) 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)
8:H:100:THR:HG23	8:H:138:GLU:HA	1.33	1.11
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.13	1.11
1:A:34:LYS:HD3	1:A:57:ARG:HH22	1.07	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	0.94	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.19	1.08
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.36	1.08
1:A:855:THR:HG21	1:A:857:ARG:HE	1.13	1.08
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.15	1.08
2:B:806:THR:HG22	2:B:808:ALA:H	1.11	1.07
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.25	1.07
2:B:467:GLY:H	2:B:475:SER:HB3	1.17	1.07
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.37	1.07
1:A:53:LEU:HD23	1:A:54:ASN:N	1.68	1.06
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.37	1.06
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.21	1.05
9:I:34:TYR:HD2	9:I:35:VAL:N	1.53	1.05
1:A:58:LEU:HD12	1:A:59:GLY:H	1.17	1.04
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.24	1.03
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.23	1.03
2:B:882:THR:HG22	2:B:884:ARG:H	1.20	1.03
2:B:65:GLU:HG3	2:B:66:ASP:H	1.21	1.02
2:B:515:HIS:H	2:B:518:HIS:HD2	1.07	1.02
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.36	1.02
2:B:214:ALA:HB3	2:B:498:THR:HA	1.42	1.02
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.23	1.02
2:B:589:VAL:HG12	2:B:590:HIS:H	1.22	1.01
7:G:15:PRO:HA	7:G:18:PHE:CD1	1.94	1.01
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.76	1.01
7:G:14:HIS:CD2	7:G:16:SER:HB2	1.95	1.01
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.44	1.00
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.43	1.00
1:A:524:VAL:HG12	1:A:525:GLN:H	1.25	1.00
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.25	0.99
10:J:1:MET:N	10:J:57:ILE:H	1.61	0.99
15:T:28:DT:H2"	15:T:29:DT:H5'	1.44	0.99
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.41	0.98
1:A:40:THR:HG22	1:A:41:MET:HG3	1.44	0.98
1:A:903:ASN:HD22	1:A:904:THR:N	1.62	0.98
15:T:16:DT:C6	15:T:17:TT:H5A2	1.98	0.98
4:D:144:THR:O	4:D:148:LEU:HB2	1.64	0.97
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.30	0.97
7:G:7:LEU:HB2	7:G:74:TYR:CE2	1.99	0.97
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.94	0.97
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.42	0.97
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.27	0.96
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.95	0.96
1:A:567:LYS:HB3	8:H:96:VAL:H	1.30	0.96
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.47	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.30	0.95
1:A:225:ASN:HD22	1:A:228:PHE:H	1.11	0.95
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.28	0.95
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.80	0.95
1:A:913:LEU:HD12	1:A:914:GLU:H	1.31	0.95
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.44	0.95
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.46	0.94
11:K:65:HIS:HD2	11:K:67:PHE:H	1.11	0.94
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.49	0.94
11:K:12:LEU:H	11:K:12:LEU:HD12	1.32	0.94
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.33	0.94
10:J:1:MET:H2	10:J:57:ILE:N	1.64	0.94
1:A:535:THR:HG21	1:A:616:VAL:HA	1.49	0.94
3:C:43:THR:HG22	3:C:44:LEU:H	1.29	0.94
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.48	0.94
1:A:709:THR:HG22	1:A:711:ARG:H	1.30	0.93
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.11	0.93
1:A:67:CYS:O	1:A:70:CYS:HB3	1.68	0.93
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.33	0.93
9:I:34:TYR:CD2	9:I:35:VAL:N	2.37	0.93
1:A:53:LEU:CD2	1:A:54:ASN:H	1.81	0.93
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.51	0.92
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.66	0.92
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.35	0.92
1:A:58:LEU:CD1	1:A:59:GLY:H	1.83	0.92
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.70	0.91
6:F:111:LEU:HD12	6:F:111:LEU:H	1.34	0.91
1:A:63:ARG:HA	1:A:74:MET:SD	2.09	0.91
1:A:754:SER:H	1:A:757:ASN:HD22	1.12	0.91
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.51	0.91
2:B:467:GLY:N	2:B:475:SER:HB3	1.84	0.91
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.35	0.91
3:C:47:ASP:HA	12:L:69:ALA:CB	2.01	0.90
9:I:85:PHE:H	9:I:85:PHE:HD2	1.19	0.90
1:A:901:LEU:H	1:A:926:GLN:NE2	1.69	0.90
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.53	0.90
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.51	0.90
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.36	0.90
15:T:17:TT:H4R	15:T:19:DT:OP2	1.69	0.90
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.87	0.90
8:H:4:THR:HA	8:H:60:ALA:HB2	1.53	0.89
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.52	0.89
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.08	0.89
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.07	0.89
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.89
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.54	0.89
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.52	0.89
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.55	0.88
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.87	0.88
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.88
8:H:36:CYS:HA	8:H:126:GLU:O	1.72	0.88
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.56	0.88
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.55	0.88
5:E:19:VAL:O	5:E:23:VAL:HG23	1.74	0.88
15:T:16:DT:C5	15:T:17:TT:H5A2	2.08	0.87
2:B:502:ILE:H	2:B:502:ILE:HD12	1.39	0.87
3:C:32:SER:O	3:C:36:VAL:HG23	1.74	0.87
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.05	0.87
14:P:5:C:H2'	14:P:6:C:O4'	1.74	0.87
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.56	0.87
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.55	0.87
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.55	0.87
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD12	2:B:113:TYR:H	1.40	0.87
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.08	0.87
4:D:134:THR:HG22	4:D:135:GLY:H	1.40	0.86
1:A:321:PRO:O	1:A:322:VAL:HB	1.76	0.86
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.55	0.86
2:B:1084:GLN:H	2:B:1084:GLN:NE2	1.73	0.86
14:P:6:C:H2'	14:P:7:A:C8	2.10	0.86
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.56	0.86
1:A:855:THR:HG21	1:A:857:ARG:NE	1.90	0.86
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.05	0.86
2:B:613:VAL:HG13	2:B:627:PHE:O	1.76	0.86
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.57	0.86
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.56	0.86
7:G:81:PRO:HG3	7:G:106:MET:SD	2.15	0.86
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.89	0.86
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.23	0.86
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.58	0.86
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.41	0.86
1:A:913:LEU:HD12	1:A:914:GLU:N	1.91	0.85
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.38	0.85
1:A:58:LEU:HD12	1:A:59:GLY:N	1.91	0.85
3:C:56:THR:HG22	3:C:57:VAL:H	1.40	0.85
2:B:515:HIS:H	2:B:518:HIS:CD2	1.95	0.85
2:B:806:THR:HG22	2:B:808:ALA:N	1.91	0.85
11:K:65:HIS:CD2	11:K:67:PHE:H	1.95	0.85
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.42	0.85
2:B:737:THR:HG21	9:I:66:PRO:HA	1.59	0.85
4:D:47:LEU:HD13	4:D:48:ILE:H	1.39	0.85
2:B:1085:ILE:N	2:B:1085:ILE:HD12	1.92	0.85
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.10	0.84
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.84
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.13	0.84
2:B:378:LEU:O	2:B:382:ILE:HG13	1.78	0.84
10:J:48:ARG:HE	10:J:49:MET:HE2	1.42	0.84
4:D:134:THR:HG22	4:D:135:GLY:N	1.92	0.84
15:T:28:DT:H2"	15:T:29:DT:C5'	2.08	0.84
2:B:549:THR:H	2:B:628:THR:HG23	1.40	0.84
2:B:654:ARG:H	2:B:657:HIS:HD2	1.22	0.84
1:A:70:CYS:O	1:A:72:GLU:HG2	1.76	0.84
1:A:1325:THR:O	5:E:148:GLU:HB2	1.78	0.84
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.77	0.83
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.14	0.83
15:T:27:DA:H2"	15:T:28:DT:H5'	1.58	0.83
2:B:98:THR:O	2:B:126:SER:HB2	1.77	0.83
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.93	0.83
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.60	0.83
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.94	0.83
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.90	0.82
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.61	0.82
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.59	0.82
2:B:879:ARG:NH1	2:B:883:LEU:HD22	1.94	0.82
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	1.95	0.82
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.62	0.82
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.43	0.82
15:T:16:DT:H72	15:T:17:TT:H5A3	1.61	0.82
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.10	0.82
6:F:82:THR:HG22	6:F:84:TYR:H	1.44	0.82
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.43	0.81
1:A:855:THR:CG2	1:A:857:ARG:HE	1.91	0.81
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.60	0.81
2:B:516:ASN:HD22	2:B:516:ASN:N	1.74	0.81
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
11:K:6:ARG:O	11:K:9:LEU:HG	1.80	0.81
1:A:646:PHE:O	1:A:650:GLN:HG3	1.80	0.81
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.11	0.81
2:B:46:GLN:HG3	2:B:47:GLN:H	1.45	0.81
9:I:50:THR:HG22	9:I:52:ILE:H	1.43	0.81
9:I:111:THR:HG22	9:I:112:SER:H	1.46	0.81
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.63	0.81
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.79	0.81
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.46	0.81
2:B:850:LEU:HD12	2:B:851:PHE:N	1.95	0.81
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.63	0.81
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.45	0.81
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.81	0.81
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.61	0.81
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.13	0.81
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.44	0.81
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.63	0.81
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.29	0.81
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG22	3:C:44:LEU:N	1.96	0.80
11:K:47:ARG:HB3	11:K:47:ARG:NH1	1.95	0.80
15:T:14:DC:H1'	15:T:15:DT:H5'	1.62	0.80
1:A:534:LEU:O	1:A:574:GLY:HA3	1.80	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.12	0.80
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.47	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.62	0.80
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.47	0.80
2:B:955:THR:HG22	2:B:956:THR:N	1.97	0.80
9:I:105:SER:O	9:I:106:CYS:HB3	1.80	0.80
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.62	0.80
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.15	0.80
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.64	0.80
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.97	0.80
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.17	0.80
2:B:863:GLU:OE2	2:B:873:THR:HA	1.82	0.80
1:A:768:GLN:CG	1:A:816:HIS:HA	2.11	0.80
1:A:1387:HIS:CE1	13:N:4:DT:H4'	2.17	0.80
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.63	0.79
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.48	0.79
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.63	0.79
6:F:69:LEU:HA	6:F:70:LYS:N	1.96	0.79
11:K:110:ASN:O	11:K:111:LEU:HD23	1.82	0.79
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.16	0.79
2:B:486:TYR:HE2	2:B:1096:ARG:HH12	1.31	0.79
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.46	0.79
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.65	0.79
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.81	0.79
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.64	0.79
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.65	0.79
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.63	0.79
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.63	0.79
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.79
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.63	0.79
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.47	0.79
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.65	0.79
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.65	0.79
1:A:524:VAL:HG12	1:A:525:GLN:N	1.98	0.79
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.63	0.79
1:A:34:LYS:CE	1:A:57:ARG:HH12	1.95	0.79
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.65	0.79
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.64	0.78
2:B:365:THR:HG23	2:B:367:LEU:H	1.48	0.78
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.63	0.78
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.66	0.78
2:B:850:LEU:HD12	2:B:851:PHE:H	1.49	0.78
1:A:450:LEU:HB3	1:A:838:GLN:NE2	1.99	0.78
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.83	0.78
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.19	0.78
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.64	0.78
2:B:65:GLU:HG3	2:B:66:ASP:N	1.99	0.78
10:J:8:PHE:H	10:J:49:MET:HE1	1.45	0.78
2:B:563:MET:HE3	2:B:580:VAL:HB	1.66	0.78
1:A:438:ASP:O	1:A:439:ASN:HB2	1.83	0.77
1:A:866:PHE:C	1:A:867:ILE:HD12	2.03	0.77
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.19	0.77
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.84	0.77
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.66	0.77
11:K:47:ARG:HH11	11:K:47:ARG:CB	1.96	0.77
2:B:114:PRO:HG2	2:B:115:GLN:H	1.50	0.77
1:A:567:LYS:HB3	8:H:96:VAL:N	1.98	0.77
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.64	0.77
3:C:172:PRO:O	3:C:235:VAL:HG23	1.84	0.77
5:E:213:ILE:HG12	5:E:214:CYS:H	1.47	0.77
15:T:27:DA:H2"	15:T:28:DT:C5'	2.13	0.77
1:A:903:ASN:ND2	1:A:905:ASP:H	1.81	0.77
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.67	0.77
2:B:467:GLY:H	2:B:475:SER:CB	1.96	0.77
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.00	0.77
8:H:59:ILE:HG22	8:H:60:ALA:N	1.98	0.77
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.65	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.99	0.77
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.85	0.77
2:B:189:LEU:O	2:B:192:LEU:N	2.16	0.77
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.85	0.77
15:T:22:BRU:H2'	15:T:23:DG:C8	2.20	0.77
1:A:254:GLU:HB2	2:B:935:ARG:NH1	1.99	0.76
1:A:450:LEU:H	1:A:450:LEU:HD12	1.50	0.76
3:C:73:GLN:NE2	3:C:74:SER:H	1.82	0.76
1:A:858:ASN:ND2	1:A:860:LEU:H	1.82	0.76
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:HG22	7:G:139:ILE:N	1.98	0.76
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.49	0.76
2:B:359:GLU:O	2:B:362:PRO:HD3	1.85	0.76
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.66	0.76
15:T:16:DT:H1'	15:T:17:TT:H5'1	1.66	0.76
2:B:486:TYR:CE2	2:B:1096:ARG:NH1	2.52	0.76
2:B:770:GLN:CD	2:B:983:ARG:HA	2.05	0.76
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.66	0.76
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.65	0.76
13:N:0:DT:H1'	13:N:1:DA:H5'	1.67	0.76
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.68	0.76
2:B:589:VAL:HG12	2:B:590:HIS:N	1.97	0.76
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.68	0.76
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.68	0.76
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.34	0.76
3:C:253:LYS:O	3:C:256:ALA:HB3	1.86	0.76
7:G:1:MET:SD	7:G:79:PHE:CD1	2.79	0.76
12:L:38:LEU:O	12:L:39:SER:HB3	1.84	0.76
1:A:61:ILE:HG22	1:A:62:ASP:H	1.50	0.76
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.84	0.76
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.67	0.76
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.20	0.76
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.85	0.76
1:A:588:LEU:O	1:A:606:LEU:HA	1.86	0.76
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.67	0.75
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.67	0.75
7:G:1:MET:SD	7:G:79:PHE:HD1	2.09	0.75
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.26	0.75
1:A:225:ASN:ND2	1:A:228:PHE:H	1.84	0.75
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.66	0.75
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.68	0.75
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.67	0.75
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.16	0.75
1:A:528:LEU:O	1:A:531:ILE:HG22	1.85	0.75
1:A:763:ALA:O	1:A:803:SER:HB3	1.87	0.75
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.34	0.75
14:P:6:C:H2'	14:P:7:A:H8	1.48	0.75
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.21	0.75
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.86	0.75
2:B:411:PRO:O	2:B:414:ALA:HB3	1.86	0.75
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.67	0.75
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.85	0.75
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.02	0.75
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.01	0.75
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.50	0.75
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.02	0.75
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.02	0.75
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.69	0.74
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.16	0.74
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.02	0.74
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.52	0.74
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.70	0.74
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.87	0.74
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.01	0.74
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.21	0.74
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.27	0.74
3:C:133:ILE:HD11	3:C:237:SER:HA	1.68	0.74
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.87	0.74
2:B:336:ARG:NH2	2:B:345:LYS:HE2	1.99	0.74
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.02	0.74
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.01	0.74
1:A:265:LYS:HD2	1:A:265:LYS:H	1.52	0.74
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.70	0.74
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.85	0.74
15:T:16:DT:H2"	15:T:17:TT:O2P	1.86	0.74
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.87	0.74
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.88	0.74
1:A:567:LYS:CB	8:H:95:TYR:HA	2.17	0.74
4:D:66:ARG:HD2	4:D:133:THR:HB	1.69	0.74
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.69	0.74
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.18	0.74
6:F:111:LEU:HD12	6:F:111:LEU:N	2.03	0.74
1:A:58:LEU:HD13	1:A:80:HIS:O	1.86	0.74
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.00	0.74
2:B:906:SER:O	2:B:941:LEU:HD23	1.88	0.74
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.68	0.74
1:A:385:ILE:HG22	1:A:386:ASP:N	2.02	0.73
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.50	0.73
2:B:776:GLN:HE22	14:P:8:G:H5'	1.51	0.73
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.19	0.73
2:B:343:ILE:HG21	2:B:348:ARG:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:GLU:O	2:B:961:LEU:HD22	1.87	0.73
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.73
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.52	0.73
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.70	0.73
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.53	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.52	0.73
1:A:886:ILE:HG22	1:A:887:GLY:N	2.04	0.73
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.24	0.73
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.88	0.73
1:A:853:ASP:O	1:A:854:ASN:HB2	1.89	0.73
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.88	0.73
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.18	0.73
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.89	0.73
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.01	0.73
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.68	0.73
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.19	0.73
1:A:885:THR:O	1:A:940:ARG:HD2	1.88	0.73
3:C:73:GLN:HE21	3:C:74:SER:H	1.37	0.73
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.73
1:A:858:ASN:C	1:A:858:ASN:HD22	1.87	0.73
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.73
1:A:1329:THR:HG22	1:A:1331:SER:N	2.04	0.73
1:A:68:GLN:C	1:A:70:CYS:H	1.92	0.72
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.72
3:C:147:LEU:HD12	3:C:151:GLN:O	1.89	0.72
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.24	0.72
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.03	0.72
1:A:472:LEU:O	1:A:475:THR:HB	1.90	0.72
1:A:541:ILE:HD13	1:A:549:MET:CE	2.19	0.72
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.89	0.72
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.71	0.72
1:A:19:PHE:O	1:A:1416:ALA:HA	1.89	0.72
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.29	0.72
2:B:825:VAL:CG1	2:B:826:ALA:N	2.51	0.72
3:C:147:LEU:N	3:C:147:LEU:HD23	2.03	0.72
15:T:17:TT:C3R	15:T:19:DT:H5"	2.20	0.72
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.52	0.72
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.71	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.04	0.72
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.19	0.72
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.69	0.72
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.55	0.72
6:F:111:LEU:C	6:F:113:GLY:H	1.92	0.72
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.20	0.72
1:A:115:LEU:O	1:A:122:MET:HE2	1.90	0.72
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.72	0.72
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.90	0.72
4:D:47:LEU:HD13	4:D:48:ILE:N	2.04	0.72
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.72	0.72
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.72	0.72
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.54	0.71
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.71	0.71
15:T:26:DC:H2"	15:T:27:DA:H5'	1.71	0.71
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.16	0.71
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.71
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.88	0.71
3:C:186:LEU:HD21	3:C:224:GLN:O	1.90	0.71
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.25	0.71
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.54	0.71
10:J:14:VAL:O	10:J:14:VAL:HG12	1.88	0.71
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.72	0.71
4:D:7:THR:HG21	4:D:32:GLU:CD	2.10	0.71
6:F:111:LEU:O	6:F:113:GLY:N	2.22	0.71
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.71	0.71
1:A:1329:THR:HG22	1:A:1331:SER:H	1.54	0.71
2:B:708:GLU:O	2:B:710:LEU:N	2.24	0.71
3:C:213:PRO:O	3:C:214:ASN:HB2	1.91	0.71
11:K:31:VAL:HG12	11:K:32:VAL:N	2.06	0.71
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.21	0.71
3:C:179:GLU:HG2	3:C:180:TYR:N	2.06	0.71
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.72	0.71
2:B:601:ARG:O	2:B:605:ARG:HG3	1.91	0.71
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.73	0.71
5:E:117:THR:HG22	5:E:119:SER:H	1.55	0.71
8:H:4:THR:HA	8:H:60:ALA:CB	2.20	0.71
8:H:64:ASN:O	8:H:65:LEU:HB2	1.89	0.71
1:A:743:VAL:O	1:A:747:VAL:HG23	1.91	0.71
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.73	0.71
3:C:208:GLU:O	3:C:210:GLU:N	2.24	0.71
1:A:106:VAL:HG13	1:A:112:LYS:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:H	1:A:233:TRP:HE3	1.38	0.70
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.56	0.70
2:B:955:THR:HG22	2:B:956:THR:H	1.53	0.70
11:K:53:ASP:OD1	11:K:55:LYS:HB2	1.91	0.70
1:A:92:HIS:O	1:A:94:GLY:N	2.24	0.70
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.72	0.70
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.73	0.70
2:B:756:ILE:O	2:B:759:PRO:HD3	1.92	0.70
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.73	0.70
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.22	0.70
4:D:189:ASP:O	4:D:193:THR:HB	1.91	0.70
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.32	0.70
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.74	0.70
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.72	0.70
9:I:75:CYS:SG	9:I:79:HIS:N	2.63	0.70
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	1.91	0.70
2:B:615:MET:C	2:B:616:ILE:HD12	2.12	0.70
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.20	0.70
8:H:61:SER:O	8:H:62:SER:HB3	1.91	0.70
2:B:365:THR:HG23	2:B:367:LEU:HG	1.71	0.70
6:F:125:LEU:HG	6:F:125:LEU:O	1.92	0.70
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.18	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.92	0.70
1:A:665:GLY:O	1:A:667:GLY:N	2.25	0.70
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.57	0.70
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.74	0.70
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.70
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.56	0.70
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.04	0.70
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.05	0.70
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.90	0.69
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.69
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.55	0.69
6:F:103:MET:O	6:F:104:ASN:HB2	1.91	0.69
7:G:111:THR:HG22	7:G:113:HIS:H	1.56	0.69
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.92	0.69
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.92	0.69
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.73	0.69
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.54	0.69
7:G:128:PRO:O	7:G:138:THR:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.57	0.69
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.27	0.69
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.89	0.69
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.74	0.69
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.07	0.69
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.75	0.69
1:A:35:ILE:HG22	1:A:35:ILE:O	1.91	0.69
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.73	0.69
10:J:48:ARG:HD2	10:J:49:MET:N	2.06	0.69
15:T:19:DT:H2"	15:T:20:DC:C5'	2.22	0.69
1:A:55:ASP:N	1:A:56:PRO:HD3	2.07	0.69
2:B:874:PHE:HA	2:B:913:GLY:O	1.91	0.69
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.23	0.69
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.23	0.69
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.72	0.69
4:D:176:GLU:C	4:D:178:ALA:H	1.95	0.69
5:E:202:SER:OG	5:E:204:THR:HG22	1.93	0.69
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.74	0.69
1:A:265:LYS:HD2	1:A:265:LYS:N	2.08	0.69
1:A:714:PHE:O	1:A:718:VAL:HG23	1.93	0.69
2:B:515:HIS:HD2	2:B:517:THR:H	1.39	0.69
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.28	0.69
1:A:1290:LYS:O	1:A:1291:VAL:HG23	1.92	0.69
2:B:168:GLY:H	2:B:450:ALA:HB1	1.57	0.69
3:C:2:SER:N	3:C:3:GLU:N	2.40	0.69
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.28	0.68
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.11	0.68
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.23	0.68
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.57	0.68
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.56	0.68
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.22	0.68
10:J:44:TYR:HA	10:J:47:ARG:CB	2.23	0.68
1:A:979:SER:OG	1:A:980:ASP:N	2.25	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	0.68
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.57	0.68
2:B:642:ASP:O	2:B:644:GLU:N	2.26	0.68
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.75	0.68
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.75	0.68
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.29	0.68
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.76	0.68
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.07	0.68
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.59	0.68
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.74	0.68
2:B:953:LEU:HD23	2:B:953:LEU:O	1.93	0.68
5:E:157:SER:OG	5:E:160:GLU:HG3	1.94	0.68
7:G:119:LEU:HD12	7:G:131:GLN:O	1.94	0.68
10:J:1:MET:H2	10:J:57:ILE:H	0.78	0.68
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.75	0.68
2:B:882:THR:HG22	2:B:884:ARG:N	2.02	0.68
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.57	0.68
13:N:1:DA:H2"	13:N:2:DA:OP2	1.93	0.68
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.28	0.68
4:D:138:ASN:OD1	4:D:141:LEU:HB2	1.94	0.68
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.24	0.68
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.29	0.68
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.23	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.59	0.68
2:B:516:ASN:N	2:B:516:ASN:ND2	2.41	0.68
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.59	0.68
5:E:114:ASN:O	5:E:115:ASN:HB3	1.92	0.68
1:A:658:LEU:HD13	2:B:831:SER:N	2.08	0.67
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.29	0.67
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.23	0.67
1:A:302:THR:HA	1:A:305:ASP:O	1.93	0.67
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.30	0.67
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.25	0.67
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.76	0.67
4:D:4:SER:OG	4:D:5:THR:N	2.27	0.67
9:I:13:MET:O	9:I:14:LEU:HD23	1.94	0.67
10:J:23:ASN:C	10:J:25:LEU:H	1.97	0.67
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.75	0.67
4:D:134:THR:CG2	4:D:135:GLY:H	2.06	0.67
6:F:76:LYS:O	6:F:79:ARG:HD3	1.95	0.67
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.24	0.67
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.22	0.67
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.76	0.67
2:B:295:GLY:H	2:B:298:LEU:HD23	1.57	0.67
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.75	0.67
1:A:869:GLY:O	5:E:204:THR:HG21	1.94	0.67
1:A:881:GLN:NE2	1:A:958:VAL:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HG2	2:B:747:MET:HB3	1.76	0.67
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.74	0.67
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.76	0.67
1:A:853:ASP:OD1	1:A:855:THR:N	2.28	0.67
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.10	0.67
2:B:314:LEU:O	2:B:317:CYS:HB3	1.95	0.67
1:A:50:ILE:C	1:A:52:GLY:H	1.99	0.67
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.09	0.67
1:A:1409:LEU:CD1	2:B:1207:LEU:HD11	2.23	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
8:H:59:ILE:HG22	8:H:60:ALA:H	1.60	0.67
1:A:69:THR:C	1:A:71:GLN:N	2.48	0.67
1:A:663:SER:OG	1:A:664:THR:N	2.24	0.67
1:A:709:THR:HG23	9:I:94:ASP:HA	1.77	0.67
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.76	0.67
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.29	0.67
1:A:254:GLU:O	1:A:256:GLN:N	2.27	0.66
1:A:548:ASN:OD1	11:K:60:ALA:HB1	1.95	0.66
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.25	0.66
3:C:179:GLU:HG2	3:C:180:TYR:H	1.60	0.66
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.30	0.66
15:T:17:TT:C4R	15:T:19:DT:OP2	2.43	0.66
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.78	0.66
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.77	0.66
2:B:336:ARG:NH2	2:B:345:LYS:HG2	2.10	0.66
10:J:44:TYR:HD2	10:J:44:TYR:N	1.94	0.66
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.30	0.66
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.30	0.66
1:A:709:THR:HG22	1:A:711:ARG:N	2.09	0.66
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.75	0.66
1:A:996:ASN:O	1:A:998:LEU:HD12	1.94	0.66
2:B:211:VAL:O	2:B:480:SER:HA	1.96	0.66
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.76	0.66
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.10	0.66
1:A:105:CYS:O	1:A:114:LEU:HG	1.95	0.66
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.77	0.66
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.66
3:C:244:VAL:O	3:C:248:ILE:HG13	1.95	0.66
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.25	0.66
13:N:3:DG:H1'	13:N:4:DT:H5'	1.77	0.66
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.30	0.66
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.59	0.66
2:B:37:PHE:HE2	2:B:542:MET:HA	1.60	0.66
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.78	0.66
2:B:880:THR:O	2:B:881:ASN:HB2	1.95	0.66
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.77	0.66
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.31	0.66
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.36	0.66
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.77	0.66
1:A:1293:SER:OG	1:A:1294:PRO:HD2	1.96	0.66
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.78	0.66
2:B:745:PRO:O	2:B:748:ILE:HG12	1.95	0.66
3:C:18:VAL:HG12	3:C:18:VAL:O	1.94	0.66
1:A:666:ILE:HD12	1:A:667:GLY:H	1.61	0.66
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.78	0.66
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.77	0.66
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.77	0.66
1:A:384:ASN:O	1:A:386:ASP:N	2.28	0.66
2:B:180:TYR:HD1	2:B:180:TYR:H	1.44	0.66
3:C:226:ASP:O	3:C:227:THR:HB	1.96	0.66
8:H:38:LEU:HD12	8:H:124:ARG:O	1.96	0.66
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.61	0.66
15:T:17:TT:H5R1	15:T:17:TT:H1'	1.77	0.66
1:A:347:PHE:H	2:B:1107:ALA:HA	1.61	0.66
1:A:512:VAL:HA	1:A:519:PRO:HA	1.77	0.66
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.66
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.11	0.66
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.77	0.66
1:A:728:LYS:O	1:A:732:LEU:HG	1.96	0.65
2:B:557:PHE:C	2:B:557:PHE:CD2	2.69	0.65
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.78	0.65
10:J:2:ILE:HG22	10:J:3:VAL:O	1.95	0.65
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.30	0.65
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.10	0.65
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.62	0.65
2:B:975:GLN:HG2	2:B:976:ILE:H	1.62	0.65
8:H:142:LEU:C	8:H:143:LEU:HD12	2.17	0.65
1:A:84:ILE:O	1:A:84:ILE:HG23	1.96	0.65
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.78	0.65
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.64	0.65
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:HD12	6:F:118:LEU:O	1.97	0.65
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.61	0.65
3:C:69:LEU:N	3:C:69:LEU:HD12	2.11	0.65
2:B:1023:VAL:O	2:B:1026:LEU:N	2.29	0.65
15:T:17:TT:C3R	15:T:19:DT:C5'	2.74	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.65
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.31	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.32	0.65
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.27	0.65
2:B:582:VAL:HA	2:B:626:ILE:O	1.97	0.65
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.26	0.65
3:C:66:ARG:NH2	10:J:3:VAL:O	2.29	0.65
4:D:118:THR:HB	4:D:121:LYS:HB2	1.79	0.65
15:T:24:DG:H2"	15:T:25:DT:O5'	1.97	0.65
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.65
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.60	0.65
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.78	0.65
1:A:144:THR:O	1:A:146:MET:HG3	1.96	0.65
1:A:675:THR:O	1:A:679:ILE:HG13	1.97	0.65
1:A:741:ASN:HD22	1:A:744:LYS:H	1.45	0.65
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.96	0.65
2:B:871:THR:HG22	2:B:872:GLU:O	1.97	0.65
4:D:22:GLU:H	4:D:22:GLU:CD	1.99	0.65
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.65
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.97	0.65
1:A:590:ARG:O	1:A:591:PHE:HB2	1.97	0.65
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.31	0.65
2:B:344:LYS:O	2:B:345:LYS:HB2	1.95	0.65
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.79	0.65
15:T:19:DT:H2"	15:T:20:DC:H5'	1.77	0.65
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.13	0.65
15:T:26:DC:H2"	15:T:27:DA:C5'	2.27	0.65
1:A:69:THR:C	1:A:71:GLN:H	1.97	0.64
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.62	0.64
2:B:336:ARG:CD	2:B:348:ARG:HH11	2.09	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.05	0.64
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.78	0.64
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.97	0.64
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.27	0.64
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.79	0.64
11:K:15:GLY:O	11:K:16:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG22	1:A:1240:CYS:CB	2.28	0.64
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.80	0.64
10:J:1:MET:H1	10:J:56:LEU:N	1.95	0.64
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.32	0.64
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.33	0.64
1:A:903:ASN:HD22	1:A:903:ASN:C	2.00	0.64
1:A:960:ILE:O	1:A:963:ILE:HG22	1.97	0.64
1:A:965:GLN:O	1:A:968:GLN:HB2	1.98	0.64
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.28	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.64
2:B:57:TYR:N	2:B:57:TYR:HD1	1.95	0.64
2:B:843:GLN:N	2:B:994:TYR:O	2.26	0.64
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.62	0.64
2:B:57:TYR:N	2:B:57:TYR:CD1	2.65	0.64
2:B:616:ILE:HD12	2:B:616:ILE:N	2.13	0.64
11:K:12:LEU:HD12	11:K:12:LEU:N	2.11	0.64
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.24	0.64
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.61	0.64
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.33	0.64
4:D:53:SER:HB3	4:D:153:ARG:H	1.61	0.64
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.26	0.64
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.79	0.64
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.97	0.64
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.33	0.64
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.32	0.64
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.12	0.64
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.64
8:H:44:VAL:O	8:H:44:VAL:HG12	1.98	0.64
15:T:15:DT:C5	15:T:16:DT:H73	2.32	0.64
1:A:320:ARG:NH2	14:P:1:U:O2'	2.31	0.64
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.96	0.64
1:A:1437:GLY:O	1:A:1439:GLY:N	2.31	0.64
2:B:305:VAL:O	2:B:305:VAL:HG12	1.98	0.64
2:B:821:GLN:HE22	2:B:851:PHE:CA	2.09	0.64
4:D:191:ALA:O	4:D:193:THR:N	2.31	0.64
8:H:89:LEU:C	8:H:91:ASP:H	2.01	0.64
13:N:6:DC:H2"	13:N:7:DT:OP2	1.97	0.64
15:T:15:DT:C6	15:T:16:DT:C7	2.80	0.64
1:A:41:MET:HB3	1:A:48:ALA:O	1.98	0.64
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.98	0.64
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.78	0.64
1:A:69:THR:O	1:A:71:GLN:N	2.30	0.64
1:A:658:LEU:HD13	2:B:831:SER:H	1.62	0.64
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.80	0.64
2:B:955:THR:HG23	12:L:54:ARG:O	1.97	0.64
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.62	0.64
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.13	0.64
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.80	0.64
15:T:16:DT:H1'	15:T:17:TT:C5'	2.28	0.64
1:A:55:ASP:C	1:A:57:ARG:H	2.01	0.63
1:A:108:MET:N	1:A:108:MET:SD	2.71	0.63
1:A:877:HIS:O	1:A:878:ILE:HG12	1.99	0.63
2:B:217:ARG:HD2	2:B:217:ARG:C	2.19	0.63
2:B:520:GLY:H	2:B:748:ILE:HG22	1.62	0.63
2:B:770:GLN:HG2	2:B:983:ARG:O	1.97	0.63
2:B:950:ASP:O	2:B:951:GLN:HB2	1.98	0.63
10:J:44:TYR:N	10:J:44:TYR:CD2	2.65	0.63
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.79	0.63
1:A:164:ARG:HG3	1:A:165:GLY:N	2.12	0.63
3:C:31:ASN:O	3:C:34:ARG:HB3	1.98	0.63
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.80	0.63
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.63
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.79	0.63
6:F:103:MET:CE	7:G:66:GLY:H	2.11	0.63
7:G:1:MET:HE1	7:G:80:LYS:H	1.62	0.63
1:A:401:GLY:C	1:A:435:HIS:HD2	2.02	0.63
1:A:471:ASN:OD1	1:A:472:LEU:N	2.31	0.63
1:A:979:SER:OG	1:A:981:LEU:HG	1.98	0.63
2:B:278:GLN:HG2	2:B:279:ASP:H	1.62	0.63
2:B:842:ASN:ND2	2:B:845:SER:H	1.96	0.63
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.13	0.63
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.63
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.98	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
2:B:121:ASN:HA	2:B:207:GLY:CA	2.27	0.63
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.63	0.63
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.09	0.63
1:A:55:ASP:CG	1:A:55:ASP:O	2.33	0.63
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.33	0.63
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.34	0.63
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:CG2	2:B:956:THR:H	2.12	0.63
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.28	0.63
4:D:176:GLU:O	4:D:178:ALA:N	2.32	0.63
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.29	0.63
9:I:52:ILE:HG13	9:I:52:ILE:O	1.97	0.63
1:A:475:THR:HG23	1:A:476:SER:N	2.13	0.63
1:A:745:GLN:HA	1:A:748:MET:HE3	1.81	0.63
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.14	0.63
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.64	0.63
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.29	0.63
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.81	0.63
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.81	0.63
11:K:61:TYR:C	11:K:61:TYR:CD2	2.71	0.63
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.81	0.63
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.34	0.63
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.63
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.81	0.62
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.62	0.62
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.33	0.62
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.34	0.62
4:D:130:LEU:O	4:D:132:GLN:N	2.30	0.62
11:K:12:LEU:H	11:K:12:LEU:CD1	2.11	0.62
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.80	0.62
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.99	0.62
1:A:782:ARG:NH2	2:B:699:GLU:O	2.31	0.62
2:B:563:MET:CE	2:B:580:VAL:HB	2.28	0.62
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.62
7:G:83:LYS:HE2	7:G:150:CYS:H	1.64	0.62
10:J:8:PHE:H	10:J:49:MET:CE	2.10	0.62
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.79	0.62
1:A:381:THR:CG2	1:A:383:TYR:H	2.12	0.62
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.34	0.62
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.62
6:F:114:GLU:OE2	6:F:119:ARG:HG2	1.99	0.62
7:G:80:LYS:HD3	7:G:80:LYS:N	2.14	0.62
8:H:127:GLY:O	8:H:128:ASN:HB2	1.99	0.62
8:H:130:ARG:H	8:H:130:ARG:HD2	1.64	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.99	0.62
1:A:384:ASN:O	1:A:385:ILE:C	2.37	0.62
7:G:143:ILE:HG22	7:G:144:ARG:N	2.13	0.62
1:A:37:PHE:N	1:A:37:PHE:CD1	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.82	0.62
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.63	0.62
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.00	0.62
3:C:164:ALA:HA	3:C:167:HIS:O	1.99	0.62
15:T:17:TT:H3R	15:T:19:DT:H5"	1.79	0.62
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.12	0.62
1:A:381:THR:HG22	1:A:383:TYR:H	1.64	0.62
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.82	0.62
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.16	0.62
3:C:183:TRP:O	3:C:185:LYS:N	2.33	0.62
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.12	0.62
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.81	0.62
1:A:450:LEU:HD12	1:A:450:LEU:N	2.14	0.62
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.34	0.62
5:E:157:SER:C	5:E:159:ASP:H	2.02	0.62
6:F:103:MET:HE2	7:G:66:GLY:H	1.64	0.62
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.35	0.62
11:K:46:ILE:O	11:K:50:LEU:HB2	1.98	0.62
11:K:111:LEU:O	11:K:112:GLN:NE2	2.30	0.62
1:A:446:ARG:HB2	1:A:487:MET:SD	2.40	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.62
1:A:844:ALA:C	1:A:845:LEU:HD23	2.20	0.62
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.82	0.62
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.99	0.62
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.35	0.62
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.80	0.62
8:H:62:SER:C	8:H:64:ASN:H	2.03	0.62
1:A:825:ILE:HG22	1:A:826:ASP:N	2.14	0.62
9:I:13:MET:HG3	9:I:14:LEU:N	2.15	0.62
1:A:353:ILE:HG21	1:A:487:MET:CE	2.25	0.61
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.80	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.15	0.61
2:B:737:THR:CG2	9:I:66:PRO:HA	2.29	0.61
4:D:5:THR:O	4:D:5:THR:HG23	2.00	0.61
10:J:44:TYR:HD2	10:J:44:TYR:H	1.48	0.61
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.34	0.61
15:T:16:DT:C1'	15:T:17:TT:H5'1	2.29	0.61
1:A:466:SER:O	2:B:1103:ILE:HD11	2.00	0.61
1:A:546:VAL:O	1:A:550:LEU:HG	2.01	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.35	0.61
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.13	0.61
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.61
7:G:18:PHE:HA	7:G:22:MET:HE2	1.82	0.61
10:J:32:GLU:CD	10:J:32:GLU:H	2.03	0.61
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.00	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.35	0.61
4:D:191:ALA:C	4:D:193:THR:H	2.03	0.61
1:A:164:ARG:HG3	1:A:165:GLY:H	1.65	0.61
1:A:1013:ASP:O	1:A:1015:VAL:N	2.33	0.61
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.30	0.61
8:H:41:ASP:O	8:H:42:ILE:HG13	2.00	0.61
1:A:698:GLN:HA	9:I:97:MET:O	2.00	0.61
1:A:901:LEU:O	1:A:921:GLY:N	2.29	0.61
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.61
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.81	0.61
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.29	0.61
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.15	0.61
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.00	0.61
2:B:35:SER:HA	2:B:811:TYR:HE2	1.65	0.61
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.16	0.61
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.81	0.61
2:B:1022:THR:HG23	2:B:1022:THR:O	1.99	0.61
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.47	0.61
2:B:1174:LYS:O	2:B:1176:ASN:N	2.34	0.61
4:D:128:VAL:O	4:D:132:GLN:HG3	2.01	0.61
4:D:195:ILE:O	4:D:197:SER:N	2.34	0.61
1:A:12:ARG:NE	2:B:1192:TYR:HE2	1.98	0.61
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.16	0.61
2:B:549:THR:N	2:B:628:THR:HG23	2.14	0.61
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.31	0.61
3:C:73:GLN:HE21	3:C:74:SER:N	1.98	0.61
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.81	0.61
15:T:16:DT:H2"	15:T:17:TT:H5'1	1.83	0.61
2:B:221:ASN:N	2:B:241:ARG:O	2.28	0.61
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.83	0.61
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.00	0.61
2:B:955:THR:CG2	2:B:956:THR:N	2.63	0.61
3:C:100:THR:HG22	3:C:101:LEU:N	2.15	0.61
12:L:39:SER:O	12:L:40:LEU:HG	2.00	0.61
1:A:252:PHE:O	1:A:253:ASN:HB2	2.01	0.61
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.83	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	2.01	0.61
1:A:866:PHE:O	1:A:867:ILE:HD12	2.00	0.61
1:A:1436:ILE:O	1:A:1437:GLY:C	2.39	0.61
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.30	0.61
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.35	0.61
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.66	0.61
6:F:69:LEU:N	6:F:70:LYS:CA	2.64	0.61
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.41	0.61
1:A:264:PHE:O	1:A:267:ALA:HB3	2.01	0.61
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.30	0.61
7:G:145:VAL:HG12	7:G:146:LYS:N	2.14	0.61
11:K:10:PHE:N	11:K:10:PHE:CD2	2.69	0.61
12:L:31:CYS:SG	12:L:34:CYS:N	2.72	0.61
1:A:4:GLN:O	1:A:5:GLN:HB2	2.01	0.60
1:A:68:GLN:O	1:A:70:CYS:N	2.33	0.60
1:A:456:MET:HB2	1:A:478:TYR:OH	2.01	0.60
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.30	0.60
2:B:357:GLN:O	2:B:366:GLN:HA	2.00	0.60
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.83	0.60
2:B:830:TYR:O	2:B:832:GLY:N	2.34	0.60
14:P:4:A:O2'	14:P:5:C:H5'	2.01	0.60
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.65	0.60
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.67	0.60
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.01	0.60
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.83	0.60
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.16	0.60
1:A:720:ARG:O	1:A:724:GLU:HB2	2.01	0.60
1:A:1193:LEU:HD22	1:A:1260:LEU:HD11	1.82	0.60
2:B:123:THR:O	2:B:125:SER:N	2.33	0.60
2:B:434:ARG:O	2:B:437:GLU:HB2	2.02	0.60
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.60	0.60
4:D:130:LEU:C	4:D:132:GLN:H	2.04	0.60
15:T:13:DA:H1'	15:T:14:DC:H5'	1.83	0.60
1:A:244:PRO:O	1:A:246:VAL:N	2.34	0.60
1:A:311:GLN:O	1:A:312:PRO:C	2.39	0.60
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.83	0.60
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.49	0.60
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.67	0.60
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.81	0.60
5:E:29:PHE:O	5:E:30:ILE:HG13	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:ILE:HG22	5:E:31:THR:N	2.16	0.60
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.60
1:A:567:LYS:CG	1:A:568:PRO:CD	2.77	0.60
1:A:1329:THR:CG2	1:A:1331:SER:H	2.15	0.60
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.83	0.60
4:D:53:SER:CB	4:D:153:ARG:H	2.14	0.60
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.83	0.60
9:I:13:MET:HG3	9:I:14:LEU:H	1.64	0.60
1:A:321:PRO:O	1:A:322:VAL:CB	2.48	0.60
2:B:833:TYR:N	2:B:833:TYR:CD1	2.67	0.60
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.37	0.60
7:G:115:MET:HB3	7:G:163:ILE:HD11	1.83	0.60
8:H:56:THR:HB	8:H:145:ARG:HG2	1.83	0.60
15:T:15:DT:H1'	15:T:16:DT:H5'	1.84	0.60
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.83	0.60
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.60
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.36	0.60
2:B:769:TYR:O	2:B:772:ALA:N	2.34	0.60
4:D:170:THR:CG2	4:D:172:LEU:HG	2.31	0.60
15:T:16:DT:C5	15:T:17:TT:C5A	2.84	0.60
2:B:801:LYS:O	10:J:52:THR:HG23	2.01	0.60
8:H:93:TYR:HB3	8:H:144:ILE:O	2.01	0.60
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.83	0.60
11:K:47:ARG:C	11:K:47:ARG:HD2	2.22	0.60
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.17	0.60
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.67	0.60
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.84	0.60
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.02	0.60
7:G:49:LEU:HG	7:G:76:ALA:HA	1.81	0.60
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.32	0.60
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.32	0.60
1:A:968:GLN:O	1:A:970:THR:N	2.35	0.60
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.60
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.49	0.60
2:B:1180:PHE:O	2:B:1181:GLU:O	2.20	0.60
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.32	0.59
1:A:345:VAL:HG23	1:A:346:ASP:O	2.02	0.59
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.84	0.59
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.35	0.59
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.62	0.59
2:B:654:ARG:N	2:B:657:HIS:HD2	1.97	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.70	0.59
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.30	0.59
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.02	0.59
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.62	0.59
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.83	0.59
2:B:192:LEU:O	2:B:193:LYS:HB2	2.02	0.59
2:B:654:ARG:H	2:B:657:HIS:CD2	2.11	0.59
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.84	0.59
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.67	0.59
2:B:825:VAL:HG13	2:B:826:ALA:H	1.66	0.59
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.84	0.59
7:G:18:PHE:HA	7:G:22:MET:CE	2.32	0.59
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.85	0.59
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.83	0.59
1:A:524:VAL:CG1	1:A:525:GLN:HE21	2.15	0.59
1:A:915:SER:O	1:A:919:ILE:HG13	2.02	0.59
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.84	0.59
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.00	0.59
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.85	0.59
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.67	0.59
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.36	0.59
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.83	0.59
6:F:69:LEU:CA	6:F:70:LYS:N	2.64	0.59
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.38	0.59
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.17	0.59
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.59
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.18	0.59
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.71	0.59
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.85	0.59
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.83	0.59
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.67	0.59
3:C:167:HIS:HD2	3:C:168:ALA:H	1.51	0.59
6:F:111:LEU:H	6:F:111:LEU:CD1	2.10	0.59
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.59
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.33	0.59
1:A:907:THR:CG2	1:A:908:LEU:N	2.65	0.59
1:A:940:ARG:HG2	1:A:940:ARG:HH11	1.67	0.59
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.32	0.59
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.01	0.59
2:B:23:ALA:H	2:B:654:ARG:HB3	1.67	0.59
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:O	1:A:96:ILE:C	2.41	0.59
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.15	0.59
2:B:125:SER:HA	2:B:171:PRO:HA	1.84	0.59
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.37	0.59
3:C:133:ILE:CD1	3:C:237:SER:HA	2.31	0.59
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.84	0.59
1:A:534:LEU:O	1:A:534:LEU:HG	2.01	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.42	0.59
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.35	0.59
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.02	0.59
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.37	0.59
1:A:317:LYS:O	1:A:318:SER:HB3	2.03	0.59
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.38	0.59
1:A:482:PHE:C	1:A:484:GLY:H	2.05	0.59
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.17	0.59
5:E:78:LEU:HD23	5:E:79:TRP:N	2.18	0.59
7:G:80:LYS:O	7:G:80:LYS:HG2	2.01	0.59
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.85	0.58
1:A:774:ARG:O	1:A:775:ILE:C	2.41	0.58
1:A:929:LEU:HD21	1:A:983:ILE:HD13	1.85	0.58
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.22	0.58
2:B:816:GLU:O	2:B:817:LEU:HD23	2.03	0.58
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.86	0.58
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.37	0.58
8:H:89:LEU:O	8:H:91:ASP:N	2.36	0.58
1:A:42:ASP:HB3	1:A:45:GLN:H	1.68	0.58
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.17	0.58
1:A:353:ILE:CG2	1:A:487:MET:HE3	2.27	0.58
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.12	0.58
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.33	0.58
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.03	0.58
7:G:149:GLY:O	7:G:159:ALA:HB1	2.03	0.58
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.38	0.58
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.31	0.58
2:B:843:GLN:O	2:B:844:SER:C	2.42	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.18	0.58
2:B:1045:SER:O	2:B:1046:PRO:O	2.21	0.58
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.34	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.30	0.58
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.33	0.58
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.34	0.58
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.84	0.58
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.58
4:D:7:THR:HB	7:G:42:PHE:CE2	2.39	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.67	0.58
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.58
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.34	0.58
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.18	0.58
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.18	0.58
2:B:112:LEU:HD12	2:B:113:TYR:N	2.15	0.58
2:B:1008:PRO:HB2	2:B:1010:LEU:O	2.03	0.58
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.85	0.58
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.03	0.58
1:A:7:SER:C	1:A:9:ALA:H	2.06	0.58
1:A:23:SER:HA	1:A:233:TRP:CD1	2.39	0.58
2:B:185:THR:H	2:B:188:ASP:HB2	1.69	0.58
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.86	0.58
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.16	0.58
11:K:93:SER:O	11:K:97:LYS:HG3	2.04	0.58
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.39	0.58
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.34	0.58
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.66	0.58
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.19	0.58
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.68	0.58
3:C:263:THR:C	3:C:265:MET:H	2.07	0.58
7:G:1:MET:SD	7:G:1:MET:O	2.62	0.58
10:J:7:CYS:SG	10:J:8:PHE:N	2.76	0.58
1:A:1409:LEU:HD13	2:B:1207:LEU:CD1	2.30	0.58
2:B:680:THR:O	2:B:684:LEU:HD12	2.02	0.58
2:B:731:VAL:HG12	2:B:732:SER:N	2.18	0.58
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.33	0.58
4:D:160:VAL:O	4:D:164:ILE:HG13	2.04	0.58
7:G:39:THR:HG22	7:G:40:GLY:N	2.18	0.58
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.33	0.58
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.32	0.58
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.58
2:B:25:ILE:HD11	2:B:653:VAL:O	2.03	0.58
2:B:705:MET:H	2:B:710:LEU:HD12	1.69	0.58
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.58
3:C:73:GLN:HB3	3:C:131:HIS:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:GLN:O	4:D:47:LEU:HD23	2.04	0.58
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.33	0.58
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.69	0.58
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.58
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.69	0.58
2:B:687:GLU:O	2:B:689:LEU:HG	2.04	0.58
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.33	0.58
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.83	0.57
2:B:265:SER:O	2:B:266:ALA:HB3	2.03	0.57
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.39	0.57
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.17	0.57
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.57
4:D:56:ARG:HD3	4:D:149:THR:HA	1.87	0.57
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.19	0.57
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.32	0.57
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.85	0.57
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.34	0.57
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.40	0.57
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.34	0.57
1:A:1064:VAL:O	1:A:1067:LEU:HB3	2.04	0.57
2:B:797:TYR:HB2	2:B:852:ARG:O	2.04	0.57
2:B:847:ASP:C	2:B:849:GLY:H	2.06	0.57
2:B:882:THR:HB	2:B:934:LYS:O	2.04	0.57
8:H:95:TYR:HE2	8:H:97:MET:CG	2.18	0.57
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.68	0.57
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.34	0.57
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.34	0.57
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.86	0.57
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.33	0.57
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.23	0.57
6:F:77:ASP:C	6:F:79:ARG:H	2.06	0.57
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.33	0.57
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.34	0.57
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.39	0.57
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.15	0.57
2:B:1176:ASN:C	2:B:1178:ASN:H	2.08	0.57
3:C:18:VAL:O	3:C:20:PHE:HD2	1.87	0.57
15:T:16:DT:H72	15:T:17:TT:C5A	2.31	0.57
1:A:42:ASP:HA	1:A:46:THR:O	2.05	0.57
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.33	0.57
1:A:406:ILE:HG22	1:A:412:ARG:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.20	0.57
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.39	0.57
7:G:39:THR:HG22	7:G:40:GLY:H	1.68	0.57
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.40	0.57
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.04	0.57
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.38	0.57
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.35	0.57
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.07	0.57
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.37	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.52	0.57
1:A:282:ASN:O	1:A:284:ALA:N	2.38	0.57
1:A:442:VAL:O	1:A:457:ALA:HA	2.05	0.57
1:A:469:ARG:HH11	1:A:469:ARG:HB3	1.69	0.57
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.04	0.57
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.57
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.39	0.57
4:D:64:VAL:C	4:D:66:ARG:H	2.07	0.57
4:D:71:LYS:HA	4:D:74:GLN:CB	2.32	0.57
5:E:10:SER:O	5:E:14:ARG:HG3	2.04	0.57
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.39	0.57
2:B:954:VAL:O	12:L:55:ILE:O	2.22	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.04	0.57
6:F:143:PHE:C	6:F:143:PHE:CD1	2.77	0.57
15:T:16:DT:C2'	15:T:17:TT:H5'1	2.34	0.57
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.40	0.57
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.39	0.57
2:B:336:ARG:HD3	2:B:348:ARG:NH1	2.18	0.57
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.04	0.57
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.38	0.57
3:C:35:ARG:NH1	11:K:41:THR:N	2.53	0.57
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.40	0.57
14:P:1:U:H2'	14:P:2:C:C6	2.39	0.57
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.86	0.57
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.86	0.57
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.40	0.57
2:B:126:SER:O	2:B:169:ARG:HA	2.03	0.57
2:B:557:PHE:C	2:B:557:PHE:HD2	2.08	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.88	0.57
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.69	0.57
2:B:873:THR:O	2:B:914:LYS:HA	2.04	0.57
2:B:916:THR:O	2:B:935:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1181:GLU:HG3	2:B:1188:LYS:HE3	1.85	0.57
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.86	0.57
4:D:4:SER:O	4:D:5:THR:HB	2.04	0.57
10:J:48:ARG:HE	10:J:49:MET:CE	2.13	0.57
1:A:399:HIS:O	1:A:401:GLY:N	2.37	0.56
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.30	0.56
1:A:596:THR:O	1:A:598:LEU:N	2.37	0.56
1:A:761:MET:HA	1:A:804:TYR:HB2	1.87	0.56
1:A:986:ILE:HG22	1:A:987:VAL:N	2.18	0.56
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.19	0.56
2:B:44:VAL:O	2:B:45:SER:C	2.44	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.39	0.56
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.20	0.56
8:H:4:THR:O	8:H:5:LEU:HD23	2.04	0.56
14:P:7:A:H2'	14:P:8:G:C8	2.40	0.56
15:T:19:DT:H2"	15:T:20:DC:O5'	2.05	0.56
1:A:17:VAL:HA	2:B:1215:ARG:O	2.05	0.56
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.70	0.56
1:A:353:ILE:HD13	1:A:487:MET:CE	2.34	0.56
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.05	0.56
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.86	0.56
2:B:378:LEU:O	2:B:378:LEU:HD12	2.03	0.56
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.86	0.56
3:C:47:ASP:CA	12:L:69:ALA:CB	2.79	0.56
3:C:73:GLN:HE21	3:C:75:MET:N	2.02	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.85	0.56
8:H:40:LEU:HD22	8:H:123:MET:CE	2.35	0.56
1:A:92:HIS:HD2	1:A:304:MET:CE	2.18	0.56
1:A:289:ILE:C	1:A:291:GLU:H	2.08	0.56
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.71	0.56
1:A:402:ALA:CB	1:A:434:ARG:HA	2.35	0.56
1:A:527:THR:HG23	1:A:650:GLN:HA	1.88	0.56
1:A:709:THR:HB	1:A:712:GLU:HG3	1.86	0.56
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.40	0.56
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.05	0.56
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.87	0.56
2:B:114:PRO:O	2:B:116:GLU:N	2.38	0.56
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.20	0.56
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.87	0.56
2:B:744:HIS:HD2	2:B:746:SER:OG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:997:GLU:CD	2:B:997:GLU:H	2.05	0.56
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.63	0.56
2:B:1166:CYS:O	2:B:1168:LEU:N	2.37	0.56
3:C:46:ILE:HD12	3:C:67:LEU:O	2.04	0.56
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.87	0.56
3:C:254:LYS:O	3:C:258:ILE:HD13	2.05	0.56
5:E:39:LEU:O	5:E:42:PHE:HB3	2.05	0.56
10:J:12:LYS:O	10:J:14:VAL:HG23	2.05	0.56
11:K:57:LEU:HD12	11:K:77:THR:O	2.05	0.56
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.86	0.56
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.56
3:C:168:ALA:O	3:C:170:TRP:N	2.38	0.56
7:G:17:PHE:N	7:G:17:PHE:CD2	2.73	0.56
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.56
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.35	0.56
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.36	0.56
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.21	0.56
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.33	0.56
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.56
7:G:154:VAL:HG12	7:G:155:SER:N	2.20	0.56
8:H:91:ASP:C	8:H:93:TYR:H	2.09	0.56
1:A:524:VAL:CG1	1:A:525:GLN:H	2.06	0.56
1:A:751:SER:O	1:A:752:LYS:HG2	2.05	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.38	0.56
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.32	0.56
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.35	0.56
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.05	0.56
8:H:102:TYR:N	8:H:102:TYR:CD2	2.73	0.56
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.88	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.70	0.56
2:B:825:VAL:HG12	2:B:826:ALA:N	2.20	0.56
1:A:107:CYS:N	1:A:114:LEU:HD21	2.20	0.56
1:A:225:ASN:ND2	1:A:227:VAL:H	2.02	0.56
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.34	0.56
1:A:541:ILE:HD13	1:A:549:MET:HE3	1.88	0.56
1:A:639:PRO:HG2	1:A:640:GLN:H	1.70	0.56
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.41	0.56
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.13	0.56
7:G:88:ASP:OD2	7:G:88:ASP:N	2.39	0.56
7:G:138:THR:CG2	7:G:139:ILE:H	1.98	0.56
8:H:143:LEU:HD12	8:H:143:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:O	9:I:3:THR:C	2.43	0.56
11:K:47:ARG:HD3	11:K:59:ALA:O	2.05	0.56
1:A:244:PRO:O	1:A:247:ARG:N	2.39	0.56
1:A:300:VAL:O	1:A:300:VAL:HG12	2.06	0.56
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.36	0.56
1:A:1369:ALA:O	1:A:1370:LEU:C	2.44	0.56
2:B:315:LYS:N	2:B:316:PRO:HD2	2.21	0.56
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.06	0.56
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.71	0.56
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.38	0.56
4:D:47:LEU:CD1	4:D:48:ILE:N	2.68	0.56
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.88	0.56
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.88	0.56
11:K:63:VAL:HG23	11:K:63:VAL:O	2.06	0.56
1:A:401:GLY:C	1:A:435:HIS:CD2	2.79	0.56
1:A:565:ILE:O	1:A:570:PRO:HA	2.06	0.56
1:A:1001:ARG:O	1:A:1002:GLY:O	2.24	0.56
1:A:1095:THR:O	1:A:1096:SER:HB2	2.05	0.56
2:B:128:LEU:O	2:B:167:ILE:N	2.31	0.56
2:B:220:GLY:O	2:B:222:ILE:HG13	2.06	0.56
3:C:124:LEU:O	3:C:127:ARG:HG2	2.06	0.56
6:F:93:ILE:HD13	6:F:148:VAL:CG1	2.36	0.56
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.87	0.55
1:A:299:HIS:O	1:A:301:ALA:N	2.39	0.55
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.54	0.55
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.71	0.55
1:A:1074:GLU:C	1:A:1076:ALA:H	2.10	0.55
2:B:464:GLY:HA2	2:B:479:VAL:O	2.05	0.55
3:C:90:ASP:O	3:C:91:HIS:HB3	2.05	0.55
6:F:143:PHE:C	6:F:143:PHE:HD1	2.09	0.55
8:H:103:LYS:HG2	8:H:104:PHE:N	2.22	0.55
1:A:61:ILE:HG22	1:A:62:ASP:N	2.18	0.55
1:A:308:ILE:HG22	1:A:309:ALA:H	1.70	0.55
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.71	0.55
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.35	0.55
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.88	0.55
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.55
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.69	0.55
3:C:189:THR:HG22	3:C:190:ASP:N	2.20	0.55
6:F:111:LEU:C	6:F:113:GLY:N	2.57	0.55
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:ASP:C	9:I:63:GLY:H	2.09	0.55
9:I:111:THR:CG2	9:I:112:SER:H	2.18	0.55
11:K:42:LEU:O	11:K:46:ILE:HG13	2.06	0.55
1:A:58:LEU:CG	1:A:59:GLY:H	2.18	0.55
1:A:726:ARG:O	1:A:729:ALA:HB3	2.05	0.55
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.88	0.55
2:B:957:ASN:O	2:B:959:ASP:N	2.39	0.55
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.35	0.55
3:C:154:LYS:O	3:C:155:LEU:HD23	2.07	0.55
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.88	0.55
4:D:13:ARG:HB2	4:D:17:LYS:NZ	2.19	0.55
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.06	0.55
1:A:130:ASP:O	1:A:133:LYS:N	2.35	0.55
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.22	0.55
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.26	0.55
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.40	0.55
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.36	0.55
2:B:63:ILE:O	2:B:67:SER:HB3	2.06	0.55
2:B:172:ILE:HG22	2:B:173:MET:N	2.22	0.55
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.72	0.55
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.39	0.55
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.41	0.55
8:H:4:THR:CA	8:H:60:ALA:HB2	2.31	0.55
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.37	0.55
12:L:58:LYS:O	12:L:58:LYS:HG2	2.06	0.55
1:A:98:LYS:O	1:A:99:ILE:C	2.44	0.55
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.22	0.55
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.21	0.55
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.89	0.55
2:B:729:ILE:O	2:B:729:ILE:HG22	2.04	0.55
8:H:11:GLN:HA	8:H:53:ASP:O	2.06	0.55
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.34	0.55
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.15	0.55
1:A:219:PHE:O	1:A:222:LEU:O	2.24	0.55
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.42	0.55
1:A:858:ASN:ND2	1:A:858:ASN:C	2.59	0.55
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.07	0.55
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.17	0.55
2:B:35:SER:O	2:B:39:ARG:HG3	2.07	0.55
2:B:498:THR:HB	2:B:537:LYS:O	2.07	0.55
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:192:ARG:HG2	5:E:192:ARG:O	2.06	0.55
7:G:80:LYS:H	7:G:80:LYS:HD3	1.72	0.55
9:I:34:TYR:CD2	9:I:34:TYR:C	2.80	0.55
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.66	0.55
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.89	0.55
1:A:492:PRO:O	1:A:493:GLN:NE2	2.40	0.55
6:F:97:ARG:O	6:F:101:ILE:HG13	2.07	0.55
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.05	0.55
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.07	0.55
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.12	0.55
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.07	0.55
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.70	0.55
2:B:745:PRO:C	2:B:747:MET:H	2.10	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.26	0.55
5:E:15:ALA:O	5:E:19:VAL:HG23	2.07	0.55
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.25	0.55
8:H:61:SER:O	8:H:62:SER:CB	2.54	0.55
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.89	0.55
11:K:46:ILE:O	11:K:46:ILE:HG22	2.06	0.55
1:A:567:LYS:CB	1:A:568:PRO:CD	2.84	0.55
1:A:842:VAL:HG12	1:A:843:LYS:N	2.21	0.55
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.88	0.55
2:B:806:THR:O	2:B:809:MET:HG3	2.06	0.55
9:I:62:ILE:O	9:I:62:ILE:HG12	2.06	0.55
15:T:22:BRU:H2'	15:T:23:DG:O4'	2.07	0.55
1:A:903:ASN:HD22	1:A:904:THR:H	1.46	0.55
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.89	0.55
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.51	0.55
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.95	0.55
2:B:833:TYR:N	2:B:833:TYR:HD1	2.04	0.55
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.89	0.55
3:C:189:THR:HG22	3:C:190:ASP:H	1.71	0.55
3:C:256:ALA:O	3:C:259:LEU:N	2.40	0.55
4:D:24:ALA:C	4:D:26:THR:H	2.10	0.55
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.28	0.55
8:H:82:PRO:C	8:H:84:ALA:H	2.10	0.55
13:N:0:DT:H1'	13:N:1:DA:C5'	2.37	0.55
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.27	0.54
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.72	0.54
1:A:504:LEU:HD12	1:A:504:LEU:N	2.22	0.54
1:A:982:THR:HB	1:A:985:ASP:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.54
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.89	0.54
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.54
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.54
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.88	0.54
4:D:51:ASN:O	4:D:52:LEU:O	2.25	0.54
4:D:167:LEU:O	4:D:170:THR:OG1	2.18	0.54
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.46	0.54
1:A:527:THR:CG2	1:A:650:GLN:HA	2.38	0.54
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.22	0.54
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.90	0.54
2:B:446:LEU:O	2:B:447:ALA:HB3	2.07	0.54
2:B:467:GLY:N	2:B:475:SER:CB	2.64	0.54
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.72	0.54
3:C:129:ILE:HG23	3:C:130:GLY:N	2.22	0.54
8:H:25:ARG:HA	8:H:41:ASP:HA	1.89	0.54
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.54
1:A:666:ILE:HD12	1:A:666:ILE:N	2.22	0.54
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.29	0.54
2:B:465:ASN:HD22	2:B:465:ASN:N	2.04	0.54
3:C:76:ASP:OD2	3:C:128:ASN:N	2.39	0.54
3:C:142:VAL:H	10:J:16:ASP:HB3	1.71	0.54
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.07	0.54
10:J:36:LEU:O	10:J:39:LEU:N	2.39	0.54
11:K:67:PHE:C	11:K:68:PHE:HD2	2.10	0.54
13:N:0:DT:H2"	13:N:1:DA:O5'	2.07	0.54
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.89	0.54
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.90	0.54
1:A:518:LYS:HE2	1:A:624:SER:O	2.08	0.54
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.89	0.54
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.07	0.54
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.07	0.54
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.88	0.54
2:B:339:THR:O	2:B:339:THR:HG22	2.07	0.54
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.42	0.54
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.37	0.54
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.72	0.54
9:I:101:PHE:N	9:I:101:PHE:CD1	2.75	0.54
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.23	0.54
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.41	0.54
2:B:221:ASN:OD1	2:B:242:SER:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:683:SER:O	2:B:687:GLU:HB2	2.07	0.54
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.25	0.54
3:C:140:ASN:O	3:C:141:GLY:O	2.26	0.54
7:G:79:PHE:HZ	7:G:106:MET:CE	2.20	0.54
10:J:27:GLU:O	10:J:29:GLU:N	2.40	0.54
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.48	0.54
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.89	0.54
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.71	0.54
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.48	0.54
2:B:388:CYS:O	2:B:391:ASP:N	2.36	0.54
2:B:549:THR:HG22	2:B:550:ASP:N	2.15	0.54
3:C:145:CYS:HA	10:J:2:ILE:HD11	1.89	0.54
3:C:168:ALA:C	3:C:170:TRP:N	2.60	0.54
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.54
7:G:4:ILE:O	7:G:4:ILE:HG22	2.06	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.88	0.54
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.73	0.54
2:B:101:MET:O	2:B:102:VAL:HG23	2.07	0.54
2:B:283:VAL:O	2:B:286:PHE:N	2.41	0.54
2:B:843:GLN:O	2:B:846:ILE:N	2.41	0.54
6:F:130:ILE:O	6:F:148:VAL:HG21	2.07	0.54
1:A:92:HIS:HD2	1:A:304:MET:HE1	1.72	0.54
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.42	0.54
1:A:317:LYS:O	1:A:318:SER:CB	2.56	0.54
1:A:332:LYS:O	1:A:334:GLY:N	2.40	0.54
1:A:471:ASN:O	1:A:474:VAL:HG12	2.08	0.54
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.41	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.73	0.54
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.48	0.54
1:A:1365:TYR:O	1:A:1367:HIS:N	2.40	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.37	0.54
2:B:1106:ARG:HH12	2:B:1110:PRO:HG2	1.71	0.54
3:C:37:MET:HA	3:C:41:ILE:CD1	2.38	0.54
4:D:64:VAL:O	4:D:66:ARG:N	2.40	0.54
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.88	0.54
1:A:385:ILE:CG2	1:A:386:ASP:N	2.71	0.54
1:A:718:VAL:O	1:A:721:PHE:HB2	2.07	0.54
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.89	0.54
2:B:46:GLN:HG3	2:B:47:GLN:N	2.21	0.54
2:B:247:GLY:C	2:B:249:ARG:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:GLY:N	2:B:748:ILE:HG22	2.22	0.54
2:B:911:ILE:O	2:B:911:ILE:HG22	2.07	0.54
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.71	0.54
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.73	0.54
11:K:31:VAL:O	11:K:74:ARG:HA	2.06	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.71	0.54
13:N:5:DA:C2	15:T:13:DA:C2	2.95	0.54
14:P:0:U:H2'	14:P:1:U:H5'	1.89	0.54
14:P:5:C:O2'	14:P:6:C:H5'	2.07	0.54
1:A:40:THR:HG22	1:A:41:MET:CG	2.29	0.54
1:A:58:LEU:CD1	1:A:59:GLY:N	2.63	0.54
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.89	0.54
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.08	0.54
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.41	0.54
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.08	0.54
1:A:858:ASN:ND2	1:A:861:GLY:H	2.05	0.54
1:A:901:LEU:N	1:A:926:GLN:NE2	2.48	0.54
1:A:1114:PRO:O	1:A:1115:SER:O	2.26	0.54
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.07	0.54
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.73	0.54
2:B:776:GLN:NE2	14:P:8:G:H5'	2.20	0.54
2:B:910:VAL:HG12	2:B:912:ILE:H	1.73	0.54
5:E:31:THR:O	5:E:35:VAL:HG23	2.07	0.54
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.43	0.54
7:G:47:CYS:O	7:G:76:ALA:HB1	2.08	0.54
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.25	0.54
10:J:45:CYS:O	10:J:48:ARG:HG3	2.08	0.54
11:K:47:ARG:HD2	11:K:47:ARG:O	2.08	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.39	0.53
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.38	0.53
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.53
2:B:1182:CYS:O	2:B:1183:LYS:O	2.26	0.53
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.53
4:D:176:GLU:C	4:D:178:ALA:N	2.61	0.53
7:G:27:LYS:O	7:G:30:LEU:HB3	2.08	0.53
7:G:51:TYR:C	7:G:51:TYR:CD2	2.81	0.53
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.08	0.53
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.43	0.53
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:ARG:HA	3:C:37:MET:HE2	1.88	0.53
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.08	0.53
1:A:366:VAL:CG2	1:A:460:VAL:HG22	2.36	0.53
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.44	0.53
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.27	0.53
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.08	0.53
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.38	0.53
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.72	0.53
5:E:55:ARG:C	5:E:57:MET:H	2.10	0.53
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.38	0.53
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.43	0.53
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.90	0.53
1:A:222:LEU:O	1:A:224:PHE:N	2.41	0.53
1:A:230:ARG:N	1:A:233:TRP:CE3	2.65	0.53
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.90	0.53
2:B:705:MET:H	2:B:710:LEU:CD1	2.22	0.53
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.89	0.53
2:B:810:GLU:HB2	2:B:815:ARG:NH2	2.22	0.53
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.08	0.53
4:D:52:LEU:C	4:D:54:GLU:H	2.11	0.53
4:D:198:LEU:O	4:D:200:ASN:N	2.40	0.53
7:G:9:LEU:HD12	7:G:10:ASN:H	1.73	0.53
11:K:41:THR:HG22	11:K:42:LEU:N	2.22	0.53
1:A:44:THR:O	1:A:45:GLN:HB2	2.09	0.53
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.44	0.53
1:A:224:PHE:HD2	1:A:229:SER:O	1.91	0.53
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.24	0.53
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.43	0.53
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.89	0.53
2:B:999:MET:HA	2:B:999:MET:CE	2.38	0.53
9:I:103:CYS:CB	9:I:106:CYS:HG	2.21	0.53
1:A:61:ILE:O	1:A:63:ARG:N	2.42	0.53
1:A:278:THR:O	1:A:278:THR:HG22	2.09	0.53
1:A:474:VAL:C	1:A:477:PRO:HD2	2.29	0.53
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.53
1:A:699:ALA:CB	1:A:701:LEU:HG	2.39	0.53
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.92	0.53
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.73	0.53
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.90	0.53
1:A:1332:PHE:O	1:A:1333:ILE:C	2.47	0.53
2:B:388:CYS:O	2:B:390:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:N	2:B:710:LEU:HD12	2.23	0.53
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.27	0.53
3:C:166:GLU:OE1	12:L:70:ARG:NH2	2.32	0.53
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.91	0.53
1:A:34:LYS:H	1:A:57:ARG:NH2	2.07	0.53
1:A:248:PRO:O	1:A:260:ASP:HB2	2.09	0.53
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.24	0.53
2:B:448:ILE:O	2:B:450:ALA:N	2.42	0.53
2:B:975:GLN:O	2:B:990:ILE:HD12	2.09	0.53
4:D:18:VAL:HG13	4:D:18:VAL:O	2.09	0.53
7:G:15:PRO:O	7:G:16:SER:C	2.46	0.53
7:G:73:LYS:HE2	7:G:74:TYR:O	2.08	0.53
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.34	0.53
10:J:28:ASP:O	10:J:30:LEU:HG	2.09	0.53
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.91	0.53
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.90	0.53
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.39	0.53
5:E:105:PHE:O	5:E:106:GLN:HB2	2.08	0.53
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.08	0.53
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.74	0.53
15:T:24:DG:H2"	15:T:25:DT:C5'	2.38	0.53
1:A:42:ASP:HB3	1:A:45:GLN:N	2.24	0.53
1:A:332:LYS:C	1:A:334:GLY:H	2.11	0.53
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.30	0.53
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.34	0.53
2:B:1156:ASP:O	2:B:1157:ALA:O	2.26	0.53
3:C:166:GLU:O	3:C:167:HIS:HB2	2.09	0.53
5:E:78:LEU:HD23	5:E:78:LEU:C	2.28	0.53
7:G:1:MET:SD	7:G:1:MET:C	2.87	0.53
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.90	0.53
8:H:58:THR:HG22	8:H:59:ILE:H	1.74	0.53
15:T:19:DT:C2'	15:T:20:DC:O5'	2.57	0.53
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.36	0.53
1:A:472:LEU:CD2	2:B:836:GLU:HG3	2.38	0.53
1:A:477:PRO:CG	1:A:521:MET:HG2	2.38	0.53
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.42	0.53
1:A:1313:LEU:O	1:A:1315:GLU:N	2.42	0.53
2:B:34:ILE:HD13	2:B:747:MET:HE2	1.90	0.53
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.91	0.53
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.39	0.53
2:B:1010:LEU:O	2:B:1011:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:NH1	11:K:41:THR:H	2.06	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.21	0.53
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.91	0.53
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.53
11:K:114:LEU:HD13	11:K:114:LEU:C	2.29	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
1:A:58:LEU:CG	1:A:59:GLY:N	2.72	0.52
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.89	0.52
1:A:774:ARG:NH2	1:A:797:LYS:HG3	2.24	0.52
1:A:1139:GLU:O	1:A:1275:GLY:HA3	2.09	0.52
3:C:27:LEU:O	3:C:28:ALA:C	2.47	0.52
5:E:134:THR:C	5:E:135:PHE:HD1	2.12	0.52
9:I:71:SER:OG	9:I:83:ASN:HB2	2.09	0.52
14:P:4:A:H2'	14:P:5:C:C6	2.44	0.52
1:A:325:ILE:O	1:A:326:ARG:C	2.45	0.52
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.29	0.52
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.09	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.61	0.52
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.73	0.52
1:A:1017:LEU:CB	5:E:205:SER:HA	2.39	0.52
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.21	0.52
4:D:17:LYS:CA	4:D:17:LYS:HE3	2.39	0.52
5:E:163:GLU:O	5:E:164:LEU:C	2.47	0.52
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.49	0.52
10:J:5:VAL:O	10:J:6:ARG:O	2.26	0.52
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.39	0.52
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.91	0.52
1:A:600:PRO:HG2	1:A:601:LYS:H	1.74	0.52
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.49	0.52
2:B:360:PHE:C	2:B:360:PHE:CD2	2.82	0.52
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.23	0.52
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.52
2:B:860:MET:HG2	2:B:861:ASP:H	1.75	0.52
3:C:45:ALA:O	3:C:159:ALA:HA	2.09	0.52
8:H:128:ASN:CG	8:H:128:ASN:O	2.47	0.52
1:A:34:LYS:CB	1:A:36:ARG:HE	2.22	0.52
1:A:353:ILE:HB	1:A:470:LEU:HD21	1.90	0.52
1:A:427:GLN:O	1:A:428:TYR:C	2.48	0.52
1:A:540:PHE:CE2	1:A:565:ILE:HD12	2.44	0.52
2:B:332:ASP:O	2:B:336:ARG:HG3	2.09	0.52
2:B:711:GLU:H	2:B:712:PRO:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.74	0.52
6:F:69:LEU:N	6:F:70:LYS:HA	2.25	0.52
1:A:92:HIS:O	1:A:95:PHE:N	2.32	0.52
1:A:108:MET:SD	1:A:210:ILE:HD13	2.49	0.52
1:A:332:LYS:C	1:A:334:GLY:N	2.62	0.52
1:A:903:ASN:ND2	1:A:904:THR:N	2.45	0.52
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.91	0.52
2:B:224:GLN:O	2:B:238:ALA:HA	2.10	0.52
2:B:461:LEU:N	2:B:461:LEU:HD12	2.23	0.52
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.40	0.52
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.22	0.52
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.30	0.52
4:D:185:CYS:HB2	4:D:211:LEU:CD2	2.37	0.52
9:I:60:GLN:NE2	9:I:107:SER:OG	2.41	0.52
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.40	0.52
14:P:0:U:C2'	14:P:1:U:H5'	2.40	0.52
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.38	0.52
1:A:323:LYS:HZ3	14:P:1:U:H4'	1.75	0.52
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.92	0.52
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.52
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.52
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.10	0.52
1:A:1341:ILE:O	1:A:1344:GLY:N	2.43	0.52
1:A:1364:ASN:O	1:A:1365:TYR:C	2.47	0.52
2:B:22:SER:HA	2:B:654:ARG:HG3	1.91	0.52
2:B:269:ILE:HG21	2:B:282:ILE:HD13	1.91	0.52
3:C:74:SER:HB2	3:C:77:ILE:HG12	1.91	0.52
1:A:34:LYS:O	1:A:35:ILE:HB	2.09	0.52
1:A:42:ASP:C	1:A:44:THR:H	2.11	0.52
1:A:381:THR:HG23	1:A:382:PRO:CD	2.39	0.52
1:A:475:THR:CG2	1:A:476:SER:H	2.23	0.52
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.44	0.52
1:A:1076:ALA:HA	1:A:1079:MET:HE3	1.91	0.52
2:B:27:ALA:O	2:B:29:ASP:N	2.43	0.52
2:B:34:ILE:O	2:B:37:PHE:N	2.42	0.52
2:B:343:ILE:HG22	2:B:345:LYS:H	1.75	0.52
2:B:942:ARG:O	2:B:944:THR:N	2.43	0.52
2:B:1151:LEU:N	2:B:1151:LEU:HD12	2.25	0.52
2:B:1177:HIS:O	2:B:1179:GLN:N	2.42	0.52
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.52
6:F:90:ARG:CG	6:F:91:ALA:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:15:DT:C6	15:T:16:DT:H73	2.43	0.52
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.44	0.52
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.45	0.52
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.10	0.52
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.92	0.52
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.43	0.52
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.92	0.52
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.45	0.52
2:B:731:VAL:HG12	2:B:732:SER:H	1.75	0.52
3:C:243:VAL:O	3:C:243:VAL:HG12	2.08	0.52
3:C:251:LEU:O	3:C:251:LEU:HD12	2.10	0.52
4:D:19:GLU:O	4:D:21:GLU:N	2.43	0.52
7:G:88:ASP:HA	7:G:144:ARG:HA	1.91	0.52
8:H:99:GLY:N	8:H:118:PHE:CD2	2.78	0.52
9:I:34:TYR:HD2	9:I:34:TYR:C	2.10	0.52
9:I:50:THR:HG22	9:I:51:ASN:N	2.25	0.52
1:A:23:SER:HA	1:A:233:TRP:NE1	2.25	0.52
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.25	0.52
1:A:577:ILE:C	1:A:579:SER:N	2.60	0.52
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.38	0.52
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.25	0.52
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.92	0.52
11:K:65:HIS:CD2	11:K:65:HIS:C	2.83	0.52
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.45	0.52
1:A:596:THR:C	1:A:598:LEU:N	2.63	0.52
1:A:613:ILE:HG22	1:A:614:PHE:HD2	1.75	0.52
1:A:647:GLY:O	1:A:651:LYS:HG3	2.10	0.52
1:A:800:VAL:HG11	1:A:808:LEU:HG	1.90	0.52
2:B:287:ARG:NH1	2:B:324:ILE:O	2.42	0.52
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.44	0.52
2:B:343:ILE:HG22	2:B:348:ARG:HG3	1.88	0.52
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.92	0.52
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.10	0.52
2:B:1106:ARG:NH1	2:B:1110:PRO:CG	2.72	0.52
3:C:236:GLY:C	3:C:238:ILE:N	2.63	0.52
5:E:35:VAL:C	5:E:37:LEU:H	2.13	0.52
10:J:13:VAL:O	10:J:14:VAL:CG2	2.58	0.52
1:A:2:VAL:HG21	2:B:1157:ALA:HB1	1.92	0.51
1:A:335:ARG:N	1:A:339:ASN:HD22	2.07	0.51
1:A:573:SER:O	1:A:576:GLN:HB2	2.10	0.51
1:A:639:PRO:HG2	1:A:640:GLN:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:MET:HA	2:B:514:LEU:HB3	1.92	0.51
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.74	0.51
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.92	0.51
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.10	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.10	0.51
2:B:918:ILE:HD12	2:B:935:ARG:HD3	1.91	0.51
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.25	0.51
3:C:146:LYS:C	3:C:147:LEU:HD23	2.31	0.51
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.74	0.51
5:E:153:HIS:O	5:E:154:ILE:CG1	2.58	0.51
7:G:1:MET:O	7:G:3:PHE:CD1	2.63	0.51
7:G:111:THR:HB	7:G:114:LEU:HB2	1.92	0.51
10:J:64:ASN:CB	10:J:65:PRO:CD	2.86	0.51
1:A:37:PHE:HD1	1:A:37:PHE:H	1.58	0.51
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.23	0.51
1:A:711:ARG:HA	9:I:97:MET:HE1	1.91	0.51
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.22	0.51
2:B:1068:GLY:O	2:B:1069:PHE:O	2.29	0.51
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.93	0.51
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.31	0.51
3:C:98:VAL:O	3:C:99:LEU:HD22	2.09	0.51
9:I:25:LEU:HB3	9:I:38:ALA:CB	2.40	0.51
1:A:93:VAL:HG21	1:A:301:ALA:O	2.11	0.51
1:A:341:MET:CE	1:A:843:LYS:NZ	2.73	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.50	0.51
1:A:867:ILE:HG22	1:A:871:ASP:H	1.75	0.51
1:A:939:ASP:O	1:A:940:ARG:C	2.49	0.51
1:A:1213:GLY:O	1:A:1214:GLU:C	2.49	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.75	0.51
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.39	0.51
2:B:343:ILE:CG2	2:B:348:ARG:N	2.73	0.51
2:B:885:MET:HA	2:B:936:ASP:HB2	1.93	0.51
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.92	0.51
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.68	0.51
3:C:209:TYR:HD1	3:C:209:TYR:H	1.57	0.51
3:C:238:ILE:HG21	3:C:242:GLN:HB2	1.90	0.51
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.92	0.51
7:G:145:VAL:CG1	7:G:146:LYS:N	2.73	0.51
9:I:99:LEU:O	9:I:111:THR:HG23	2.10	0.51
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.28	0.51
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.46	0.51
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.46	0.51
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.92	0.51
2:B:860:MET:HG2	2:B:861:ASP:N	2.26	0.51
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.51
7:G:51:TYR:O	7:G:54:ILE:HG13	2.10	0.51
9:I:59:VAL:C	9:I:61:ASP:H	2.14	0.51
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.72	0.51
1:A:958:VAL:O	1:A:958:VAL:HG12	2.09	0.51
2:B:232:SER:CB	2:B:261:ARG:HH21	2.12	0.51
2:B:388:CYS:C	2:B:390:LEU:H	2.13	0.51
2:B:707:PRO:O	2:B:711:GLU:HG3	2.10	0.51
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.75	0.51
9:I:51:ASN:O	9:I:54:GLU:HG3	2.11	0.51
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.76	0.51
14:P:3:G:H2'	14:P:4:A:C8	2.46	0.51
15:T:20:DC:C2'	15:T:21:DC:O5'	2.58	0.51
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.45	0.51
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.91	0.51
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.93	0.51
3:C:226:ASP:O	3:C:227:THR:CB	2.58	0.51
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.45	0.51
7:G:66:GLY:O	7:G:67:SER:C	2.48	0.51
11:K:69:ALA:O	11:K:70:ARG:HB3	2.10	0.51
1:A:244:PRO:CB	1:A:245:PRO:CD	2.89	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.25	0.51
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.92	0.51
2:B:515:HIS:O	2:B:518:HIS:HB2	2.10	0.51
5:E:177:ARG:HD3	5:E:215:MET:CG	2.41	0.51
7:G:74:TYR:H	7:G:74:TYR:HD2	1.59	0.51
9:I:106:CYS:O	9:I:107:SER:HB2	2.10	0.51
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.75	0.51
1:A:754:SER:H	1:A:757:ASN:ND2	1.93	0.51
1:A:921:GLY:O	1:A:922:ASP:C	2.47	0.51
1:A:984:LYS:O	1:A:988:LEU:HB2	2.09	0.51
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.10	0.51
2:B:25:ILE:HD11	2:B:653:VAL:C	2.31	0.51
2:B:337:ARG:C	2:B:338:GLY:N	2.64	0.51
2:B:484:ASN:HB3	2:B:486:TYR:HD1	1.74	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.30	0.51
5:E:14:ARG:O	5:E:17:ARG:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.11	0.51
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.92	0.51
7:G:143:ILE:CG2	7:G:144:ARG:N	2.74	0.51
8:H:22:LYS:O	8:H:23:VAL:HG23	2.11	0.51
10:J:27:GLU:C	10:J:29:GLU:H	2.12	0.51
1:A:260:ASP:OD1	1:A:261:ASP:N	2.44	0.51
1:A:685:GLU:HG3	1:A:686:ALA:N	2.26	0.51
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.76	0.51
1:A:832:ALA:HB1	15:T:19:DT:OP1	2.10	0.51
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.45	0.51
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.41	0.51
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.75	0.51
4:D:8:PHE:O	4:D:9:GLN:HB2	2.11	0.51
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.76	0.51
9:I:101:PHE:HE1	9:I:112:SER:HB2	1.76	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.74	0.51
15:T:22:BRU:C2'	15:T:23:DG:O4'	2.59	0.51
1:A:316:GLN:O	1:A:317:LYS:C	2.49	0.51
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.21	0.51
1:A:877:HIS:C	1:A:878:ILE:CG1	2.80	0.51
1:A:974:ASP:C	1:A:976:THR:H	2.15	0.51
2:B:237:VAL:HG12	2:B:238:ALA:N	2.26	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.65	0.51
3:C:82:TYR:O	3:C:83:SER:C	2.49	0.51
3:C:112:ASN:HD22	3:C:112:ASN:N	2.09	0.51
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.11	0.51
6:F:147:SER:OG	6:F:150:GLU:HG3	2.10	0.51
7:G:125:SER:OG	7:G:128:PRO:HA	2.11	0.51
14:P:0:U:O2'	14:P:1:U:H5'	2.11	0.51
1:A:853:ASP:OD1	1:A:855:THR:HB	2.10	0.50
1:A:903:ASN:ND2	1:A:903:ASN:C	2.64	0.50
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.10	0.50
2:B:848:ARG:HD2	10:J:7:CYS:O	2.11	0.50
2:B:905:VAL:HG23	2:B:941:LEU:HD22	1.93	0.50
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.26	0.50
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.41	0.50
8:H:83:GLN:C	8:H:85:GLY:H	2.13	0.50
9:I:16:PRO:HB3	9:I:27:PHE:CD2	2.47	0.50
9:I:111:THR:CG2	9:I:112:SER:N	2.74	0.50
1:A:75:ASN:O	1:A:76:GLU:CB	2.58	0.50
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.93	0.50
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.40	0.50
1:A:1444:MET:CG	7:G:60:ARG:HA	2.38	0.50
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.50
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.92	0.50
2:B:796:LEU:HD12	2:B:852:ARG:O	2.11	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.25	0.50
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.42	0.50
3:C:167:HIS:CD2	3:C:168:ALA:N	2.79	0.50
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.51	0.50
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.93	0.50
5:E:157:SER:HG	5:E:160:GLU:HG3	1.74	0.50
8:H:139:ASN:O	8:H:140:ALA:HB2	2.11	0.50
9:I:85:PHE:CD2	9:I:85:PHE:N	2.67	0.50
11:K:31:VAL:HG12	11:K:32:VAL:H	1.75	0.50
1:A:203:SER:OG	1:A:206:GLU:HB2	2.11	0.50
1:A:262:LEU:O	1:A:264:PHE:N	2.45	0.50
2:B:129:PHE:HA	2:B:165:VAL:O	2.12	0.50
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.26	0.50
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.26	0.50
2:B:803:LEU:HB2	2:B:1032:SER:OG	2.10	0.50
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.92	0.50
2:B:1202:LEU:O	2:B:1203:LEU:C	2.48	0.50
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.93	0.50
1:A:43:GLU:O	1:A:44:THR:CB	2.59	0.50
1:A:50:ILE:C	1:A:52:GLY:N	2.63	0.50
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.94	0.50
1:A:326:ARG:HH22	1:A:1407:GLU:CG	2.23	0.50
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.93	0.50
1:A:998:LEU:HD12	1:A:998:LEU:H	1.77	0.50
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.11	0.50
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.93	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.76	0.50
3:C:208:GLU:C	3:C:210:GLU:H	2.14	0.50
7:G:39:THR:HG22	7:G:41:LYS:H	1.76	0.50
11:K:60:ALA:O	11:K:73:LEU:HD12	2.11	0.50
1:A:71:GLN:C	1:A:73:GLY:H	2.14	0.50
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.27	0.50
2:B:814:PHE:C	2:B:816:GLU:H	2.13	0.50
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.50
3:C:167:HIS:CD2	3:C:168:ALA:H	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.41	0.50
10:J:23:ASN:O	10:J:25:LEU:N	2.45	0.50
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.47	0.50
1:A:535:THR:HG22	1:A:536:LEU:N	2.26	0.50
1:A:873:MET:C	1:A:1058:VAL:HG23	2.32	0.50
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.11	0.50
1:A:1299:VAL:CG1	1:A:1300:LYS:H	2.25	0.50
2:B:516:ASN:ND2	2:B:516:ASN:H	2.10	0.50
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.45	0.50
5:E:153:HIS:O	5:E:154:ILE:HG13	2.10	0.50
1:A:33:ALA:O	1:A:83:HIS:HD2	1.95	0.50
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.77	0.50
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.50
2:B:1172:ILE:HG22	2:B:1172:ILE:O	2.11	0.50
3:C:255:VAL:O	3:C:255:VAL:HG12	2.12	0.50
9:I:82:GLU:O	9:I:104:LEU:HG	2.11	0.50
14:P:4:A:H2'	14:P:5:C:O4'	2.11	0.50
1:A:57:ARG:O	1:A:68:GLN:HG3	2.11	0.50
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.47	0.50
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.94	0.50
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.46	0.50
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.77	0.50
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.93	0.50
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.12	0.50
2:B:344:LYS:O	2:B:345:LYS:CB	2.58	0.50
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.46	0.50
2:B:957:ASN:O	2:B:960:GLY:N	2.43	0.50
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.50
3:C:183:TRP:O	3:C:185:LYS:HG3	2.12	0.50
3:C:236:GLY:O	3:C:238:ILE:N	2.45	0.50
15:T:10:DA:H2"	15:T:11:DG:OP2	2.11	0.50
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.92	0.50
1:A:577:ILE:O	1:A:578:LEU:C	2.51	0.50
1:A:1418:LEU:HD12	1:A:1419:ASP:H	1.77	0.50
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.47	0.50
2:B:744:HIS:HD2	2:B:746:SER:CB	2.25	0.50
7:G:80:LYS:O	7:G:82:PHE:CE1	2.65	0.50
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.93	0.50
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.46	0.50
12:L:36:SER:O	12:L:37:LYS:C	2.49	0.50
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ALA:O	1:A:845:LEU:HD23	2.12	0.49
1:A:947:PHE:CD2	1:A:954:TRP:CE2	3.00	0.49
2:B:234:ILE:HD12	2:B:234:ILE:N	2.26	0.49
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.94	0.49
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.26	0.49
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.27	0.49
3:C:232:VAL:HG21	3:C:244:VAL:CG2	2.39	0.49
4:D:151:PHE:CD1	4:D:151:PHE:N	2.78	0.49
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.73	0.49
5:E:144:ILE:HG13	5:E:145:THR:N	2.25	0.49
8:H:58:THR:HG22	8:H:59:ILE:N	2.27	0.49
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.59	0.49
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.94	0.49
1:A:909:ASP:C	1:A:911:SER:H	2.16	0.49
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.93	0.49
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.60	0.49
2:B:794:ASN:O	2:B:795:ILE:HD12	2.12	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.60	0.49
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	2.86	0.49
3:C:56:THR:HG22	3:C:57:VAL:N	2.18	0.49
4:D:145:MET:O	4:D:149:THR:N	2.44	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.12	0.49
14:P:5:C:C2'	14:P:6:C:O4'	2.55	0.49
1:A:68:GLN:C	1:A:70:CYS:N	2.62	0.49
1:A:130:ASP:O	1:A:131:SER:C	2.50	0.49
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.34	0.49
1:A:403:LYS:O	1:A:404:TYR:CD2	2.66	0.49
1:A:600:PRO:C	1:A:602:ASP:H	2.15	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.13	0.49
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.60	0.49
2:B:258:LEU:HG	2:B:258:LEU:O	2.13	0.49
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
4:D:66:ARG:O	4:D:70:PHE:HB2	2.12	0.49
8:H:98:TYR:C	8:H:118:PHE:HD2	2.15	0.49
10:J:32:GLU:O	10:J:33:GLY:C	2.50	0.49
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.94	0.49
2:B:466:TRP:O	2:B:468:GLU:N	2.46	0.49
3:C:241:ASP:O	3:C:245:VAL:HG23	2.12	0.49
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.13	0.49
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.94	0.49
1:A:299:HIS:C	1:A:301:ALA:H	2.15	0.49
1:A:367:PRO:HA	1:A:463:ILE:O	2.13	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.49
1:A:1334:ASP:O	1:A:1336:MET:N	2.45	0.49
2:B:29:ASP:O	2:B:30:SER:C	2.50	0.49
2:B:702:LEU:HD12	2:B:703:ILE:H	1.76	0.49
2:B:778:MET:CE	2:B:1094:ARG:CD	2.89	0.49
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.48	0.49
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.01	0.49
2:B:830:TYR:O	2:B:831:SER:C	2.50	0.49
3:C:70:ILE:O	3:C:70:ILE:HG22	2.11	0.49
3:C:242:GLN:C	3:C:244:VAL:H	2.14	0.49
3:C:263:THR:C	3:C:265:MET:N	2.66	0.49
4:D:27:LEU:HD22	4:D:173:HIS:HD2	1.76	0.49
4:D:52:LEU:O	4:D:54:GLU:N	2.44	0.49
4:D:64:VAL:C	4:D:66:ARG:N	2.66	0.49
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.94	0.49
7:G:29:LYS:O	7:G:30:LEU:C	2.51	0.49
8:H:103:LYS:HG2	8:H:104:PHE:H	1.78	0.49
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.93	0.49
1:A:853:ASP:OD1	1:A:853:ASP:C	2.50	0.49
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.41	0.49
1:A:971:PHE:O	1:A:972:HIS:C	2.51	0.49
1:A:1116:LEU:CB	1:A:1308:THR:HG21	2.42	0.49
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.95	0.49
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.93	0.49
3:C:77:ILE:O	3:C:79:GLN:N	2.46	0.49
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.38	0.49
4:D:156:ASP:C	4:D:158:GLU:H	2.15	0.49
7:G:61:ILE:HG23	7:G:66:GLY:O	2.12	0.49
12:L:28:LYS:HB2	12:L:39:SER:HA	1.95	0.49
1:A:24:PRO:HB3	1:A:237:THR:HB	1.94	0.49
1:A:53:LEU:CD2	1:A:54:ASN:N	2.56	0.49
1:A:115:LEU:HB2	1:A:122:MET:CE	2.43	0.49
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.93	0.49
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.13	0.49
2:B:51:PHE:HE2	2:B:172:ILE:HG23	1.77	0.49
2:B:205:ILE:N	2:B:205:ILE:HD12	2.27	0.49
2:B:222:ILE:O	2:B:240:ILE:HA	2.12	0.49
2:B:882:THR:O	2:B:883:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.37	0.49
3:C:258:ILE:HD12	3:C:258:ILE:N	2.26	0.49
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.42	0.49
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.28	0.49
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.93	0.49
8:H:35:GLN:O	8:H:37:LYS:HG3	2.12	0.49
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.28	0.49
1:A:464:PRO:O	1:A:465:TYR:O	2.30	0.49
1:A:701:LEU:HD23	9:I:115:LYS:HG3	1.95	0.49
2:B:95:ILE:HG13	2:B:129:PHE:O	2.12	0.49
2:B:217:ARG:HD2	2:B:217:ARG:O	2.13	0.49
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.41	0.49
2:B:654:ARG:C	2:B:656:GLY:H	2.16	0.49
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.49
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.12	0.49
4:D:195:ILE:N	4:D:196:PRO:CD	2.75	0.49
11:K:65:HIS:CD2	11:K:66:PRO:HG2	2.48	0.49
1:A:241:VAL:O	1:A:242:PRO:C	2.51	0.49
1:A:595:THR:O	1:A:596:THR:HG23	2.12	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.94	0.49
1:A:853:ASP:OD1	1:A:855:THR:CB	2.61	0.49
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.95	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.11	0.49
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.41	0.49
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.25	0.49
4:D:145:MET:O	4:D:149:THR:HB	2.13	0.49
8:H:40:LEU:HD12	8:H:122:LEU:O	2.13	0.49
13:N:3:DG:H1'	13:N:4:DT:C5'	2.42	0.49
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.13	0.49
1:A:388:LEU:HD22	1:A:432:VAL:HG21	1.95	0.49
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.43	0.49
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.95	0.49
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.77	0.49
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.93	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.48	0.49
2:B:405:ARG:HA	2:B:631:GLY:O	2.13	0.49
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.13	0.49
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.80	0.49
3:C:74:SER:CB	3:C:77:ILE:HG12	2.43	0.49
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.47	0.49
6:F:77:ASP:O	6:F:78:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:THR:HG23	6:F:89:GLU:CD	2.33	0.49
9:I:103:CYS:CB	9:I:106:CYS:SG	3.01	0.49
10:J:2:ILE:CG2	10:J:3:VAL:N	2.75	0.49
10:J:7:CYS:SG	10:J:49:MET:HE3	2.53	0.49
12:L:43:THR:HG22	12:L:43:THR:O	2.13	0.49
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.26	0.48
1:A:53:LEU:O	1:A:54:ASN:C	2.50	0.48
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.48
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.95	0.48
1:A:618:GLU:O	1:A:619:LYS:C	2.52	0.48
1:A:719:VAL:O	1:A:721:PHE:N	2.46	0.48
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.13	0.48
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.95	0.48
2:B:181:LEU:HD22	2:B:189:LEU:HD22	1.95	0.48
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.48
3:C:147:LEU:N	3:C:147:LEU:CD2	2.75	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.45	0.48
3:C:187:LYS:C	3:C:189:THR:H	2.15	0.48
10:J:2:ILE:H	10:J:57:ILE:HG22	1.78	0.48
14:P:0:U:H2'	14:P:1:U:C5'	2.43	0.48
1:A:310:GLY:O	1:A:312:PRO:HD2	2.14	0.48
1:A:503:GLN:C	1:A:504:LEU:HD12	2.34	0.48
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.95	0.48
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.28	0.48
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.94	0.48
2:B:189:LEU:CA	2:B:192:LEU:HD12	2.25	0.48
2:B:281:PRO:O	2:B:283:VAL:N	2.46	0.48
11:K:50:LEU:CD2	11:K:56:VAL:HG21	2.43	0.48
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.78	0.48
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.95	0.48
1:A:556:TRP:C	1:A:558:GLY:H	2.17	0.48
1:A:639:PRO:CG	1:A:640:GLN:H	2.25	0.48
1:A:881:GLN:O	1:A:953:ASN:HA	2.13	0.48
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.96	0.48
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.77	0.48
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.94	0.48
5:E:29:PHE:C	5:E:30:ILE:HG13	2.33	0.48
5:E:177:ARG:O	5:E:212:ARG:CD	2.61	0.48
7:G:115:MET:CB	7:G:116:PRO:HD2	2.43	0.48
9:I:100:PHE:N	9:I:100:PHE:CD1	2.81	0.48
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:A:369:SER:C	2.51	0.48
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.13	0.48
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.43	0.48
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.14	0.48
1:A:1216:ILE:O	1:A:1219:THR:HB	2.12	0.48
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.48	0.48
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.94	0.48
2:B:449:ASN:C	2:B:451:LYS:H	2.17	0.48
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.77	0.48
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	0.48
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.94	0.48
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.35	0.48
3:C:9:LYS:O	3:C:10:ILE:C	2.52	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.13	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
5:E:154:ILE:HG22	5:E:155:ARG:O	2.12	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.43	0.48
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.78	0.48
15:T:24:DG:C2'	15:T:25:DT:O5'	2.62	0.48
1:A:323:LYS:NZ	14:P:1:U:H4'	2.29	0.48
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.94	0.48
1:A:873:MET:HG2	1:A:957:PRO:HB3	1.95	0.48
1:A:1010:ALA:O	1:A:1011:GLN:C	2.52	0.48
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.27	0.48
2:B:911:ILE:O	2:B:912:ILE:HG13	2.14	0.48
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.34	0.48
3:C:73:GLN:NE2	3:C:74:SER:N	2.57	0.48
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.28	0.48
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.94	0.48
11:K:91:CYS:O	11:K:94:ILE:HB	2.13	0.48
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.78	0.48
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.94	0.48
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.14	0.48
1:A:1445:ILE:HG21	7:G:18:PHE:CD2	2.48	0.48
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.02	0.48
3:C:66:ARG:NH1	3:C:144:ILE:O	2.47	0.48
4:D:13:ARG:C	4:D:17:LYS:HZ3	2.16	0.48
8:H:111:LEU:HD23	8:H:127:GLY:O	2.13	0.48
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.96	0.48
1:A:116:ASP:C	1:A:118:HIS:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:VAL:O	1:A:653:VAL:C	2.52	0.48
1:A:710:LEU:H	1:A:710:LEU:HD12	1.79	0.48
1:A:774:ARG:HB2	1:A:797:LYS:HB3	1.96	0.48
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.01	0.48
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.47	0.48
2:B:640:VAL:O	2:B:640:VAL:HG12	2.13	0.48
2:B:831:SER:HB3	2:B:994:TYR:OH	2.14	0.48
2:B:843:GLN:CG	11:K:6:ARG:HH21	2.27	0.48
4:D:20:GLU:HA	4:D:20:GLU:OE2	2.13	0.48
6:F:123:LYS:O	6:F:124:GLU:C	2.52	0.48
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.79	0.48
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.01	0.48
13:N:5:DA:H2"	13:N:6:DC:OP2	2.13	0.48
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.77	0.48
1:A:84:ILE:O	1:A:84:ILE:CG2	2.61	0.48
1:A:117:GLU:H	1:A:117:GLU:CD	2.17	0.48
1:A:295:LEU:O	1:A:298:PHE:HB3	2.13	0.48
1:A:577:ILE:O	1:A:579:SER:N	2.47	0.48
1:A:901:LEU:HA	1:A:907:THR:OG1	2.13	0.48
1:A:1070:GLN:O	1:A:1072:ILE:N	2.46	0.48
1:A:1259:MET:C	1:A:1261:LYS:H	2.16	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.09	0.48
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.94	0.48
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.32	0.48
3:C:100:THR:CG2	3:C:101:LEU:N	2.77	0.48
3:C:114:TYR:HB3	3:C:140:ASN:O	2.13	0.48
4:D:51:ASN:O	4:D:54:GLU:HB3	2.14	0.48
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.43	0.48
5:E:147:HIS:O	5:E:148:GLU:C	2.52	0.48
7:G:1:MET:O	7:G:3:PHE:CE1	2.67	0.48
7:G:91:VAL:HB	7:G:139:ILE:O	2.13	0.48
13:N:5:DA:H1'	13:N:6:DC:O5'	2.13	0.48
1:A:38:PRO:HB3	1:A:270:LEU:HG	1.95	0.48
1:A:53:LEU:CD2	1:A:54:ASN:HD22	2.27	0.48
1:A:313:GLN:O	1:A:314:ALA:HB3	2.13	0.48
1:A:639:PRO:CG	1:A:640:GLN:N	2.77	0.48
1:A:773:LYS:H	1:A:773:LYS:HG3	1.45	0.48
1:A:847:ASP:OD1	1:A:848:ILE:HG13	2.14	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.76	0.48
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.48
2:B:1060:ARG:C	2:B:1062:HIS:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:NH2	10:J:5:VAL:CG2	2.76	0.48
7:G:139:ILE:HG22	7:G:140:LYS:N	2.29	0.48
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.44	0.48
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.43	0.48
1:A:92:HIS:O	1:A:93:VAL:C	2.52	0.48
1:A:442:VAL:CB	1:A:489:LEU:HD11	2.40	0.48
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.13	0.48
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.78	0.48
2:B:308:TRP:CA	2:B:311:LEU:HD12	2.38	0.48
2:B:825:VAL:HG13	2:B:826:ALA:N	2.24	0.48
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.96	0.48
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.67	0.48
7:G:111:THR:HG22	7:G:113:HIS:N	2.27	0.48
1:A:334:GLY:O	1:A:335:ARG:C	2.52	0.47
1:A:445:ASN:ND2	1:A:446:ARG:N	2.61	0.47
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.94	0.47
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.29	0.47
2:B:34:ILE:O	2:B:35:SER:C	2.53	0.47
2:B:387:LEU:O	2:B:392:ARG:HB2	2.14	0.47
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.49	0.47
2:B:882:THR:HG21	2:B:884:ARG:HB2	1.96	0.47
3:C:254:LYS:C	3:C:256:ALA:N	2.65	0.47
3:C:259:LEU:HD13	11:K:91:CYS:HB2	1.96	0.47
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.49	0.47
10:J:16:ASP:O	10:J:18:TRP:N	2.47	0.47
1:A:49:LYS:CE	1:A:61:ILE:HD12	2.42	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.45	0.47
1:A:220:THR:O	1:A:221:SER:C	2.53	0.47
1:A:532:ARG:O	1:A:535:THR:HB	2.14	0.47
1:A:598:LEU:O	1:A:599:SER:C	2.53	0.47
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.79	0.47
1:A:684:ALA:O	1:A:687:LYS:HB2	2.14	0.47
1:A:967:ALA:O	1:A:968:GLN:O	2.32	0.47
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.96	0.47
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.29	0.47
1:A:1279:ILE:HG22	1:A:1279:ILE:O	2.14	0.47
2:B:189:LEU:O	2:B:190:TYR:C	2.53	0.47
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.97	0.47
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.29	0.47
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.92	0.47
3:C:33:LEU:O	3:C:34:ARG:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ILE:N	3:C:258:ILE:CD1	2.78	0.47
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.26	0.47
7:G:79:PHE:HZ	7:G:106:MET:HE1	1.80	0.47
12:L:27:LEU:O	12:L:28:LYS:HG2	2.14	0.47
1:A:243:PRO:O	1:A:244:PRO:C	2.52	0.47
1:A:500:GLU:OE2	2:B:1145:SER:CB	2.62	0.47
1:A:645:LEU:O	1:A:646:PHE:C	2.53	0.47
1:A:697:ALA:C	1:A:699:ALA:H	2.17	0.47
1:A:783:THR:HG22	1:A:784:LEU:HG	1.96	0.47
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.96	0.47
1:A:1151:GLU:HA	9:I:44:TYR:O	2.13	0.47
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.44	0.47
3:C:8:VAL:HG12	3:C:9:LYS:N	2.29	0.47
3:C:213:PRO:HG2	3:C:214:ASN:H	1.79	0.47
3:C:254:LYS:C	3:C:256:ALA:H	2.17	0.47
4:D:159:THR:O	4:D:163:VAL:HG23	2.13	0.47
5:E:67:GLU:O	5:E:70:SER:HB3	2.15	0.47
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.44	0.47
6:F:140:ASP:C	6:F:140:ASP:OD1	2.53	0.47
7:G:20:PRO:HG2	7:G:21:ARG:H	1.79	0.47
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.43	0.47
11:K:111:LEU:O	11:K:112:GLN:CB	2.62	0.47
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.94	0.47
1:A:528:LEU:HG	1:A:529:CYS:N	2.30	0.47
1:A:827:THR:O	1:A:831:THR:HB	2.13	0.47
1:A:901:LEU:H	1:A:926:GLN:HE21	1.58	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.47
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.77	0.47
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.97	0.47
2:B:637:LEU:O	2:B:690:VAL:HG13	2.14	0.47
2:B:785:TYR:CD1	2:B:785:TYR:C	2.87	0.47
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.78	0.47
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.22	0.47
5:E:136:ASN:OD1	5:E:137:GLU:N	2.48	0.47
8:H:89:LEU:C	8:H:91:ASP:N	2.67	0.47
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.97	0.47
1:A:242:PRO:HD3	2:B:1209:ALA:CB	2.44	0.47
1:A:699:ALA:O	1:A:700:ASN:CB	2.62	0.47
1:A:800:VAL:CG1	1:A:808:LEU:HG	2.43	0.47
1:A:964:ILE:O	1:A:967:ALA:HB3	2.14	0.47
1:A:1152:ILE:HG13	9:I:44:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:THR:HB	1:A:1406:VAL:H	1.47	0.47
2:B:130:VAL:HB	2:B:167:ILE:HD12	1.97	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.46	0.47
2:B:782:LEU:HD12	2:B:788:ARG:NH1	2.24	0.47
2:B:999:MET:HA	2:B:999:MET:HE3	1.96	0.47
2:B:1034:VAL:O	2:B:1037:LEU:N	2.42	0.47
3:C:31:ASN:O	3:C:32:SER:C	2.50	0.47
3:C:254:LYS:O	3:C:256:ALA:N	2.48	0.47
5:E:55:ARG:HD2	5:E:83:CYS:O	2.14	0.47
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.45	0.47
7:G:96:GLN:HG3	7:G:97:HIS:CD2	2.49	0.47
9:I:61:ASP:C	9:I:63:GLY:N	2.66	0.47
11:K:111:LEU:C	11:K:112:GLN:HE21	2.17	0.47
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.40	0.47
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.35	0.47
1:A:230:ARG:HB2	1:A:233:TRP:CE3	2.50	0.47
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.50	0.47
1:A:560:ILE:H	1:A:560:ILE:HG12	1.43	0.47
1:A:613:ILE:O	1:A:614:PHE:HB3	2.15	0.47
1:A:858:ASN:ND2	1:A:860:LEU:N	2.57	0.47
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.28	0.47
1:A:1327:ILE:O	1:A:1327:ILE:HG23	2.13	0.47
2:B:46:GLN:CG	2:B:47:GLN:H	2.21	0.47
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.45	0.47
2:B:1099:VAL:O	2:B:1101:ASP:N	2.47	0.47
2:B:1106:ARG:HH11	2:B:1110:PRO:HG2	1.77	0.47
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.45	0.47
8:H:93:TYR:CD1	8:H:93:TYR:N	2.82	0.47
11:K:109:TRP:O	11:K:111:LEU:N	2.47	0.47
1:A:166:GLY:O	1:A:167:CYS:CB	2.63	0.47
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.61	0.47
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.14	0.47
1:A:506:ALA:O	1:A:509:LEU:HB2	2.14	0.47
1:A:658:LEU:CD1	2:B:831:SER:H	2.26	0.47
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.44	0.47
1:A:947:PHE:HD2	1:A:954:TRP:CZ2	2.32	0.47
1:A:1067:LEU:HD12	1:A:1367:HIS:CE1	2.49	0.47
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.45	0.47
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.14	0.47
1:A:1454:MET:O	1:A:1454:MET:HG3	2.14	0.47
2:B:324:ILE:CG2	2:B:325:GLN:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.57	0.47
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.97	0.47
2:B:864:LYS:N	2:B:872:GLU:OE1	2.47	0.47
2:B:1142:GLY:O	2:B:1144:ALA:N	2.47	0.47
3:C:18:VAL:O	3:C:19:ASP:C	2.53	0.47
3:C:22:LEU:HD13	3:C:230:MET:CE	2.45	0.47
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.95	0.47
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.96	0.47
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.44	0.47
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.45	0.47
1:A:806:ARG:NH1	2:B:729:ILE:HG13	2.29	0.47
1:A:845:LEU:O	1:A:846:GLU:C	2.51	0.47
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.63	0.47
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.61	0.47
2:B:37:PHE:CE2	2:B:542:MET:HA	2.47	0.47
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:681:TRP:O	2:B:684:LEU:N	2.48	0.47
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.50	0.47
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.95	0.47
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.47
8:H:123:MET:HG2	8:H:124:ARG:N	2.29	0.47
10:J:36:LEU:O	10:J:37:SER:C	2.53	0.47
11:K:82:ASP:O	11:K:85:ASP:HB2	2.15	0.47
1:A:31:SER:OG	1:A:82:GLY:HA2	2.15	0.47
1:A:42:ASP:O	1:A:44:THR:N	2.36	0.47
1:A:58:LEU:O	1:A:59:GLY:O	2.33	0.47
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.30	0.47
1:A:1005:GLU:O	1:A:1006:ILE:C	2.53	0.47
1:A:1265:ASN:O	1:A:1268:LEU:N	2.46	0.47
2:B:472:ALA:C	2:B:474:SER:H	2.17	0.47
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.49	0.47
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.96	0.47
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.47
2:B:889:THR:HG22	2:B:891:ASP:HB2	1.97	0.47
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.97	0.47
2:B:1110:PRO:HG3	2:B:1124:ARG:O	2.14	0.47
2:B:1125:ASP:O	2:B:1125:ASP:OD1	2.33	0.47
2:B:1151:LEU:N	2:B:1151:LEU:CD1	2.77	0.47
4:D:191:ALA:C	4:D:193:THR:N	2.68	0.47
5:E:17:ARG:O	5:E:20:LYS:HB2	2.15	0.47
5:E:168:TYR:C	5:E:169:ARG:HG3	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG12	6:F:110:ASP:N	2.30	0.47
8:H:113:ALA:HB1	8:H:125:LEU:O	2.15	0.47
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.32	0.47
9:I:58:VAL:O	9:I:58:VAL:HG12	2.15	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.91	0.47
1:A:840:ARG:O	1:A:841:LEU:C	2.53	0.47
2:B:240:ILE:CD1	2:B:377:PHE:HE2	2.28	0.47
2:B:400:HIS:O	2:B:402:GLY:N	2.48	0.47
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.44	0.47
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.97	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
2:B:862:GLN:CG	2:B:963:PHE:HD1	2.25	0.47
3:C:16:ASP:O	3:C:17:ASN:CG	2.54	0.47
3:C:26:ASP:O	3:C:27:LEU:C	2.51	0.47
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.45	0.47
5:E:90:VAL:O	5:E:90:VAL:HG22	2.15	0.47
6:F:77:ASP:C	6:F:79:ARG:N	2.68	0.47
6:F:90:ARG:HD3	6:F:155:LEU:HD12	1.94	0.47
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.97	0.47
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.45	0.47
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.30	0.46
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.30	0.46
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.80	0.46
1:A:393:ARG:O	1:A:394:ASN:C	2.52	0.46
1:A:534:LEU:HD13	1:A:656:TRP:CD2	2.49	0.46
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.15	0.46
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.81	0.46
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.79	0.46
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.16	0.46
3:C:76:ASP:O	3:C:79:GLN:HG2	2.16	0.46
3:C:168:ALA:O	3:C:169:LYS:C	2.51	0.46
3:C:213:PRO:O	3:C:214:ASN:CB	2.62	0.46
6:F:143:PHE:HD1	6:F:143:PHE:O	1.99	0.46
7:G:110:VAL:HG22	7:G:161:GLY:O	2.15	0.46
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.38	0.46
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.80	0.46
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.40	0.46
1:A:577:ILE:O	1:A:580:VAL:N	2.46	0.46
1:A:877:HIS:O	1:A:878:ILE:CG1	2.63	0.46
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.16	0.46
1:A:1118:VAL:HG12	1:A:1327:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:THR:O	1:A:1325:THR:CG2	2.63	0.46
2:B:175:ARG:HH11	2:B:175:ARG:CG	2.20	0.46
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.78	0.46
2:B:459:TYR:CE1	2:B:469:GLN:HG2	2.51	0.46
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.15	0.46
3:C:67:LEU:HD13	3:C:157:CYS:SG	2.56	0.46
4:D:7:THR:O	4:D:7:THR:HG23	2.14	0.46
5:E:178:ILE:HG22	5:E:213:ILE:O	2.14	0.46
6:F:130:ILE:O	6:F:148:VAL:CG2	2.63	0.46
7:G:1:MET:SD	7:G:79:PHE:CE1	3.08	0.46
12:L:58:LYS:O	12:L:59:ALA:O	2.33	0.46
15:T:17:TT:H3R	15:T:19:DT:C5'	2.41	0.46
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.97	0.46
1:A:107:CYS:H	1:A:114:LEU:HD21	1.80	0.46
1:A:650:GLN:O	1:A:654:ASN:ND2	2.48	0.46
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.50	0.46
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.51	0.46
1:A:1163:ILE:HG22	1:A:1164:PRO:HD2	1.98	0.46
2:B:806:THR:HG22	2:B:808:ALA:CB	2.45	0.46
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.31	0.46
2:B:1197:PRO:O	2:B:1200:ALA:N	2.48	0.46
3:C:69:LEU:N	3:C:69:LEU:CD1	2.78	0.46
3:C:186:LEU:N	3:C:186:LEU:HD12	2.31	0.46
3:C:242:GLN:C	3:C:244:VAL:N	2.69	0.46
5:E:207:ARG:NH1	5:E:207:ARG:HB2	2.31	0.46
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.97	0.46
10:J:13:VAL:C	10:J:14:VAL:HG23	2.36	0.46
11:K:53:ASP:C	11:K:55:LYS:H	2.19	0.46
15:T:16:DT:C7	15:T:17:TT:C5A	2.93	0.46
1:A:511:ILE:O	1:A:519:PRO:HA	2.16	0.46
1:A:709:THR:HG22	1:A:710:LEU:N	2.29	0.46
1:A:873:MET:C	1:A:1058:VAL:CG2	2.84	0.46
1:A:940:ARG:HB3	1:A:941:LYS:HE3	1.98	0.46
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.45	0.46
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.46
2:B:654:ARG:O	2:B:656:GLY:N	2.49	0.46
2:B:1096:ARG:HH21	14:P:7:A:H4'	1.80	0.46
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.26	0.46
3:C:35:ARG:HH12	11:K:41:THR:H	1.63	0.46
3:C:74:SER:HB2	3:C:77:ILE:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:GLU:O	3:C:216:GLY:C	2.53	0.46
3:C:263:THR:O	3:C:265:MET:N	2.49	0.46
5:E:136:ASN:OD1	5:E:138:ALA:N	2.48	0.46
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.97	0.46
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.45	0.46
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.43	0.46
11:K:5:ASP:O	11:K:6:ARG:C	2.53	0.46
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.50	0.46
14:P:5:C:C2'	14:P:6:C:H5'	2.45	0.46
1:A:325:ILE:HG21	2:B:1210:MET:CG	2.40	0.46
1:A:335:ARG:HB3	1:A:336:ILE:H	1.63	0.46
1:A:525:GLN:CB	2:B:835:GLN:HG2	2.44	0.46
1:A:699:ALA:HB1	9:I:114:GLN:HB2	1.98	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.14	0.46
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.97	0.46
1:A:1364:ASN:O	1:A:1366:ARG:HG3	2.16	0.46
2:B:185:THR:H	2:B:188:ASP:CB	2.29	0.46
2:B:363:HIS:O	2:B:364:ILE:CB	2.53	0.46
2:B:908:GLU:O	2:B:909:ASP:O	2.33	0.46
3:C:86:CYS:O	3:C:88:CYS:N	2.49	0.46
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.03	0.46
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.46	0.46
9:I:15:TYR:N	9:I:15:TYR:CD1	2.84	0.46
11:K:65:HIS:HD2	11:K:67:PHE:N	1.94	0.46
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.81	0.46
1:A:537:ARG:NH1	8:H:120:GLY:O	2.48	0.46
1:A:722:LEU:O	1:A:725:ALA:HB3	2.14	0.46
1:A:815:PHE:O	1:A:816:HIS:C	2.53	0.46
1:A:841:LEU:O	1:A:845:LEU:HG	2.15	0.46
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.46
1:A:966:ASN:O	1:A:967:ALA:C	2.54	0.46
1:A:1236:LEU:O	1:A:1237:ILE:HG13	2.16	0.46
1:A:1260:LEU:O	1:A:1260:LEU:HG	2.15	0.46
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.98	0.46
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.97	0.46
4:D:53:SER:HB3	4:D:152:SER:CA	2.46	0.46
4:D:135:GLY:C	4:D:137:ASN:H	2.18	0.46
4:D:209:ARG:O	4:D:212:LYS:HB2	2.16	0.46
7:G:79:PHE:CZ	7:G:106:MET:HE1	2.51	0.46
9:I:100:PHE:N	9:I:100:PHE:HD1	2.13	0.46
11:K:29:ASN:O	11:K:76:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:85:ASP:O	11:K:88:LYS:HB2	2.16	0.46
12:L:46:VAL:O	12:L:46:VAL:HG12	2.16	0.46
13:N:2:DA:H2"	13:N:3:DG:OP2	2.16	0.46
1:A:195:ASP:O	1:A:196:GLU:HB3	2.16	0.46
1:A:575:LYS:NZ	1:A:615:GLY:H	2.13	0.46
1:A:816:HIS:CD2	2:B:764:SER:H	2.34	0.46
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.15	0.46
1:A:964:ILE:O	1:A:967:ALA:N	2.48	0.46
1:A:1019:CYS:O	1:A:1022:LEU:N	2.49	0.46
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.45	0.46
2:B:51:PHE:O	2:B:54:PHE:HB3	2.16	0.46
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.97	0.46
2:B:228:LYS:CB	2:B:261:ARG:HH22	2.29	0.46
2:B:906:SER:O	2:B:907:GLY:O	2.33	0.46
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.48	0.46
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.46
3:C:160:LYS:O	3:C:161:LYS:O	2.34	0.46
5:E:205:SER:O	5:E:206:GLY:C	2.53	0.46
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.61	0.46
1:A:326:ARG:HG2	1:A:327:ALA:N	2.30	0.46
1:A:443:LEU:O	1:A:489:LEU:HD12	2.16	0.46
1:A:847:ASP:O	1:A:858:ASN:HA	2.16	0.46
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.15	0.46
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.73	0.46
1:A:1265:ASN:C	1:A:1267:MET:N	2.68	0.46
2:B:114:PRO:HG2	2:B:115:GLN:N	2.27	0.46
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.46	0.46
2:B:311:LEU:O	2:B:312:GLU:C	2.54	0.46
2:B:1029:CYS:HA	2:B:1089:PRO:O	2.16	0.46
2:B:1081:LEU:O	2:B:1082:MET:C	2.54	0.46
2:B:1099:VAL:C	2:B:1101:ASP:H	2.19	0.46
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.30	0.46
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.46
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.51	0.46
9:I:112:SER:O	9:I:114:GLN:N	2.48	0.46
10:J:43:ARG:O	10:J:47:ARG:HB2	2.16	0.46
1:A:58:LEU:HD11	1:A:80:HIS:H	1.81	0.46
1:A:71:GLN:O	1:A:73:GLY:N	2.43	0.46
1:A:146:MET:HA	1:A:171:GLN:HB2	1.98	0.46
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.97	0.46
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:SER:O	1:A:327:ALA:HB3	2.15	0.46
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.81	0.46
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.98	0.46
1:A:909:ASP:O	1:A:911:SER:N	2.49	0.46
1:A:996:ASN:C	1:A:998:LEU:HD12	2.36	0.46
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.80	0.46
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.78	0.46
2:B:469:GLN:HB2	2:B:470:LYS:H	1.45	0.46
2:B:502:ILE:HD12	2:B:502:ILE:N	2.19	0.46
2:B:957:ASN:O	2:B:958:GLN:C	2.54	0.46
2:B:979:LYS:HG2	2:B:1095:LEU:HD13	1.98	0.46
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.50	0.46
3:C:37:MET:HA	3:C:41:ILE:HD11	1.98	0.46
3:C:239:PRO:O	3:C:240:VAL:C	2.53	0.46
4:D:53:SER:HB3	4:D:152:SER:HA	1.97	0.46
4:D:213:GLU:O	4:D:217:LEU:HG	2.16	0.46
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.31	0.46
7:G:22:MET:O	7:G:23:LYS:C	2.54	0.46
1:A:40:THR:C	1:A:41:MET:HG3	2.36	0.46
1:A:608:ILE:C	1:A:610:GLY:N	2.68	0.46
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.46
1:A:809:THR:H	1:A:812:GLU:HB2	1.81	0.46
1:A:960:ILE:O	1:A:961:ARG:C	2.54	0.46
2:B:29:ASP:HB3	2:B:658:ILE:HD11	1.97	0.46
2:B:897:GLY:O	2:B:898:LEU:HD23	2.16	0.46
2:B:942:ARG:NH2	15:T:25:DT:OP2	2.48	0.46
2:B:990:ILE:HG22	2:B:991:GLY:N	2.31	0.46
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.76	0.46
3:C:204:SER:C	3:C:206:ASN:N	2.70	0.46
7:G:20:PRO:CG	7:G:21:ARG:H	2.29	0.46
7:G:56:ILE:O	7:G:57:GLN:HB2	2.16	0.46
11:K:110:ASN:C	11:K:111:LEU:HG	2.36	0.46
1:A:298:PHE:O	1:A:301:ALA:HB3	2.16	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.98	0.45
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.45
2:B:828:ALA:O	2:B:834:ASN:ND2	2.49	0.45
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	0.45
4:D:7:THR:O	4:D:9:GLN:N	2.49	0.45
4:D:173:HIS:O	4:D:177:VAL:HG23	2.16	0.45
7:G:14:HIS:HD1	7:G:15:PRO:HD2	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:GLN:C	7:G:119:LEU:H	2.18	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.45	0.45
11:K:19:LEU:HD21	11:K:35:PHE:CE2	2.51	0.45
12:L:27:LEU:HD23	12:L:27:LEU:N	2.31	0.45
1:A:37:PHE:N	1:A:37:PHE:HD1	2.10	0.45
1:A:70:CYS:O	1:A:70:CYS:SG	2.74	0.45
1:A:119:ASN:O	1:A:122:MET:HB3	2.16	0.45
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.80	0.45
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.36	0.45
1:A:569:LYS:O	1:A:571:LEU:HD13	2.15	0.45
1:A:774:ARG:H	1:A:774:ARG:HG2	1.42	0.45
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.63	0.45
2:B:225:VAL:HA	2:B:237:VAL:O	2.16	0.45
2:B:230:ALA:N	2:B:231:PRO:HD2	2.31	0.45
2:B:259:TYR:HD1	2:B:259:TYR:H	1.65	0.45
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.31	0.45
2:B:764:SER:HB3	2:B:765:PRO:CD	2.46	0.45
2:B:842:ASN:HD22	2:B:845:SER:CB	2.30	0.45
2:B:844:SER:O	2:B:847:ASP:N	2.49	0.45
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.16	0.45
3:C:31:ASN:O	3:C:34:ARG:N	2.49	0.45
1:A:75:ASN:HA	2:B:1116:ARG:HH22	1.81	0.45
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.97	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.99	0.45
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.46	0.45
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.98	0.45
1:A:979:SER:HG	1:A:981:LEU:HG	1.80	0.45
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.45
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.45
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.98	0.45
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.50	0.45
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.97	0.45
8:H:62:SER:C	8:H:64:ASN:N	2.69	0.45
9:I:14:LEU:HD22	9:I:28:GLU:O	2.17	0.45
10:J:2:ILE:H	10:J:57:ILE:CG2	2.29	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.45
2:B:210:LYS:HD3	2:B:481:GLN:O	2.17	0.45
2:B:286:PHE:CD1	2:B:297:ILE:HG23	2.51	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.33	0.45
2:B:365:THR:HG23	2:B:367:LEU:N	2.25	0.45
2:B:776:GLN:O	2:B:1095:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.97	0.45
2:B:980:PHE:CA	2:B:1095:LEU:HD11	2.46	0.45
2:B:1011:ILE:O	2:B:1011:ILE:HG22	2.16	0.45
3:C:77:ILE:C	3:C:79:GLN:H	2.19	0.45
4:D:17:LYS:HE3	4:D:17:LYS:N	2.32	0.45
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.48	0.45
7:G:44:TYR:O	7:G:78:VAL:HG12	2.17	0.45
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.45
12:L:31:CYS:HB3	12:L:34:CYS:C	2.37	0.45
1:A:81:PHE:CZ	2:B:1208:MET:HB2	2.52	0.45
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.52	0.45
1:A:367:PRO:HB3	1:A:465:TYR:O	2.16	0.45
1:A:408:ASP:C	1:A:410:GLY:H	2.18	0.45
1:A:834:THR:HG21	1:A:1077:THR:HA	1.99	0.45
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.46	0.45
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.32	0.45
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.98	0.45
2:B:763:GLN:O	2:B:764:SER:C	2.55	0.45
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.99	0.45
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.98	0.45
3:C:66:ARG:HH21	10:J:5:VAL:H	1.65	0.45
5:E:55:ARG:O	5:E:57:MET:N	2.50	0.45
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.44	0.45
5:E:124:VAL:N	5:E:125:PRO:HD2	2.32	0.45
8:H:99:GLY:N	8:H:118:PHE:HD2	2.14	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.54	0.45
12:L:49:LYS:O	12:L:50:ASP:CB	2.64	0.45
1:A:58:LEU:CD1	1:A:80:HIS:H	2.29	0.45
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.45
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.81	0.45
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.51	0.45
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.46	0.45
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.98	0.45
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.78	0.45
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.82	0.45
2:B:388:CYS:C	2:B:390:LEU:N	2.69	0.45
2:B:847:ASP:C	2:B:849:GLY:N	2.70	0.45
2:B:1138:MET:HA	2:B:1138:MET:CE	2.46	0.45
3:C:161:LYS:O	3:C:170:TRP:NE1	2.49	0.45
10:J:2:ILE:HG22	10:J:3:VAL:N	2.32	0.45
11:K:111:LEU:C	11:K:112:GLN:HG2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:O	1:A:435:HIS:CD2	2.70	0.45
1:A:741:ASN:ND2	1:A:744:LYS:H	2.14	0.45
1:A:920:LEU:HD23	1:A:920:LEU:C	2.37	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.81	0.45
1:A:1323:ASP:C	1:A:1325:THR:H	2.19	0.45
1:A:1325:THR:O	1:A:1325:THR:HG22	2.17	0.45
2:B:383:ASN:O	2:B:384:ARG:C	2.55	0.45
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.45
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.80	0.45
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.47	0.45
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.17	0.45
2:B:1182:CYS:O	2:B:1183:LYS:C	2.54	0.45
4:D:146:GLN:O	4:D:149:THR:HG22	2.16	0.45
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.19	0.45
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.17	0.45
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.98	0.45
8:H:4:THR:HG22	8:H:5:LEU:H	1.82	0.45
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.98	0.45
1:A:26:GLU:O	1:A:27:VAL:C	2.54	0.45
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.45
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.98	0.45
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.80	0.45
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.99	0.45
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.23	0.45
1:A:723:ASN:C	1:A:725:ALA:N	2.69	0.45
1:A:1074:GLU:C	1:A:1076:ALA:N	2.69	0.45
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.82	0.45
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.99	0.45
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.98	0.45
2:B:240:ILE:HG23	2:B:240:ILE:O	2.17	0.45
2:B:446:LEU:N	2:B:446:LEU:HD23	2.32	0.45
2:B:879:ARG:O	2:B:880:THR:HB	2.17	0.45
2:B:1223:ASP:O	2:B:1224:PHE:HB2	2.17	0.45
3:C:8:VAL:HG12	3:C:9:LYS:H	1.82	0.45
3:C:55:THR:O	3:C:55:THR:HG22	2.16	0.45
3:C:99:LEU:CD1	3:C:118:LEU:HB3	2.43	0.45
4:D:137:ASN:C	4:D:137:ASN:HD22	2.21	0.45
4:D:187:THR:HG22	4:D:188:ALA:H	1.82	0.45
7:G:77:VAL:O	7:G:77:VAL:HG12	2.16	0.45
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.77	0.45
9:I:34:TYR:HD2	9:I:35:VAL:CA	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LEU:O	1:A:939:ASP:HB2	2.16	0.45
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.17	0.45
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.17	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.98	0.45
2:B:948:ILE:HG22	2:B:949:VAL:O	2.16	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.51	0.45
2:B:1031:LEU:HD23	2:B:1044:ALA:HB2	1.97	0.45
3:C:88:CYS:SG	3:C:91:HIS:HA	2.57	0.45
4:D:51:ASN:C	4:D:52:LEU:O	2.54	0.45
9:I:61:ASP:O	9:I:63:GLY:N	2.50	0.45
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.47	0.45
15:T:24:DG:H2"	15:T:25:DT:H5'	1.99	0.45
1:A:326:ARG:CG	1:A:327:ALA:N	2.79	0.45
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.81	0.45
1:A:590:ARG:HB3	1:A:605:MET:N	2.31	0.45
1:A:696:GLU:O	1:A:696:GLU:HG2	2.17	0.45
2:B:18:PHE:N	2:B:19:GLU:N	2.65	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.99	0.45
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.98	0.45
2:B:769:TYR:C	2:B:771:SER:N	2.70	0.45
2:B:976:ILE:O	2:B:990:ILE:HB	2.16	0.45
2:B:998:ASP:HB3	2:B:1076:HIS:HE1	1.82	0.45
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.17	0.45
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.81	0.45
5:E:30:ILE:CG2	5:E:31:THR:N	2.79	0.45
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.47	0.45
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.52	0.45
11:K:98:LEU:O	11:K:101:LEU:N	2.50	0.45
12:L:30:ILE:HG22	12:L:31:CYS:N	2.32	0.45
1:A:277:GLU:C	1:A:279:LEU:H	2.19	0.44
1:A:500:GLU:O	1:A:504:LEU:HD13	2.17	0.44
1:A:665:GLY:O	1:A:666:ILE:C	2.56	0.44
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.17	0.44
2:B:189:LEU:O	2:B:192:LEU:HB2	2.16	0.44
2:B:226:PHE:CD1	2:B:398:ARG:NH2	2.85	0.44
2:B:460:ALA:C	2:B:462:ALA:H	2.20	0.44
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.38	0.44
2:B:834:ASN:ND2	2:B:1013:ASN:HB2	2.32	0.44
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.44
4:D:151:PHE:H	4:D:151:PHE:HD1	1.63	0.44
7:G:106:MET:CG	7:G:107:LYS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:HG22	1:A:175:ARG:N	2.33	0.44
1:A:381:THR:HG22	1:A:383:TYR:N	2.32	0.44
1:A:453:MET:C	1:A:455:MET:N	2.70	0.44
1:A:925:LEU:C	1:A:927:VAL:H	2.21	0.44
1:A:1132:LYS:O	1:A:1135:ARG:N	2.50	0.44
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.52	0.44
2:B:848:ARG:NH1	10:J:8:PHE:O	2.50	0.44
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.99	0.44
2:B:1147:LEU:C	2:B:1147:LEU:HD23	2.37	0.44
3:C:39:ALA:HA	3:C:164:ALA:CB	2.44	0.44
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.00	0.44
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.34	0.44
7:G:1:MET:HE1	7:G:80:LYS:N	2.29	0.44
8:H:10:PHE:HA	8:H:29:ALA:O	2.17	0.44
1:A:71:GLN:HG3	1:A:72:GLU:N	2.33	0.44
1:A:494:SER:O	1:A:497:THR:N	2.45	0.44
1:A:779:PHE:CE1	1:A:785:PRO:CD	2.93	0.44
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.99	0.44
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.52	0.44
2:B:310:MET:O	2:B:313:MET:HB2	2.18	0.44
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.50	0.44
2:B:694:ASP:O	2:B:698:GLU:HB2	2.17	0.44
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.65	0.44
2:B:910:VAL:HG12	2:B:911:ILE:N	2.32	0.44
5:E:161:LYS:C	5:E:163:GLU:H	2.20	0.44
7:G:34:VAL:O	7:G:36:GLY:N	2.51	0.44
8:H:39:THR:O	8:H:123:MET:HA	2.18	0.44
10:J:52:THR:O	10:J:53:HIS:C	2.56	0.44
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.47	0.44
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.44
1:A:329:LEU:HD12	1:A:1406:VAL:HG22	2.00	0.44
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.50	0.44
1:A:679:ILE:O	1:A:683:ILE:HG13	2.17	0.44
1:A:826:ASP:HB2	1:A:830:LYS:HD3	2.00	0.44
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.98	0.44
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.52	0.44
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.99	0.44
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.99	0.44
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.52	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.83	0.44
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:LYS:HB2	2:B:261:ARG:HH22	1.82	0.44
2:B:258:LEU:O	2:B:258:LEU:CG	2.64	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:424:LEU:O	2:B:428:ILE:HG13	2.17	0.44
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.45	0.44
2:B:785:TYR:CD1	2:B:786:ASN:N	2.86	0.44
3:C:77:ILE:HG22	3:C:78:GLU:N	2.33	0.44
3:C:83:SER:OG	3:C:160:LYS:HD3	2.16	0.44
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.32	0.44
3:C:252:GLN:O	3:C:253:LYS:C	2.54	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
9:I:32:CYS:SG	9:I:33:SER:N	2.90	0.44
10:J:41:LEU:HD23	10:J:41:LEU:N	2.32	0.44
15:T:16:DT:C2'	15:T:17:TT:O2P	2.54	0.44
1:A:107:CYS:O	1:A:111:GLY:HA2	2.17	0.44
1:A:322:VAL:O	1:A:322:VAL:HG12	2.16	0.44
1:A:399:HIS:CG	1:A:400:PRO:N	2.85	0.44
1:A:528:LEU:C	1:A:528:LEU:HD12	2.38	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.44
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.33	0.44
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.44
2:B:838:SER:HA	2:B:989:THR:O	2.18	0.44
2:B:844:SER:O	2:B:847:ASP:HB2	2.18	0.44
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.77	0.44
3:C:10:ILE:HG22	3:C:11:ARG:O	2.18	0.44
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.44
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.53	0.44
10:J:34:THR:O	10:J:35:ALA:C	2.56	0.44
11:K:7:PHE:CD1	11:K:7:PHE:C	2.90	0.44
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.00	0.44
1:A:166:GLY:O	1:A:167:CYS:SG	2.76	0.44
1:A:268:ASP:O	1:A:269:ILE:C	2.54	0.44
1:A:289:ILE:C	1:A:291:GLU:N	2.70	0.44
1:A:463:ILE:HD12	1:A:469:ARG:CD	2.47	0.44
1:A:786:HIS:N	1:A:786:HIS:CD2	2.84	0.44
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.97	0.44
1:A:940:ARG:HG2	1:A:940:ARG:NH1	2.33	0.44
2:B:45:SER:OG	2:B:46:GLN:N	2.47	0.44
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.48	0.44
2:B:641:GLU:C	2:B:643:ASP:H	2.21	0.44
2:B:792:MET:H	2:B:857:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.18	0.44
7:G:8:SER:HB3	7:G:73:LYS:HD2	2.00	0.44
10:J:57:ILE:CA	10:J:60:PHE:HD2	2.24	0.44
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.47	0.44
1:A:71:GLN:C	1:A:73:GLY:N	2.71	0.44
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.82	0.44
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.82	0.44
1:A:767:GLN:HA	1:A:799:PHE:HA	1.99	0.44
1:A:867:ILE:HG22	1:A:872:GLY:N	2.33	0.44
1:A:896:ARG:HH22	1:A:1030:ARG:HH21	1.65	0.44
1:A:1343:ALA:HB1	5:E:149:LEU:HB2	1.99	0.44
2:B:30:SER:HB3	2:B:743:ILE:O	2.17	0.44
2:B:327:ARG:O	2:B:331:LEU:HD13	2.18	0.44
2:B:558:LEU:O	2:B:561:TRP:N	2.49	0.44
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.47	0.44
2:B:948:ILE:HD12	2:B:969:ARG:HH12	1.82	0.44
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.00	0.44
3:C:79:GLN:O	3:C:127:ARG:NH1	2.51	0.44
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.53	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.31	0.44
6:F:100:GLN:O	6:F:103:MET:HB2	2.18	0.44
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.53	0.44
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.48	0.44
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.52	0.44
11:K:57:LEU:N	11:K:76:GLN:O	2.51	0.44
1:A:58:LEU:HD11	1:A:243:PRO:HB2	1.96	0.44
1:A:1036:ARG:HH11	1:A:1036:ARG:CG	2.31	0.44
1:A:1095:THR:O	1:A:1096:SER:CB	2.66	0.44
2:B:641:GLU:HB3	2:B:643:ASP:OD2	2.17	0.44
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.00	0.44
3:C:58:LEU:HD22	3:C:58:LEU:N	2.33	0.44
4:D:53:SER:HB3	4:D:153:ARG:N	2.31	0.44
4:D:146:GLN:O	4:D:147:TYR:C	2.55	0.44
4:D:153:ARG:C	4:D:154:PHE:CD1	2.91	0.44
4:D:170:THR:HG21	4:D:172:LEU:CD1	2.48	0.44
15:T:22:BRU:H2'	15:T:23:DG:H8	1.76	0.44
1:A:23:SER:CB	1:A:233:TRP:NE1	2.81	0.44
1:A:32:VAL:O	1:A:32:VAL:HG23	2.17	0.44
1:A:55:ASP:C	1:A:57:ARG:N	2.68	0.44
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.99	0.44
1:A:1205:LYS:O	1:A:1206:ASP:C	2.56	0.44
2:B:616:ILE:N	2:B:616:ILE:CD1	2.81	0.44
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.53	0.44
2:B:880:THR:HB	2:B:934:LYS:HD2	1.98	0.44
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.30	0.44
3:C:255:VAL:HG12	11:K:91:CYS:HB3	1.99	0.44
5:E:93:MET:SD	5:E:97:VAL:HG23	2.58	0.44
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.74	0.44
12:L:48:CYS:SG	12:L:49:LYS:N	2.91	0.44
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.98	0.43
1:A:541:ILE:N	1:A:572:TRP:O	2.42	0.43
1:A:682:THR:HA	1:A:685:GLU:HG2	2.00	0.43
1:A:968:GLN:C	1:A:970:THR:H	2.21	0.43
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.18	0.43
2:B:244:LEU:C	2:B:246:LYS:N	2.71	0.43
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.43
2:B:681:TRP:O	2:B:683:SER:N	2.51	0.43
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.59	0.43
2:B:1002:THR:O	2:B:1003:ALA:C	2.56	0.43
2:B:1087:PHE:CD2	2:B:1087:PHE:C	2.92	0.43
3:C:69:LEU:HD12	3:C:69:LEU:H	1.79	0.43
4:D:63:LEU:O	4:D:129:LEU:HD11	2.18	0.43
4:D:130:LEU:C	4:D:132:GLN:N	2.70	0.43
5:E:191:LYS:O	5:E:193:GLY:N	2.50	0.43
7:G:1:MET:O	7:G:1:MET:CE	2.66	0.43
7:G:45:ILE:HD13	7:G:45:ILE:HA	1.88	0.43
7:G:106:MET:HE2	7:G:106:MET:HB3	1.61	0.43
13:N:0:DT:H71	13:N:1:DA:N6	2.33	0.43
1:A:164:ARG:CG	1:A:165:GLY:N	2.77	0.43
1:A:973:ILE:HD13	1:A:1036:ARG:O	2.17	0.43
2:B:54:PHE:O	2:B:58:THR:HB	2.17	0.43
2:B:172:ILE:CG2	2:B:173:MET:N	2.82	0.43
2:B:903:VAL:HG12	2:B:904:ARG:N	2.33	0.43
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.52	0.43
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	2.16	0.43
1:A:35:ILE:O	1:A:35:ILE:CG2	2.63	0.43
1:A:208:LEU:HD21	1:A:212:LYS:HE3	2.00	0.43
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.98	0.43
1:A:821:ARG:HD2	1:A:825:ILE:CD1	2.45	0.43
1:A:1037:LEU:HD12	1:A:1042:PHE:HD1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.81	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.51	0.43
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.43
2:B:231:PRO:O	2:B:232:SER:HB2	2.18	0.43
2:B:235:SER:HA	2:B:261:ARG:NH1	2.33	0.43
2:B:433:GLN:O	2:B:437:GLU:HG3	2.19	0.43
2:B:759:PRO:C	2:B:761:HIS:H	2.21	0.43
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.38	0.43
2:B:877:PRO:C	2:B:878:GLN:HG3	2.38	0.43
2:B:1102:LYS:O	2:B:1103:ILE:C	2.56	0.43
2:B:1196:ILE:O	2:B:1196:ILE:HG13	2.17	0.43
3:C:53:THR:O	3:C:153:LEU:HA	2.17	0.43
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.53	0.43
5:E:61:GLN:HG2	5:E:62:ALA:N	2.33	0.43
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.66	0.43
8:H:18:GLY:O	8:H:19:ARG:HB2	2.19	0.43
8:H:31:THR:O	8:H:31:THR:HG22	2.18	0.43
9:I:75:CYS:SG	9:I:78:CYS:C	2.96	0.43
10:J:14:VAL:O	10:J:14:VAL:CG1	2.60	0.43
1:A:584:ASN:O	1:A:637:LYS:HE3	2.18	0.43
1:A:618:GLU:O	1:A:620:LYS:N	2.52	0.43
1:A:710:LEU:HD12	1:A:710:LEU:N	2.33	0.43
1:A:815:PHE:C	1:A:817:ALA:N	2.69	0.43
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.00	0.43
1:A:1226:VAL:HG13	1:A:1239:ARG:O	2.19	0.43
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	2.01	0.43
1:A:1315:GLU:C	1:A:1317:MET:N	2.71	0.43
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.82	0.43
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.53	0.43
2:B:360:PHE:O	2:B:361:LEU:C	2.56	0.43
2:B:459:TYR:C	2:B:459:TYR:CD2	2.92	0.43
2:B:806:THR:C	2:B:808:ALA:N	2.69	0.43
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.83	0.43
3:C:124:LEU:O	3:C:125:MET:HB2	2.18	0.43
4:D:195:ILE:C	4:D:197:SER:H	2.22	0.43
7:G:13:LEU:O	7:G:67:SER:HA	2.18	0.43
8:H:47:PHE:CD2	8:H:47:PHE:O	2.72	0.43
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.99	0.43
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.43
1:A:115:LEU:HB2	1:A:122:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.83	0.43
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.16	0.43
2:B:34:ILE:O	2:B:37:PHE:HB3	2.18	0.43
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.53	0.43
2:B:899:ILE:HD13	2:B:905:VAL:HG11	2.00	0.43
2:B:1023:VAL:O	2:B:1024:ALA:C	2.57	0.43
2:B:1047:PHE:CD1	2:B:1047:PHE:N	2.76	0.43
2:B:1200:ALA:O	2:B:1203:LEU:HB3	2.18	0.43
3:C:123:ASN:ND2	3:C:125:MET:SD	2.91	0.43
7:G:138:THR:O	7:G:139:ILE:O	2.37	0.43
10:J:53:HIS:CD2	10:J:54:VAL:N	2.86	0.43
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.00	0.43
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.33	0.43
15:T:11:DG:H2"	15:T:12:DT:OP2	2.18	0.43
1:A:89:PRO:HB3	1:A:208:LEU:HD12	2.00	0.43
1:A:406:ILE:HG13	1:A:431:LYS:HB2	2.00	0.43
1:A:450:LEU:HB3	1:A:838:GLN:HE21	1.79	0.43
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.81	0.43
1:A:897:TYR:N	1:A:897:TYR:CD1	2.87	0.43
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.43
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.52	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.34	0.43
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.35	0.43
2:B:865:LYS:NZ	2:B:869:SER:HA	2.34	0.43
2:B:980:PHE:HE2	2:B:1094:ARG:CG	2.31	0.43
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.84	0.43
3:C:168:ALA:C	3:C:170:TRP:H	2.20	0.43
4:D:194:LEU:C	4:D:195:ILE:HG13	2.39	0.43
8:H:59:ILE:O	8:H:60:ALA:HB3	2.18	0.43
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.83	0.43
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.31	0.43
1:A:43:GLU:O	1:A:44:THR:HB	2.19	0.43
1:A:262:LEU:C	1:A:264:PHE:N	2.72	0.43
1:A:402:ALA:HB1	1:A:433:GLU:O	2.19	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.53	0.43
1:A:742:ASN:O	1:A:745:GLN:N	2.52	0.43
1:A:935:GLN:O	1:A:936:LEU:C	2.56	0.43
2:B:90:ILE:HD11	2:B:432:MET:SD	2.59	0.43
2:B:263:GLY:O	2:B:264:SER:C	2.56	0.43
2:B:329:THR:O	2:B:332:ASP:HB3	2.19	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.45	0.43
2:B:1106:ARG:NH1	2:B:1110:PRO:CD	2.81	0.43
3:C:67:LEU:HD11	3:C:155:LEU:HD12	1.99	0.43
3:C:83:SER:O	3:C:85:ASP:N	2.52	0.43
3:C:120:ILE:HD13	3:C:124:LEU:HD21	2.01	0.43
4:D:14:ARG:O	4:D:15:LEU:HB3	2.19	0.43
5:E:157:SER:OG	5:E:159:ASP:HB2	2.17	0.43
7:G:106:MET:HG2	7:G:107:LYS:N	2.33	0.43
11:K:88:LYS:O	11:K:91:CYS:N	2.47	0.43
1:A:75:ASN:O	1:A:76:GLU:HB2	2.19	0.43
1:A:907:THR:HG23	1:A:908:LEU:N	2.33	0.43
1:A:1291:VAL:CG1	1:A:1292:PRO:N	2.81	0.43
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.91	0.43
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.99	0.43
2:B:336:ARG:NH2	2:B:345:LYS:CE	2.78	0.43
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.83	0.43
2:B:784:ASN:O	2:B:788:ARG:HG3	2.19	0.43
2:B:842:ASN:O	2:B:846:ILE:HG13	2.19	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.01	0.43
3:C:141:GLY:HA2	10:J:16:ASP:HB3	2.00	0.43
4:D:193:THR:O	4:D:196:PRO:HD3	2.19	0.43
5:E:9:ILE:HD11	5:E:53:PRO:HD3	2.01	0.43
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.66	0.43
1:A:35:ILE:HD13	1:A:241:VAL:HG21	2.00	0.43
1:A:56:PRO:O	1:A:57:ARG:HG3	2.19	0.43
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.43
1:A:482:PHE:C	1:A:484:GLY:N	2.70	0.43
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.49	0.43
1:A:1163:ILE:CG2	1:A:1164:PRO:HD2	2.49	0.43
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.39	0.43
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.48	0.43
2:B:251:ILE:O	2:B:251:ILE:HG22	2.19	0.43
2:B:726:ALA:O	2:B:727:LYS:O	2.36	0.43
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.36	0.43
2:B:1106:ARG:HH12	2:B:1110:PRO:CG	2.31	0.43
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.84	0.43
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.43
8:H:116:TYR:HB2	8:H:123:MET:HB3	2.00	0.43
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.54	0.43
1:A:662:PHE:HB3	2:B:829:CYS:HB2	2.01	0.43
1:A:682:THR:HG23	1:A:728:LYS:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ALA:O	1:A:818:MET:C	2.56	0.43
1:A:817:ALA:O	1:A:820:GLY:N	2.52	0.43
1:A:1125:ALA:C	1:A:1127:ASP:H	2.22	0.43
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.19	0.43
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.43
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.54	0.43
1:A:1348:LEU:CG	1:A:1372:VAL:HG22	2.47	0.43
2:B:683:SER:C	2:B:685:LEU:N	2.73	0.43
2:B:809:MET:O	2:B:812:LEU:N	2.49	0.43
2:B:820:GLY:C	2:B:1091:TYR:CE1	2.92	0.43
2:B:821:GLN:HE22	2:B:851:PHE:N	2.17	0.43
2:B:1072:MET:CE	2:B:1087:PHE:HD1	2.32	0.43
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.67	0.43
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.43
5:E:177:ARG:HD3	5:E:215:MET:HG2	2.01	0.43
15:T:26:DC:C2'	15:T:27:DA:O5'	2.67	0.43
1:A:335:ARG:O	1:A:336:ILE:C	2.55	0.42
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.42
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.49	0.42
1:A:1193:LEU:HD22	1:A:1260:LEU:CD1	2.47	0.42
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.49	0.42
2:B:54:PHE:HA	2:B:58:THR:HB	2.01	0.42
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.42
2:B:579:ARG:N	2:B:589:VAL:HG13	2.34	0.42
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.39	0.42
6:F:88:TYR:CD1	6:F:88:TYR:N	2.87	0.42
1:A:12:ARG:NE	2:B:1192:TYR:CE2	2.83	0.42
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.31	0.42
1:A:276:LEU:O	1:A:279:LEU:HB2	2.19	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.54	0.42
1:A:742:ASN:O	1:A:745:GLN:HB2	2.18	0.42
1:A:867:ILE:CG2	1:A:872:GLY:N	2.82	0.42
1:A:1053:PHE:O	1:A:1055:ARG:N	2.53	0.42
1:A:1225:PHE:HE2	1:A:1227:ILE:HD11	1.84	0.42
2:B:312:GLU:O	2:B:315:LYS:HB2	2.20	0.42
2:B:487:THR:O	2:B:490:SER:HB3	2.19	0.42
2:B:604:ARG:O	2:B:606:LYS:N	2.52	0.42
2:B:952:VAL:HG12	2:B:953:LEU:N	2.34	0.42
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	2.15	0.42
4:D:7:THR:HB	7:G:42:PHE:CZ	2.54	0.42
4:D:50:LEU:HD11	4:D:58:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ILE:HG22	5:E:117:THR:N	2.34	0.42
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.40	0.42
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.42
9:I:4:PHE:CD1	9:I:4:PHE:C	2.92	0.42
1:A:58:LEU:HG	1:A:244:PRO:HD2	2.00	0.42
1:A:218:ASP:HA	1:A:221:SER:OG	2.19	0.42
1:A:332:LYS:HA	1:A:337:ARG:HD2	2.02	0.42
1:A:353:ILE:HD11	1:A:480:ALA:HB1	2.00	0.42
1:A:709:THR:HG21	9:I:93:LYS:O	2.18	0.42
1:A:731:ARG:O	1:A:735:VAL:HG23	2.18	0.42
1:A:858:ASN:HD22	1:A:861:GLY:H	1.67	0.42
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.30	0.42
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.54	0.42
1:A:1277:GLU:C	1:A:1279:ILE:H	2.21	0.42
1:A:1373:ASP:O	1:A:1376:THR:N	2.49	0.42
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.19	0.42
2:B:102:VAL:HG12	2:B:104:GLU:HG2	2.01	0.42
2:B:196:PRO:HG2	2:B:197:PHE:N	2.34	0.42
2:B:497:ARG:NH2	2:B:775:LYS:HZ1	2.17	0.42
2:B:521:LEU:HD13	2:B:633:VAL:HB	2.01	0.42
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.54	0.42
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.01	0.42
3:C:179:GLU:O	3:C:180:TYR:HB3	2.18	0.42
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.02	0.42
5:E:177:ARG:O	5:E:212:ARG:HD3	2.18	0.42
6:F:120:ILE:O	6:F:123:LYS:HB3	2.19	0.42
7:G:91:VAL:HG23	7:G:141:SER:O	2.18	0.42
7:G:137:ILE:HG21	7:G:143:ILE:HD11	2.01	0.42
8:H:55:LEU:HD22	8:H:144:ILE:HG21	2.00	0.42
11:K:84:LYS:O	11:K:87:LEU:HB3	2.19	0.42
12:L:61:THR:HG22	12:L:63:ARG:HG2	2.02	0.42
1:A:388:LEU:O	1:A:392:VAL:HG23	2.19	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.42
1:A:848:ILE:HA	1:A:857:ARG:O	2.20	0.42
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.42
2:B:419:THR:O	2:B:419:THR:HG22	2.19	0.42
2:B:582:VAL:HG12	2:B:582:VAL:O	2.19	0.42
2:B:778:MET:SD	2:B:794:ASN:HB3	2.59	0.42
2:B:873:THR:HG22	2:B:874:PHE:N	2.34	0.42
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.43	0.42
3:C:144:ILE:O	3:C:145:CYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:PRO:O	3:C:241:ASP:N	2.53	0.42
4:D:40:HIS:CG	4:D:41:GLN:N	2.87	0.42
5:E:63:ASN:HA	5:E:64:PRO:HD3	1.86	0.42
8:H:127:GLY:O	8:H:128:ASN:CB	2.65	0.42
10:J:13:VAL:O	10:J:14:VAL:HG23	2.19	0.42
13:N:4:DT:H5'	13:N:4:DT:C6	2.55	0.42
15:T:17:TT:H1'	15:T:17:TT:C5R	2.48	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.68	0.42
1:A:299:HIS:C	1:A:301:ALA:N	2.73	0.42
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.38	0.42
1:A:499:ALA:O	1:A:503:GLN:HG2	2.20	0.42
1:A:723:ASN:O	1:A:725:ALA:N	2.53	0.42
1:A:935:GLN:O	1:A:938:LYS:N	2.52	0.42
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.81	0.42
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.80	0.42
2:B:294:ASP:O	2:B:296:GLU:N	2.49	0.42
2:B:365:THR:HG23	2:B:367:LEU:CG	2.45	0.42
2:B:582:VAL:O	2:B:582:VAL:CG1	2.67	0.42
2:B:597:MET:C	2:B:599:THR:H	2.23	0.42
2:B:610:ASN:O	2:B:612:GLU:N	2.52	0.42
2:B:640:VAL:HB	2:B:738:PHE:O	2.20	0.42
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.19	0.42
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.20	0.42
2:B:1121:GLY:C	2:B:1123:SER:N	2.69	0.42
2:B:1182:CYS:C	2:B:1183:LYS:O	2.56	0.42
4:D:131:GLU:O	4:D:132:GLN:HG2	2.19	0.42
5:E:168:TYR:CB	5:E:170:LEU:HG	2.49	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
11:K:95:ILE:O	11:K:98:LEU:N	2.53	0.42
1:A:24:PRO:O	1:A:28:ARG:HG3	2.19	0.42
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.54	0.42
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.20	0.42
1:A:340:LEU:HD23	2:B:1199:ALA:HB3	2.01	0.42
1:A:402:ALA:HB1	1:A:434:ARG:HA	2.02	0.42
1:A:482:PHE:O	1:A:484:GLY:N	2.48	0.42
1:A:586:ILE:CD1	1:A:633:VAL:HG22	2.50	0.42
1:A:857:ARG:HD3	1:A:861:GLY:O	2.20	0.42
1:A:1157:ASP:C	1:A:1159:ARG:H	2.23	0.42
1:A:1423:GLY:O	1:A:1426:GLU:HB2	2.20	0.42
2:B:101:MET:O	2:B:102:VAL:CG2	2.68	0.42
2:B:185:THR:O	2:B:186:GLU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:O	2:B:607:GLY:N	2.53	0.42
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.01	0.42
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.34	0.42
2:B:1087:PHE:HD2	2:B:1087:PHE:C	2.23	0.42
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.83	0.42
7:G:27:LYS:O	7:G:28:THR:C	2.57	0.42
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.54	0.42
10:J:57:ILE:O	10:J:60:PHE:HB2	2.19	0.42
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.20	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.84	0.42
1:A:981:LEU:HD21	1:A:1038:THR:C	2.40	0.42
1:A:1013:ASP:C	1:A:1015:VAL:H	2.20	0.42
1:A:1402:PHE:O	1:A:1402:PHE:CG	2.73	0.42
2:B:128:LEU:HB2	2:B:168:GLY:O	2.20	0.42
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.85	0.42
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.07	0.42
2:B:336:ARG:NE	2:B:348:ARG:HH11	2.17	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.01	0.42
2:B:683:SER:C	2:B:685:LEU:H	2.22	0.42
2:B:769:TYR:O	2:B:771:SER:N	2.52	0.42
2:B:970:THR:HG22	2:B:971:THR:N	2.35	0.42
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.50	0.42
4:D:68:ARG:C	4:D:70:PHE:H	2.23	0.42
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.55	0.42
4:D:163:VAL:O	4:D:166:LEU:HB3	2.19	0.42
5:E:154:ILE:H	5:E:196:VAL:HG13	1.84	0.42
8:H:62:SER:HB2	8:H:64:ASN:HD22	1.83	0.42
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.54	0.42
10:J:48:ARG:NE	10:J:49:MET:HE2	2.23	0.42
11:K:30:ALA:HA	11:K:75:ILE:O	2.20	0.42
1:A:47:ARG:O	1:A:48:ALA:HB2	2.20	0.42
1:A:55:ASP:HA	1:A:58:LEU:HB3	2.02	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.99	0.42
1:A:242:PRO:HD3	2:B:1209:ALA:HB1	2.02	0.42
1:A:503:GLN:HB2	1:A:504:LEU:HD12	2.00	0.42
1:A:657:LEU:O	1:A:657:LEU:HD12	2.20	0.42
1:A:1070:GLN:O	1:A:1071:SER:C	2.57	0.42
1:A:1115:SER:O	1:A:1116:LEU:HB3	2.20	0.42
1:A:1315:GLU:C	1:A:1317:MET:H	2.22	0.42
1:A:1334:ASP:O	1:A:1337:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HE2	6:F:135:ARG:HB2	2.01	0.42
2:B:179:CYS:O	2:B:181:LEU:N	2.52	0.42
2:B:185:THR:O	2:B:188:ASP:HB2	2.20	0.42
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.73	0.42
2:B:807:ARG:O	2:B:811:TYR:HE1	2.01	0.42
2:B:1072:MET:O	2:B:1081:LEU:HG	2.19	0.42
3:C:97:VAL:HG11	3:C:130:GLY:HA3	2.01	0.42
3:C:105:GLY:O	3:C:149:LYS:O	2.38	0.42
3:C:173:ALA:O	3:C:174:ALA:HB3	2.19	0.42
3:C:236:GLY:O	3:C:237:SER:C	2.58	0.42
4:D:46:GLU:C	4:D:47:LEU:O	2.58	0.42
7:G:20:PRO:CD	7:G:21:ARG:H	2.32	0.42
15:T:17:TT:H2R2	15:T:17:TT:H2'1	2.02	0.42
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.20	0.42
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.85	0.42
2:B:386:LEU:O	2:B:388:CYS:N	2.53	0.42
2:B:492:LEU:O	2:B:493:SER:C	2.58	0.42
2:B:798:TYR:CE2	3:C:62:PHE:HZ	2.33	0.42
2:B:1196:ILE:HD12	2:B:1200:ALA:HB3	2.01	0.42
3:C:69:LEU:CD1	3:C:69:LEU:H	2.33	0.42
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.31	0.42
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.42
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.01	0.42
5:E:29:PHE:O	5:E:30:ILE:CG1	2.66	0.42
8:H:7:ASP:O	8:H:8:ASP:HB2	2.20	0.42
8:H:91:ASP:O	8:H:93:TYR:N	2.52	0.42
10:J:31:ASP:O	10:J:32:GLU:C	2.57	0.42
1:A:14:VAL:HG21	2:B:1216:LEU:CD1	2.36	0.42
1:A:204:THR:O	1:A:206:GLU:N	2.53	0.42
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.41	0.42
1:A:600:PRO:C	1:A:602:ASP:N	2.73	0.42
1:A:606:LEU:O	1:A:613:ILE:HB	2.20	0.42
1:A:608:ILE:HG13	1:A:613:ILE:HD12	2.01	0.42
1:A:682:THR:O	1:A:682:THR:HG22	2.20	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.19	0.42
1:A:722:LEU:HD22	1:A:799:PHE:CG	2.55	0.42
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.42
1:A:1007:ILE:C	1:A:1009:ASN:H	2.23	0.42
1:A:1017:LEU:HB2	5:E:205:SER:HA	2.01	0.42
1:A:1215:ARG:O	1:A:1216:ILE:C	2.58	0.42
1:A:1280:GLU:O	1:A:1281:ARG:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:SER:O	2:B:182:SER:HB3	2.20	0.42
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.67	0.42
2:B:806:THR:HG22	2:B:808:ALA:HB3	2.02	0.42
2:B:842:ASN:ND2	2:B:845:SER:OG	2.53	0.42
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.53	0.42
3:C:18:VAL:O	3:C:20:PHE:CD2	2.70	0.42
4:D:122:GLU:HA	4:D:125:SER:OG	2.19	0.42
4:D:141:LEU:HD12	4:D:141:LEU:HA	1.79	0.42
5:E:46:TYR:CE2	5:E:58:MET:HA	2.55	0.42
7:G:79:PHE:HZ	7:G:106:MET:HE2	1.85	0.42
8:H:95:TYR:CE2	8:H:97:MET:CG	2.98	0.42
8:H:128:ASN:O	8:H:128:ASN:OD1	2.37	0.42
10:J:19:GLU:O	10:J:23:ASN:HB2	2.20	0.42
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.20	0.42
12:L:55:ILE:O	12:L:56:LEU:HB2	2.19	0.42
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.01	0.41
1:A:846:GLU:HB2	1:A:847:ASP:H	1.73	0.41
1:A:869:GLY:O	1:A:870:GLU:HB2	2.19	0.41
1:A:1142:THR:O	1:A:1143:LEU:C	2.58	0.41
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.26	0.41
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.33	0.41
2:B:882:THR:HG21	2:B:935:ARG:HA	2.01	0.41
2:B:1034:VAL:C	2:B:1036:ALA:N	2.73	0.41
3:C:174:ALA:O	10:J:10:CYS:O	2.37	0.41
3:C:179:GLU:CG	3:C:180:TYR:N	2.79	0.41
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.78	0.41
7:G:1:MET:HE3	7:G:80:LYS:C	2.39	0.41
7:G:20:PRO:CG	7:G:21:ARG:N	2.83	0.41
9:I:80:SER:OG	9:I:105:SER:HB2	2.19	0.41
11:K:88:LYS:O	11:K:89:ASN:C	2.59	0.41
11:K:111:LEU:C	11:K:112:GLN:CG	2.88	0.41
15:T:15:DT:C6	15:T:16:DT:H71	2.54	0.41
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.41
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.41
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.49	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.85	0.41
1:A:600:PRO:O	1:A:602:ASP:N	2.53	0.41
1:A:661:GLY:O	1:A:662:PHE:HB2	2.20	0.41
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.20	0.41
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.41
2:B:549:THR:CG2	2:B:550:ASP:H	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1216:LEU:HD23	2:B:1216:LEU:N	2.35	0.41
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.18	0.41
4:D:177:VAL:O	4:D:177:VAL:HG12	2.21	0.41
5:E:84:ASP:O	5:E:86:PRO:HD3	2.21	0.41
1:A:336:ILE:HG22	1:A:337:ARG:N	2.35	0.41
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.17	0.41
1:A:630:ILE:O	1:A:631:HIS:C	2.58	0.41
1:A:699:ALA:HB3	1:A:701:LEU:HG	2.01	0.41
1:A:825:ILE:O	1:A:826:ASP:C	2.57	0.41
1:A:901:LEU:H	1:A:926:GLN:CD	2.20	0.41
1:A:942:PHE:CD2	1:A:942:PHE:C	2.93	0.41
1:A:988:LEU:HA	1:A:988:LEU:HD23	1.85	0.41
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.50	0.41
2:B:244:LEU:O	2:B:246:LYS:N	2.54	0.41
2:B:554:ILE:O	2:B:554:ILE:HG22	2.20	0.41
2:B:604:ARG:NH2	2:B:613:VAL:O	2.54	0.41
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.82	0.41
2:B:834:ASN:HA	2:B:838:SER:O	2.20	0.41
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.20	0.41
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.35	0.41
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.55	0.41
6:F:82:THR:HA	6:F:83:PRO:HD3	1.74	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.20	0.41
8:H:62:SER:O	8:H:64:ASN:N	2.50	0.41
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.35	0.41
1:A:7:SER:C	1:A:9:ALA:N	2.72	0.41
1:A:77:CYS:C	1:A:78:PRO:O	2.55	0.41
1:A:91:PHE:HB2	1:A:297:GLN:NE2	2.35	0.41
1:A:167:CYS:SG	1:A:167:CYS:O	2.78	0.41
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.86	0.41
1:A:650:GLN:C	1:A:654:ASN:ND2	2.73	0.41
1:A:866:PHE:HE1	5:E:211:TYR:H	1.67	0.41
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.51	0.41
1:A:1376:THR:HG23	1:A:1377:THR:H	1.86	0.41
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.03	0.41
2:B:203:PHE:N	2:B:203:PHE:CD1	2.88	0.41
2:B:237:VAL:CG1	2:B:238:ALA:N	2.82	0.41
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.50	0.41
2:B:685:LEU:C	2:B:687:GLU:H	2.24	0.41
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.84	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.21	0.41
3:C:47:ASP:C	12:L:69:ALA:HB2	2.40	0.41
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.55	0.41
4:D:118:THR:HG22	4:D:118:THR:O	2.20	0.41
4:D:135:GLY:O	4:D:137:ASN:N	2.53	0.41
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.41
7:G:115:MET:CB	7:G:116:PRO:CD	2.99	0.41
10:J:56:LEU:O	10:J:57:ILE:C	2.57	0.41
1:A:18:GLN:H	2:B:1215:ARG:HB2	1.85	0.41
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.41
1:A:367:PRO:O	1:A:368:LYS:C	2.59	0.41
1:A:408:ASP:O	1:A:410:GLY:N	2.45	0.41
1:A:420:ARG:O	1:A:421:ALA:C	2.58	0.41
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.02	0.41
1:A:608:ILE:CG1	1:A:613:ILE:HD12	2.51	0.41
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.85	0.41
1:A:826:ASP:OD1	1:A:827:THR:N	2.53	0.41
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	2.03	0.41
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.20	0.41
2:B:48:LEU:O	2:B:49:ASP:C	2.58	0.41
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.56	0.41
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.02	0.41
2:B:234:ILE:O	2:B:261:ARG:NH2	2.53	0.41
2:B:310:MET:HE1	2:B:387:LEU:HD12	2.02	0.41
2:B:317:CYS:O	2:B:318:VAL:C	2.57	0.41
2:B:467:GLY:CA	2:B:475:SER:HB3	2.50	0.41
2:B:542:MET:HB3	2:B:636:PRO:CD	2.48	0.41
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.55	0.41
2:B:758:PHE:N	2:B:759:PRO:CD	2.83	0.41
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.51	0.41
3:C:87:PHE:H	3:C:87:PHE:HD1	1.66	0.41
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.44	0.41
7:G:79:PHE:CZ	7:G:106:MET:CE	3.02	0.41
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.47	0.41
9:I:55:THR:HG21	9:I:109:ILE:HD13	2.02	0.41
11:K:53:ASP:C	11:K:55:LYS:N	2.74	0.41
1:A:65:LEU:O	1:A:66:LYS:C	2.59	0.41
1:A:284:ALA:O	1:A:286:HIS:N	2.45	0.41
1:A:472:LEU:O	1:A:475:THR:CB	2.63	0.41
1:A:474:VAL:O	1:A:477:PRO:HD2	2.20	0.41
1:A:568:PRO:HG2	1:A:569:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.48	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.37	0.41
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.01	0.41
2:B:303:TYR:N	2:B:303:TYR:CD2	2.87	0.41
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.03	0.41
2:B:805:THR:HB	2:B:809:MET:SD	2.60	0.41
2:B:1069:PHE:O	2:B:1070:GLU:HG2	2.19	0.41
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.41
3:C:48:SER:N	12:L:69:ALA:HB2	2.35	0.41
4:D:30:GLY:O	4:D:32:GLU:N	2.54	0.41
7:G:99:PHE:CD1	7:G:99:PHE:C	2.93	0.41
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.36	0.41
8:H:44:VAL:HG13	8:H:48:PRO:HA	2.03	0.41
9:I:84:VAL:HG13	9:I:84:VAL:O	2.20	0.41
11:K:110:ASN:O	11:K:111:LEU:CD2	2.61	0.41
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.50	0.41
1:A:332:LYS:H	1:A:337:ARG:HB3	1.85	0.41
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.33	0.41
1:A:380:VAL:HG23	1:A:430:TRP:O	2.21	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.55	0.41
1:A:765:VAL:HG23	1:A:802:ASN:O	2.21	0.41
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.20	0.41
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.20	0.41
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.41
2:B:96:TYR:HE1	2:B:131:ASP:OD2	2.02	0.41
2:B:336:ARG:HH22	2:B:345:LYS:CE	2.11	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.53	0.41
2:B:871:THR:HG22	2:B:872:GLU:N	2.35	0.41
2:B:911:ILE:HG22	2:B:966:VAL:HG21	2.03	0.41
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.50	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.54	0.41
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.10	0.41
7:G:9:LEU:HD12	7:G:10:ASN:N	2.35	0.41
7:G:101:VAL:N	7:G:108:VAL:O	2.52	0.41
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.41
12:L:49:LYS:O	12:L:50:ASP:HB3	2.21	0.41
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.02	0.41
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.85	0.41
1:A:95:PHE:O	1:A:98:LYS:N	2.53	0.41
1:A:150:THR:HG22	1:A:150:THR:O	2.21	0.41
1:A:263:THR:HG22	1:A:263:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:VAL:HG11	2:B:1130:PHE:HB2	2.03	0.41
1:A:417:TYR:N	1:A:417:TYR:CD2	2.88	0.41
1:A:577:ILE:O	1:A:580:VAL:HG23	2.21	0.41
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.41
1:A:621:THR:O	1:A:629:LEU:HB2	2.20	0.41
1:A:779:PHE:O	1:A:780:VAL:C	2.59	0.41
1:A:806:ARG:HH12	2:B:729:ILE:HD12	1.83	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.21	0.41
1:A:1377:THR:O	1:A:1379:GLY:N	2.53	0.41
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.20	0.41
2:B:355:ILE:O	2:B:359:GLU:HB2	2.21	0.41
2:B:570:VAL:HG23	2:B:573:GLN:HB3	2.03	0.41
2:B:936:ASP:OD1	2:B:938:SER:N	2.48	0.41
2:B:992:ILE:HG12	2:B:993:THR:N	2.35	0.41
3:C:35:ARG:HH11	11:K:41:THR:HA	1.85	0.41
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.85	0.41
6:F:85:MET:HE1	6:F:148:VAL:HG12	2.02	0.41
6:F:95:GLY:O	6:F:96:THR:C	2.59	0.41
6:F:143:PHE:CD1	6:F:143:PHE:O	2.74	0.41
11:K:6:ARG:O	11:K:8:GLU:N	2.54	0.41
12:L:27:LEU:HD13	12:L:37:LYS:HG2	2.03	0.41
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.54	0.41
1:A:21:LEU:HG	1:A:1413:GLY:O	2.21	0.41
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.35	0.41
1:A:285:PRO:O	1:A:287:HIS:N	2.53	0.41
1:A:453:MET:C	1:A:455:MET:H	2.23	0.41
1:A:666:ILE:CD1	1:A:667:GLY:H	2.29	0.41
1:A:667:GLY:HA3	3:C:192:TRP:HH2	1.84	0.41
1:A:874:ASP:O	1:A:875:ALA:C	2.59	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.86	0.41
1:A:907:THR:HG23	1:A:908:LEU:H	1.86	0.41
1:A:919:ILE:O	1:A:920:LEU:C	2.59	0.41
1:A:1328:TYR:HD1	1:A:1335:ILE:CD1	2.34	0.41
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.56	0.41
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.21	0.41
2:B:245:GLU:C	2:B:246:LYS:HG3	2.41	0.41
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.26	0.41
2:B:591:ARG:O	2:B:593:PRO:HD3	2.20	0.41
2:B:597:MET:O	2:B:599:THR:N	2.54	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.96	0.41
2:B:770:GLN:C	2:B:772:ALA:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:VAL:HG21	10:J:56:LEU:HD11	2.03	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.51	0.41
2:B:1040:ASN:O	2:B:1042:GLY:N	2.54	0.41
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.84	0.41
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.85	0.41
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.74	0.41
4:D:35:LEU:HD13	4:D:173:HIS:ND1	2.36	0.41
4:D:63:LEU:HD22	4:D:63:LEU:HA	1.84	0.41
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.55	0.41
7:G:112:LYS:O	7:G:115:MET:HG3	2.21	0.41
8:H:59:ILE:CG2	8:H:60:ALA:N	2.69	0.41
8:H:91:ASP:C	8:H:93:TYR:N	2.74	0.41
8:H:107:VAL:O	8:H:111:LEU:HB2	2.21	0.41
10:J:7:CYS:SG	10:J:49:MET:CE	3.09	0.41
10:J:32:GLU:O	10:J:35:ALA:N	2.54	0.41
11:K:31:VAL:CG1	11:K:32:VAL:H	2.30	0.41
11:K:68:PHE:HD2	11:K:68:PHE:N	2.18	0.41
11:K:111:LEU:O	11:K:112:GLN:HB3	2.21	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.80	0.41
1:A:89:PRO:HB2	1:A:204:THR:HG21	2.03	0.41
1:A:162:VAL:HG12	1:A:163:SER:N	2.36	0.41
1:A:351:THR:HB	2:B:1103:ILE:HD11	2.02	0.41
1:A:590:ARG:O	1:A:591:PHE:CB	2.68	0.41
1:A:710:LEU:HD13	9:I:94:ASP:O	2.21	0.41
1:A:719:VAL:C	1:A:721:PHE:N	2.74	0.41
1:A:780:VAL:HG23	2:B:699:GLU:OE1	2.20	0.41
1:A:786:HIS:O	1:A:787:PHE:CD2	2.74	0.41
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.41
2:B:841:MET:SD	2:B:846:ILE:HD11	2.61	0.41
2:B:842:ASN:HB3	2:B:845:SER:OG	2.20	0.41
4:D:30:GLY:O	4:D:31:GLN:C	2.59	0.41
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.56	0.41
7:G:101:VAL:HG12	7:G:102:GLN:N	2.36	0.41
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.41
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.47	0.40
1:A:362:ASP:HB3	1:A:508:PRO:HG3	2.03	0.40
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.51	0.40
1:A:420:ARG:HB3	1:A:423:ASP:HB3	2.02	0.40
1:A:794:PRO:C	1:A:796:SER:H	2.23	0.40
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.35	0.40
1:A:1115:SER:OG	1:A:1116:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.21	0.40
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.40
4:D:24:ALA:C	4:D:26:THR:N	2.73	0.40
5:E:8:ASN:OD1	5:E:8:ASN:O	2.39	0.40
8:H:82:PRO:O	8:H:83:GLN:HB2	2.21	0.40
8:H:107:VAL:O	8:H:108:SER:O	2.39	0.40
9:I:95:THR:HG22	9:I:96:SER:N	2.35	0.40
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.19	0.40
12:L:27:LEU:HB3	12:L:37:LYS:HD3	2.03	0.40
1:A:23:SER:O	1:A:26:GLU:N	2.54	0.40
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.62	0.40
1:A:723:ASN:O	1:A:724:GLU:C	2.60	0.40
1:A:742:ASN:O	1:A:743:VAL:C	2.59	0.40
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	2.02	0.40
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.86	0.40
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.92	0.40
1:A:1406:VAL:O	1:A:1407:GLU:C	2.59	0.40
2:B:175:ARG:HG2	2:B:175:ARG:NH1	2.21	0.40
2:B:326:ASP:O	2:B:327:ARG:C	2.58	0.40
2:B:581:PHE:HA	2:B:585:VAL:O	2.21	0.40
2:B:1060:ARG:C	2:B:1062:HIS:N	2.75	0.40
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.22	0.40
2:B:1115:THR:HG21	2:B:1117:GLN:CG	2.51	0.40
3:C:152:GLU:HG2	3:C:153:LEU:H	1.86	0.40
7:G:37:SER:OG	7:G:45:ILE:HB	2.20	0.40
7:G:154:VAL:CG1	7:G:155:SER:N	2.83	0.40
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.56	0.40
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.89	0.40
1:A:60:SER:C	1:A:61:ILE:HG13	2.41	0.40
1:A:116:ASP:C	1:A:118:HIS:H	2.25	0.40
1:A:577:ILE:HG13	1:A:578:LEU:N	2.36	0.40
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.03	0.40
1:A:1116:LEU:CB	1:A:1308:THR:CG2	3.00	0.40
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	2.03	0.40
1:A:1239:ARG:NH1	1:A:1239:ARG:HB3	2.36	0.40
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.51	0.40
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.04	0.40
2:B:283:VAL:O	2:B:284:ILE:C	2.59	0.40
2:B:640:VAL:HG23	2:B:740:HIS:HA	2.02	0.40
2:B:654:ARG:C	2:B:656:GLY:N	2.74	0.40
4:D:202:ILE:O	4:D:202:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:LYS:O	5:E:21:GLU:C	2.59	0.40
5:E:35:VAL:O	5:E:37:LEU:N	2.53	0.40
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.21	0.40
8:H:11:GLN:O	8:H:28:ALA:HB1	2.21	0.40
12:L:55:ILE:H	12:L:55:ILE:HG12	1.37	0.40
15:T:25:DT:H2"	15:T:26:DC:H5'	2.04	0.40
1:A:68:GLN:HE22	1:A:80:HIS:CG	2.39	0.40
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.51	0.40
1:A:353:ILE:HG21	1:A:487:MET:CG	2.51	0.40
1:A:417:TYR:O	1:A:418:SER:C	2.59	0.40
1:A:478:TYR:O	1:A:479:ASN:HB3	2.21	0.40
1:A:543:LEU:O	1:A:545:GLN:N	2.53	0.40
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.62	0.40
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.51	0.40
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	2.03	0.40
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	2.04	0.40
2:B:465:ASN:N	2:B:465:ASN:ND2	2.69	0.40
2:B:551:PRO:HG2	2:B:552:MET:H	1.86	0.40
2:B:558:LEU:C	2:B:560:GLU:N	2.74	0.40
2:B:744:HIS:CD2	2:B:746:SER:OG	2.71	0.40
2:B:902:GLY:O	12:L:65:VAL:HG11	2.21	0.40
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.04	0.40
2:B:1162:ILE:HG23	2:B:1168:LEU:O	2.22	0.40
2:B:1201:LYS:O	2:B:1204:PHE:HB2	2.22	0.40
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.86	0.40
3:C:154:LYS:C	3:C:155:LEU:HD23	2.41	0.40
3:C:176:ILE:HG22	3:C:177:GLU:N	2.36	0.40
4:D:162:ALA:O	4:D:163:VAL:C	2.59	0.40
5:E:128:PRO:HA	5:E:129:PRO:C	2.42	0.40
7:G:15:PRO:HG2	7:G:66:GLY:HA3	2.04	0.40
7:G:17:PHE:C	7:G:19:GLY:H	2.24	0.40
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.97	0.40
9:I:33:SER:O	9:I:35:VAL:HG23	2.22	0.40
1:A:61:ILE:CG2	1:A:62:ASP:H	2.20	0.40
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.81	0.40
1:A:571:LEU:HD22	8:H:46:LEU:HD11	2.02	0.40
1:A:635:ARG:HA	1:A:635:ARG:HH11	1.86	0.40
1:A:722:LEU:HD21	1:A:794:PRO:CB	2.52	0.40
1:A:1366:ARG:HH11	1:A:1366:ARG:HG2	1.87	0.40
2:B:19:GLU:O	2:B:20:ASP:C	2.60	0.40
2:B:23:ALA:O	2:B:654:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ALA:C	2:B:29:ASP:N	2.73	0.40
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.51	0.40
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.40
2:B:593:PRO:O	2:B:594:ALA:C	2.60	0.40
2:B:1152:MET:O	2:B:1153:GLU:C	2.60	0.40
2:B:1208:MET:O	2:B:1211:ASN:N	2.46	0.40
3:C:133:ILE:CD1	3:C:237:SER:CA	2.99	0.40
4:D:25:ALA:C	4:D:27:LEU:H	2.25	0.40
4:D:156:ASP:C	4:D:158:GLU:N	2.75	0.40
5:E:24:LYS:CG	5:E:25:ASP:N	2.84	0.40
11:K:10:PHE:N	11:K:10:PHE:HD2	2.19	0.40
15:T:26:DC:H2"	15:T:27:DA:O5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1410/1733 (81%)	947 (67%)	306 (22%)	157 (11%)	0 7
2	B	1096/1224 (90%)	754 (69%)	222 (20%)	120 (11%)	0 7
3	C	264/318 (83%)	164 (62%)	62 (24%)	38 (14%)	0 3
4	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	0 10
5	E	212/215 (99%)	153 (72%)	42 (20%)	17 (8%)	1 14
6	F	84/155 (54%)	65 (77%)	13 (16%)	6 (7%)	1 16
7	G	169/171 (99%)	128 (76%)	30 (18%)	11 (6%)	1 18
8	H	131/146 (90%)	87 (66%)	26 (20%)	18 (14%)	0 4
9	I	114/122 (93%)	77 (68%)	26 (23%)	11 (10%)	0 10
10	J	63/70 (90%)	34 (54%)	12 (19%)	17 (27%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	112/120 (93%)	82 (73%)	20 (18%)	10 (9%)	1 12
12	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0 0
All	All	3872/4565 (85%)	2627 (68%)	810 (21%)	435 (11%)	0 7

All (435) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	93	VAL
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	223	GLY
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	536	LEU
1	A	567	LYS
1	A	619	LYS
1	A	636	GLU
1	A	666	ILE
1	A	789	LYS
1	A	847	ASP
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1014	ALA
1	A	1036	ARG
1	A	1114	PRO
1	A	1115	SER

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Mol	Chain	Res	Type
1	A	1122	PRO
1	A	1212	VAL
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1392	SER
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	258	LEU
2	B	259	TYR
2	B	266	ALA
2	B	345	LYS
2	B	367	LEU
2	B	467	GLY
2	B	470	LYS
2	B	474	SER
2	B	613	VAL
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	831	SER
2	B	881	ASN
2	B	907	GLY
2	B	909	ASP
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1155	SER
2	B	1156	ASP
2	B	1157	ALA

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Mol	Chain	Res	Type
2	B	1171	VAL
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
3	C	4	GLU
3	C	56	THR
3	C	78	GLU
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	9	GLN
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	177	VAL
4	D	192	LYS
4	D	199	ASN
5	E	3	GLN
5	E	59	SER
5	E	73	PRO
5	E	106	GLN
5	E	130	ALA
6	F	81	THR
7	G	62	LEU
7	G	63	PRO
7	G	139	ILE
8	H	62	SER
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
8	H	140	ALA
9	I	3	THR
9	I	9	ASP

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Mol	Chain	Res	Type
9	I	79	HIS
10	J	2	ILE
10	J	6	ARG
10	J	32	GLU
10	J	64	ASN
11	K	7	PHE
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	66	LYS
1	A	69	THR
1	A	74	MET
1	A	76	GLU
1	A	84	ILE
1	A	96	ILE
1	A	219	PHE
1	A	244	PRO
1	A	253	ASN
1	A	283	GLY
1	A	300	VAL
1	A	322	VAL
1	A	331	GLY
1	A	332	LYS
1	A	336	ILE
1	A	409	SER
1	A	418	SER
1	A	424	ILE
1	A	439	ASN
1	A	465	TYR
1	A	543	LEU
1	A	544	ASP
1	A	597	LEU
1	A	720	ARG
1	A	753	GLY
1	A	780	VAL
1	A	852	TYR
1	A	871	ASP

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Mol	Chain	Res	Type
1	A	979	SER
1	A	1071	SER
1	A	1096	SER
1	A	1116	LEU
1	A	1165	GLU
1	A	1233	ASP
1	A	1280	GLU
1	A	1335	ILE
1	A	1389	PHE
1	A	1402	PHE
1	A	1405	THR
2	B	28	GLU
2	B	124	TYR
2	B	184	ALA
2	B	260	GLY
2	B	264	SER
2	B	282	ILE
2	B	283	VAL
2	B	389	ALA
2	B	401	PHE
2	B	450	ALA
2	B	540	SER
2	B	559	SER
2	B	605	ARG
2	B	619	ILE
2	B	629	ASP
2	B	655	LYS
2	B	708	GLU
2	B	746	SER
2	B	752	ALA
2	B	754	SER
2	B	792	MET
2	B	951	GLN
2	B	1011	ILE
2	B	1041	GLU
2	B	1065	GLN
2	B	1096	ARG
2	B	1100	ASP
2	B	1167	GLY
2	B	1186	ASP
2	B	1188	LYS
3	C	10	ILE

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Mol	Chain	Res	Type
3	C	51	VAL
3	C	84	ARG
3	C	87	PHE
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
4	D	21	GLU
4	D	65	GLU
4	D	131	GLU
4	D	196	PRO
5	E	36	GLU
5	E	74	ASP
5	E	115	ASN
5	E	192	ARG
5	E	206	GLY
6	F	112	GLU
7	G	19	GLY
7	G	35	GLU
7	G	154	VAL
8	H	17	PRO
8	H	21	ASN
8	H	59	ILE
8	H	77	ARG
8	H	81	PRO
8	H	90	ALA
9	I	11	ASN
9	I	47	GLU
9	I	57	GLY
9	I	106	CYS
10	J	14	VAL
10	J	17	LYS
10	J	24	LEU
10	J	28	ASP
10	J	29	GLU
10	J	33	GLY
11	K	15	GLY
11	K	29	ASN
11	K	88	LYS
12	L	53	HIS
1	A	8	SER
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	61	ILE
1	A	70	CYS
1	A	73	GLY
1	A	169	ASN
1	A	232	GLU
1	A	245	PRO
1	A	263	THR
1	A	278	THR
1	A	333	GLU
1	A	386	ASP
1	A	483	ASP
1	A	846	GLU
1	A	1013	ASP
1	A	1164	PRO
1	A	1221	LYS
1	A	1277	GLU
2	B	48	LEU
2	B	65	GLU
2	B	114	PRO
2	B	257	LYS
2	B	364	ILE
2	B	365	THR
2	B	369	GLY
2	B	449	ASN
2	B	460	ALA
2	B	461	LEU
2	B	571	PRO
2	B	591	ARG
2	B	641	GLU
2	B	711	GLU
2	B	764	SER
2	B	818	PRO
2	B	867	GLY
2	B	878	GLN
2	B	880	THR
2	B	891	ASP
2	B	894	ASP
2	B	1108	ARG
3	C	81	GLU
3	C	148	ARG
3	C	164	ALA
3	C	212	PRO

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Mol	Chain	Res	Type
3	C	237	SER
3	C	240	VAL
3	C	264	GLN
4	D	53	SER
5	E	44	ALA
5	E	45	LYS
7	G	20	PRO
7	G	64	THR
8	H	32	THR
8	H	36	CYS
8	H	84	ALA
8	H	92	ASP
8	H	135	LEU
9	I	78	CYS
10	J	8	PHE
10	J	9	SER
10	J	27	GLU
10	J	55	ASP
11	K	53	ASP
11	K	112	GLN
1	A	131	SER
1	A	399	HIS
1	A	400	PRO
1	A	591	PHE
1	A	601	LYS
1	A	605	MET
1	A	759	ALA
1	A	825	ILE
1	A	1054	LEU
1	A	1133	LEU
1	A	1224	LEU
1	A	1397	LEU
1	A	1448	GLU
2	B	22	SER
2	B	30	SER
2	B	61	ASP
2	B	94	LYS
2	B	180	TYR
2	B	309	GLN
2	B	466	TRP
2	B	682	SER
2	B	728	ARG

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Mol	Chain	Res	Type
2	B	844	SER
2	B	869	SER
2	B	945	GLU
3	C	48	SER
3	C	138	GLU
3	C	139	GLY
3	C	142	VAL
3	C	167	HIS
3	C	208	GLU
4	D	47	LEU
5	E	148	GLU
6	F	154	ASP
8	H	44	VAL
9	I	34	TYR
9	I	107	SER
10	J	45	CYS
11	K	70	ARG
12	L	26	THR
12	L	28	LYS
12	L	39	SER
12	L	56	LEU
1	A	5	GLN
1	A	55	ASP
1	A	111	GLY
1	A	205	GLU
1	A	517	ASN
1	A	639	PRO
1	A	649	ILE
1	A	673	GLY
1	A	775	ILE
1	A	910	PRO
1	A	940	ARG
1	A	958	VAL
1	A	972	HIS
1	A	1124	HIS
1	A	1309	ASP
1	A	1386	ARG
1	A	1395	GLY
2	B	598	GLU
2	B	734	HIS
2	B	848	ARG
2	B	1017	ILE

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Mol	Chain	Res	Type
2	B	1061	GLU
2	B	1214	PRO
3	C	6	PRO
4	D	12	ARG
6	F	89	GLU
6	F	150	GLU
6	F	151	LEU
7	G	81	PRO
8	H	78	SER
12	L	40	LEU
12	L	52	GLY
12	L	54	ARG
1	A	196	GLU
1	A	492	PRO
1	A	599	SER
1	A	626	ASN
1	A	648	ASN
1	A	755	PHE
1	A	1016	THR
1	A	1127	ASP
1	A	1260	LEU
1	A	1302	PRO
1	A	1369	ALA
2	B	56	ASP
2	B	206	ASN
2	B	387	LEU
2	B	611	PRO
2	B	1112	GLN
3	C	95	CYS
4	D	146	GLN
5	E	43	LYS
7	G	115	MET
10	J	18	TRP
11	K	104	ASN
12	L	55	ILE
1	A	197	PRO
1	A	380	VAL
1	A	719	VAL
2	B	511	PRO
2	B	551	PRO
2	B	712	PRO
2	B	832	GLY

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Mol	Chain	Res	Type
3	C	18	VAL
3	C	172	PRO
10	J	57	ILE
1	A	1158	PRO
2	B	102	VAL
5	E	76	GLY
9	I	62	ILE
11	K	66	PRO
1	A	35	ILE
1	A	661	GLY
2	B	688	GLY
2	B	729	ILE
2	B	903	VAL
3	C	129	ILE
3	C	217	ASP
1	A	99	ILE
1	A	357	PRO
1	A	396	PRO
1	A	652	VAL
2	B	55	VAL
7	G	34	VAL
5	E	38	PRO
5	E	129	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	1244/1520 (82%)	1123 (90%)	121 (10%)	8 30
2	B	967/1061 (91%)	886 (92%)	81 (8%)	11 37
3	C	235/274 (86%)	218 (93%)	17 (7%)	14 42
4	D	159/200 (80%)	138 (87%)	21 (13%)	4 21
5	E	196/197 (100%)	191 (97%)	5 (3%)	46 67
6	F	77/137 (56%)	71 (92%)	6 (8%)	12 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	152/152 (100%)	140 (92%)	12 (8%)	12 39
8	H	119/128 (93%)	112 (94%)	7 (6%)	19 48
9	I	110/116 (95%)	98 (89%)	12 (11%)	6 26
10	J	60/65 (92%)	52 (87%)	8 (13%)	4 21
11	K	99/102 (97%)	87 (88%)	12 (12%)	5 23
12	L	40/57 (70%)	36 (90%)	4 (10%)	7 29
All	All	3458/4009 (86%)	3152 (91%)	306 (9%)	10 35

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	11	LEU
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	62	ASP
1	A	67	CYS
1	A	70	CYS
1	A	83	HIS
1	A	93	VAL
1	A	108	MET
1	A	122	MET
1	A	130	ASP
1	A	142	CYS
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	221	SER
1	A	245	PRO
1	A	270	LEU
1	A	275	SER
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	326	ARG
1	A	335	ARG
1	A	344	ARG
1	A	345	VAL
1	A	350	ARG

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Mol	Chain	Res	Type
1	A	381	THR
1	A	385	ILE
1	A	396	PRO
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	425	GLN
1	A	434	ARG
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	460	VAL
1	A	462	VAL
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	481	ASP
1	A	493	GLN
1	A	512	VAL
1	A	515	GLN
1	A	526	ASP
1	A	560	ILE
1	A	562	THR
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	635	ARG
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	739	ASP
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	827	THR
1	A	858	ASN
1	A	859	SER
1	A	871	ASP

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Mol	Chain	Res	Type
1	A	886	ILE
1	A	890	ASP
1	A	903	ASN
1	A	906	HIS
1	A	907	THR
1	A	929	LEU
1	A	939	ASP
1	A	940	ARG
1	A	969	GLN
1	A	983	ILE
1	A	992	ASP
1	A	1001	ARG
1	A	1009	ASN
1	A	1017	LEU
1	A	1029	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1146	VAL
1	A	1152	ILE
1	A	1155	ASP
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1271	ILE
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1362	TYR
1	A	1364	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1389	PHE

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Mol	Chain	Res	Type
1	A	1405	THR
1	A	1418	LEU
1	A	1425	SER
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
1	A	1447	GLU
2	B	35	SER
2	B	57	TYR
2	B	61	ASP
2	B	106	ASP
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	223	VAL
2	B	258	LEU
2	B	268	THR
2	B	286	PHE
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	401	PHE
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	466	TRP
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	502	ILE
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	628	THR

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Mol	Chain	Res	Type
2	B	635	ARG
2	B	644	GLU
2	B	682	SER
2	B	684	LEU
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	755	ILE
2	B	795	ILE
2	B	830	TYR
2	B	833	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	844	SER
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	953	LEU
2	B	978	ASP
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1047	PHE
2	B	1060	ARG
2	B	1069	PHE
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1099	VAL
2	B	1106	ARG
2	B	1108	ARG
2	B	1120	GLU
2	B	1122	ARG
2	B	1133	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1169	MET
2	B	1170	THR

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Mol	Chain	Res	Type
2	B	1176	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	22	LEU
3	C	57	VAL
3	C	62	PHE
3	C	77	ILE
3	C	89	GLU
3	C	99	LEU
3	C	104	PHE
3	C	129	ILE
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	163	ILE
3	C	172	PRO
3	C	193	TYR
3	C	214	ASN
3	C	240	VAL
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	17	LYS
4	D	19	GLU
4	D	22	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	151	PHE
4	D	152	SER
4	D	156	ASP
4	D	170	THR
4	D	174	PRO
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	208	GLU

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Mol	Chain	Res	Type
4	D	221	TYR
5	E	60	PHE
5	E	74	ASP
5	E	104	ASN
5	E	114	ASN
5	E	132	ILE
6	F	79	ARG
6	F	90	ARG
6	F	116	ASP
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	11	ILE
7	G	13	LEU
7	G	17	PHE
7	G	45	ILE
7	G	74	TYR
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	115	MET
7	G	126	ASN
7	G	171	ILE
8	H	86	ASP
8	H	93	TYR
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	141	TYR
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	34	TYR
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	99	LEU
9	I	100	PHE

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Mol	Chain	Res	Type
9	I	101	PHE
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	16	ASP
10	J	28	ASP
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	5	ASP
11	K	10	PHE
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	65	HIS
11	K	78	THR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	71	GLN
1	A	83	HIS
1	A	92	HIS
1	A	225	ASN
1	A	256	GLN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS
1	A	479	ASN
1	A	493	GLN
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	603	ASN
1	A	631	HIS
1	A	654	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	1106	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1265	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	363	HIS
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	776	GLN
2	B	821	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1176	ASN
2	B	1179	GLN

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Mol	Chain	Res	Type
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
4	D	39	ASN
4	D	40	HIS
4	D	137	ASN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	97	HIS
7	G	126	ASN
8	H	64	ASN
9	I	12	ASN
9	I	89	GLN
9	I	90	GLN
10	J	53	HIS
10	J	64	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

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

2 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	$\#\|Z\| > 2$
15	BRU	T	22	15,14	18,21,22	0.94	1 (5%)	26,30,33	0.98	1 (3%)
15	TT	T	17	15	40,43,44	4.79	9 (22%)	59,69,72	2.52	16 (27%)

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
15	BRU	T	22	15,14	-	2/7/21/22	0/2/2/2
15	TT	T	17	15	-	10/18/105/106	0/5/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C5T-C6T	-20.32	1.31	1.55
15	T	17	TT	C5-C6	-19.74	1.32	1.55
15	T	17	TT	C6T-N1T	-4.77	1.39	1.46
15	T	17	TT	C1'-N1	3.99	1.50	1.45
15	T	17	TT	C6-N1	-3.80	1.40	1.46
15	T	17	TT	C5T-C4T	-3.54	1.45	1.51
15	T	22	BRU	O5'-C5'	-3.17	1.37	1.44
15	T	17	TT	C6T-C6	2.95	1.65	1.56
15	T	17	TT	O4-C4	2.29	1.26	1.22
15	T	17	TT	C2T-N1T	2.05	1.40	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	17	TT	C2R-C1R-N1T	8.38	126.91	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	17	TT	C5T-C5-C6	7.24	97.39	88.38
15	T	17	TT	C5-C6-C6T	-6.25	79.03	89.28
15	T	17	TT	C5-C6-N1	5.98	123.99	115.61
15	T	17	TT	N3T-C2T-N1T	-4.60	111.92	116.69
15	T	17	TT	C5-C5T-C6T	-4.25	83.09	88.38
15	T	17	TT	C5T-C6T-N1T	3.84	120.99	115.61
15	T	17	TT	C5A-C5-C5T	-3.83	105.32	116.39
15	T	17	TT	O4R-C4R-C5R	3.72	121.61	109.37
15	T	17	TT	C3R-C2R-C1R	-3.55	93.64	102.54
15	T	17	TT	O4R-C1R-N1T	3.22	112.47	108.65
15	T	17	TT	O4-C4-C5	3.21	125.44	122.88
15	T	22	BRU	C6-C5-C4	-2.88	117.75	120.67
15	T	17	TT	O3R-C3R-C4R	-2.59	100.18	110.10
15	T	17	TT	C5-C4-N3	-2.30	114.05	116.06
15	T	17	TT	C5T-C6T-C6	2.22	92.93	89.28
15	T	17	TT	C6-C6T-N1T	2.08	126.50	118.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	17	TT	C3R-C4R-C5R-O5R
15	T	17	TT	O4'-C4'-C5'-O5'
15	T	17	TT	O3'-C7-O5R-C5R
15	T	17	TT	C2'-C1'-N1-C6
15	T	17	TT	C2'-C1'-N1-C2
15	T	17	TT	O4'-C1'-N1-C6
15	T	17	TT	O4R-C4R-C5R-O5R
15	T	17	TT	O4'-C1'-N1-C2
15	T	22	BRU	O4'-C4'-C5'-O5'
15	T	17	TT	O4R-C1R-N1T-C6T
15	T	17	TT	O4R-C1R-N1T-C2T
15	T	22	BRU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	22	BRU	4	0
15	T	17	TT	22	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
3	C	1
1	A	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	18:PHE	C	19:GLU	N	3.98
1	C	2:SER	C	3:GLU	N	3.88
1	A	1175:SER	C	1176:LEU	N	3.69
1	F	69:LEU	C	70:LYS	N	3.59
1	B	337:ARG	C	338:GLY	N	2.64

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.