Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 AM GMT

PDB ID	:	3HOY
Title	:	Complete RNA polymerase II elongation complex VI
Authors	:	Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on	:	2009-06-03
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

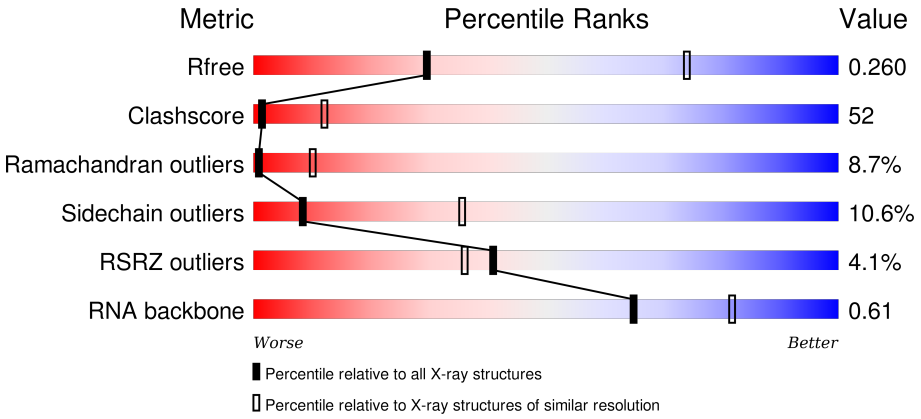
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	2% 28% 43% 10% • 18%
2	B	1224	4% 27% 51% 11% • 10%
3	C	347	% 22% 43% 12% 23%
4	D	221	29% 42% 10% 19%

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Mol	Chain	Length	Quality of chain
5	E	215	11% 29% 59% 11%
6	F	155	18% 32% 6% 44%
7	G	171	% 40% 50% 9%
8	H	146	11% 21% 54% 16% 9%
9	I	122	8% 26% 55% 15%
10	J	70	% 19% 59% 13% 7%
11	K	120	2% 33% 56% 5% 5%
12	L	70	9% 7% 40% 16% 34%
13	T	41	17% 10% 32% 5% 54%
14	N	41	17% 15% 83%
15	P	20	10% 20% 30% 50%

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
13	BRU	T	20	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31803 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11166	7036	1953	2115	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1105	Total	C	N	O	S	0	0	0
			8786	5564	1541	1627	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP P16370
C	-27	GLY	-	EXPRESSION TAG	UNP P16370
C	-26	SER	-	EXPRESSION TAG	UNP P16370
C	-25	HIS	-	EXPRESSION TAG	UNP P16370
C	-24	HIS	-	EXPRESSION TAG	UNP P16370
C	-23	HIS	-	EXPRESSION TAG	UNP P16370
C	-22	HIS	-	EXPRESSION TAG	UNP P16370
C	-21	HIS	-	EXPRESSION TAG	UNP P16370
C	-20	HIS	-	EXPRESSION TAG	UNP P16370
C	-19	SER	-	EXPRESSION TAG	UNP P16370
C	-18	ASN	-	EXPRESSION TAG	UNP P16370
C	-17	SER	-	EXPRESSION TAG	UNP P16370
C	-16	GLY	-	EXPRESSION TAG	UNP P16370
C	-15	LEU	-	EXPRESSION TAG	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	EXPRESSION TAG	UNP P16370
C	-13	ASP	-	EXPRESSION TAG	UNP P16370
C	-12	ILE	-	EXPRESSION TAG	UNP P16370
C	-11	PHE	-	EXPRESSION TAG	UNP P16370
C	-10	GLU	-	EXPRESSION TAG	UNP P16370
C	-9	ALA	-	EXPRESSION TAG	UNP P16370
C	-8	GLN	-	EXPRESSION TAG	UNP P16370
C	-7	LYS	-	EXPRESSION TAG	UNP P16370
C	-6	ILE	-	EXPRESSION TAG	UNP P16370
C	-5	GLU	-	EXPRESSION TAG	UNP P16370
C	-4	TRP	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	GLU	-	EXPRESSION TAG	UNP P16370
C	-1	ASP	-	EXPRESSION TAG	UNP P16370
C	0	THR	-	EXPRESSION TAG	UNP P16370
C	1	GLY	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1365	845	242	276	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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 subunit RPB7.

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 subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

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 subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	19	Total	Br	C	N	O	P	8	0	0
			382	1	184	64	115	18			

- Molecule 14 is a DNA chain called 5'-D(*CP*CP*GP*GP*CP*AP*GP*TP*AP*CP*TP*A P*GP*TP*AP*AP*AP*CP*TP*AP*GP*TP*AP*TP*T*GP*AP*AP*AP*GP*TP*AP*C P*TP*TP*GP*AP*GP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	11	0	0
			145	70	32	37	6			

- Molecule 15 is a RNA chain called 5'-R(*UP*AP*UP*AP*UP*GP*CP*A*UP*AP*AP*AP *GP*AP*CP*CP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			213	97	43	64	9			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

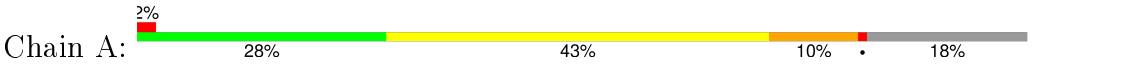
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

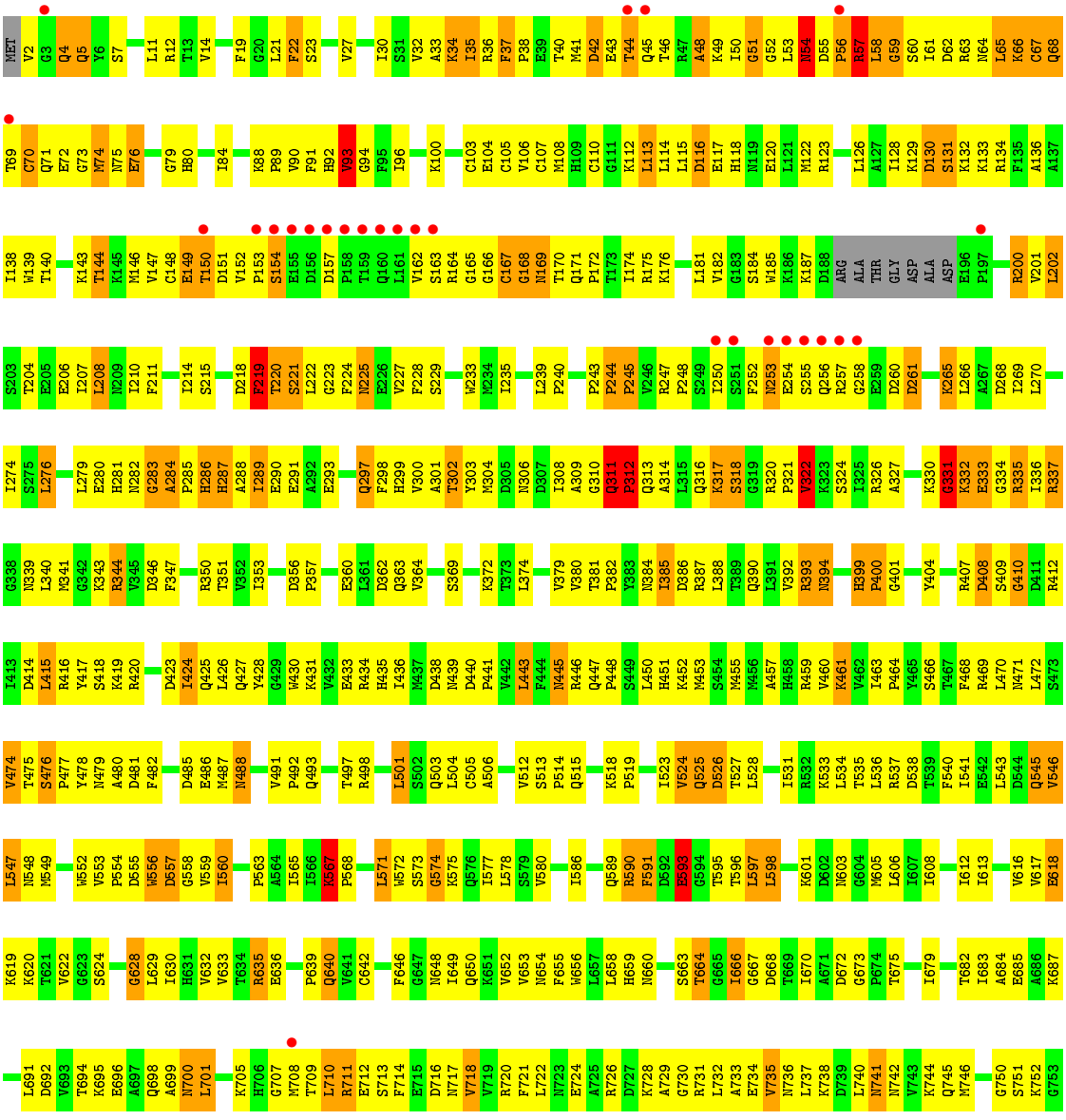
3 Residue-property plots (i)

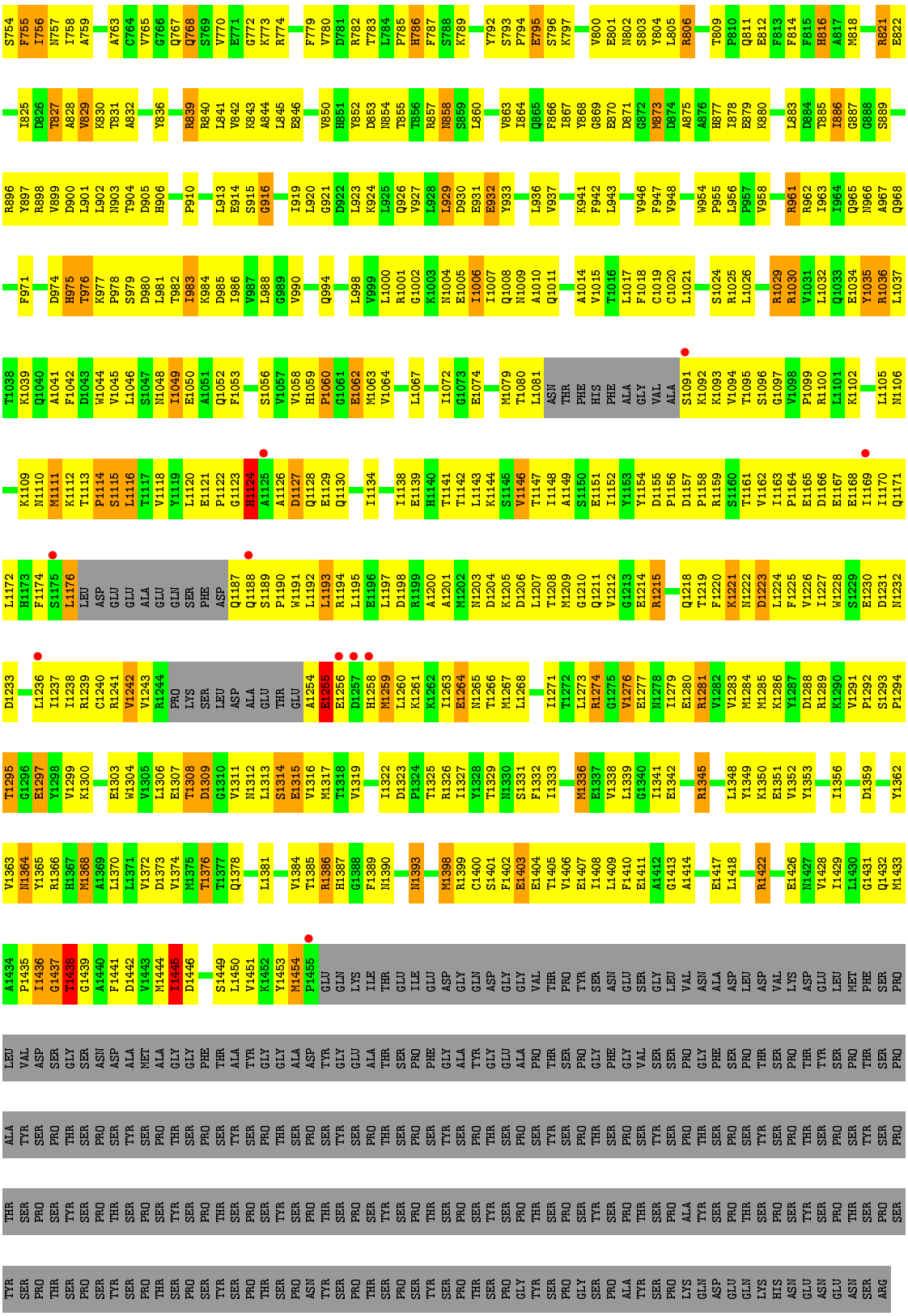
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:

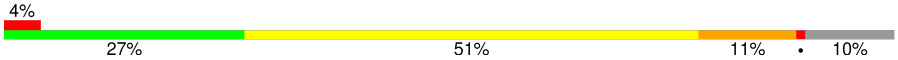


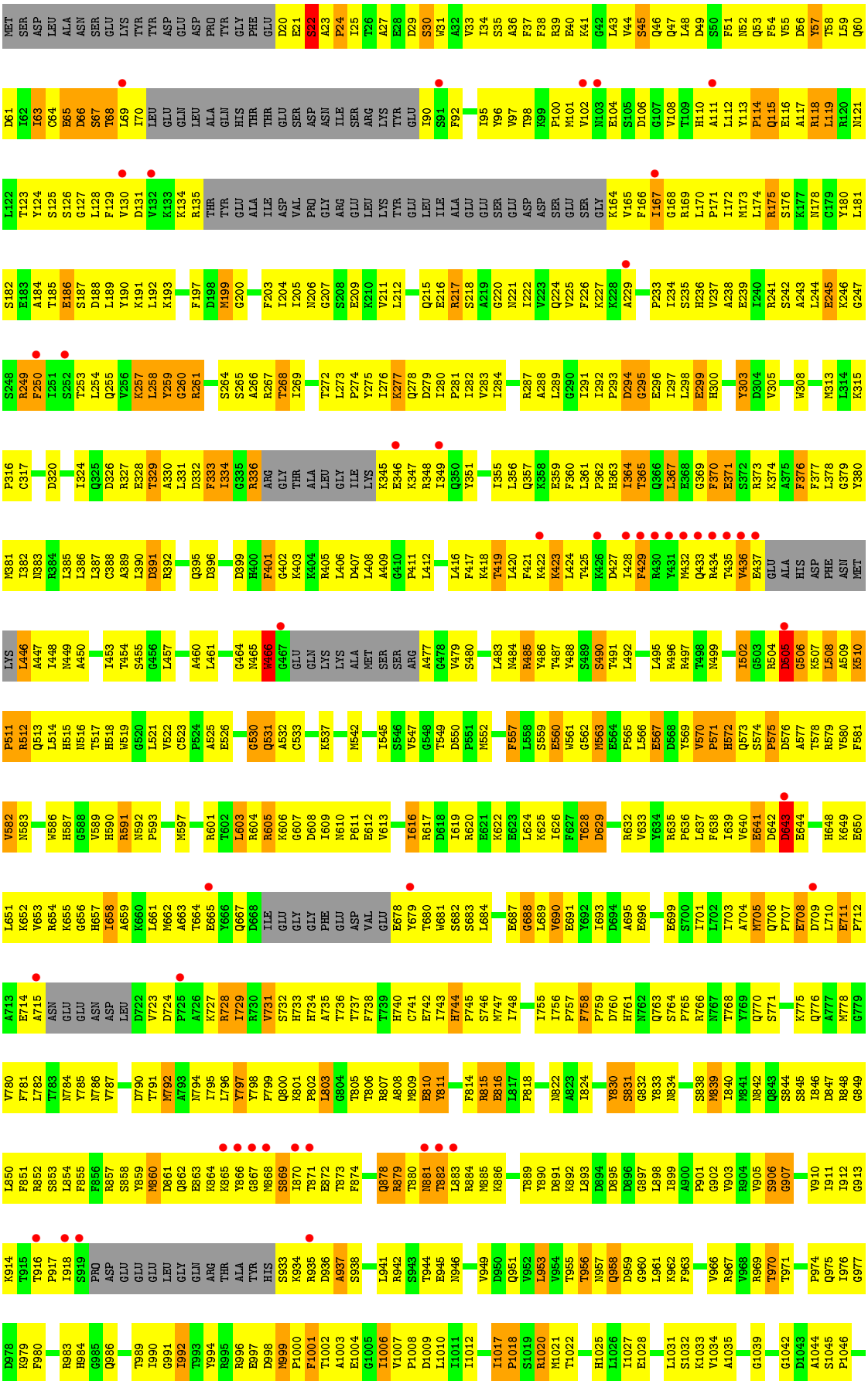


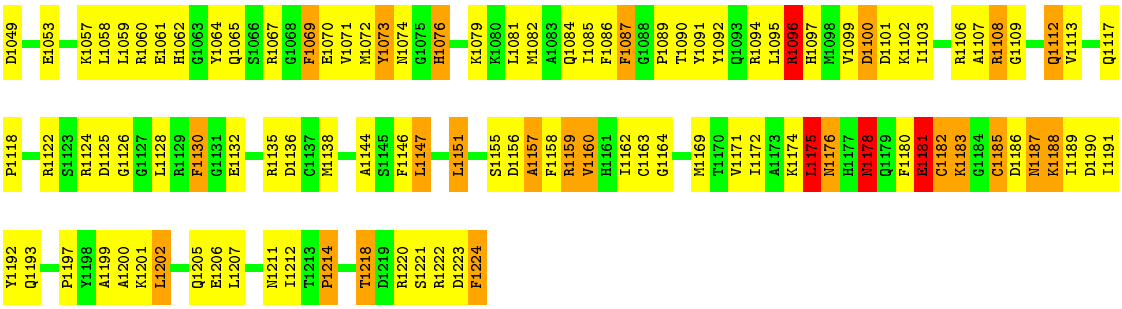


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

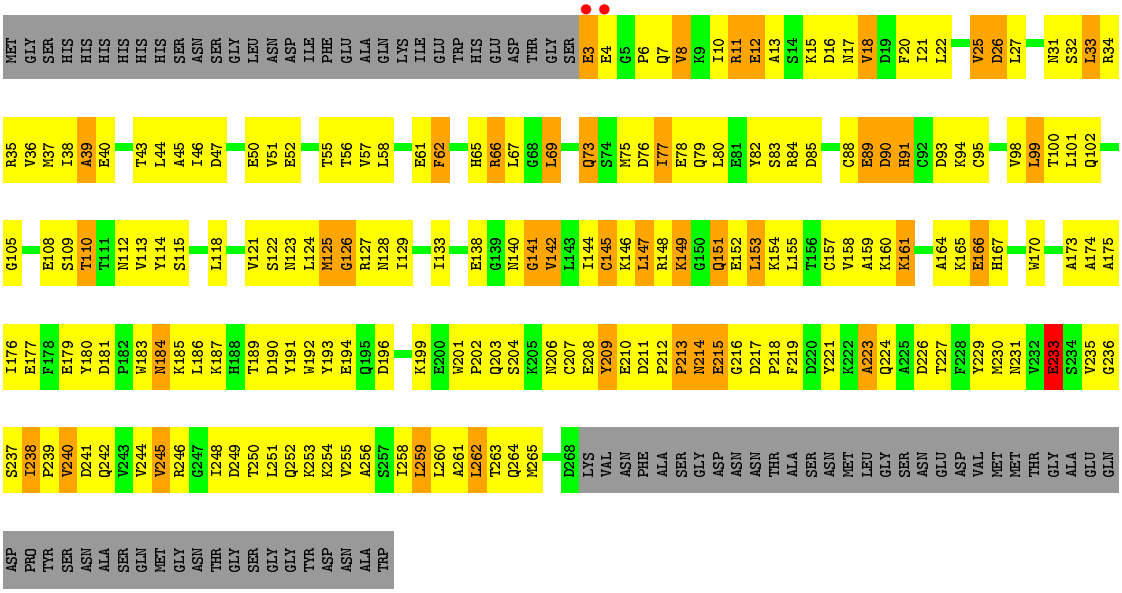






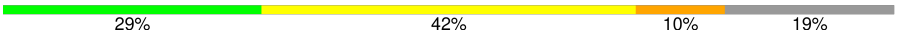
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

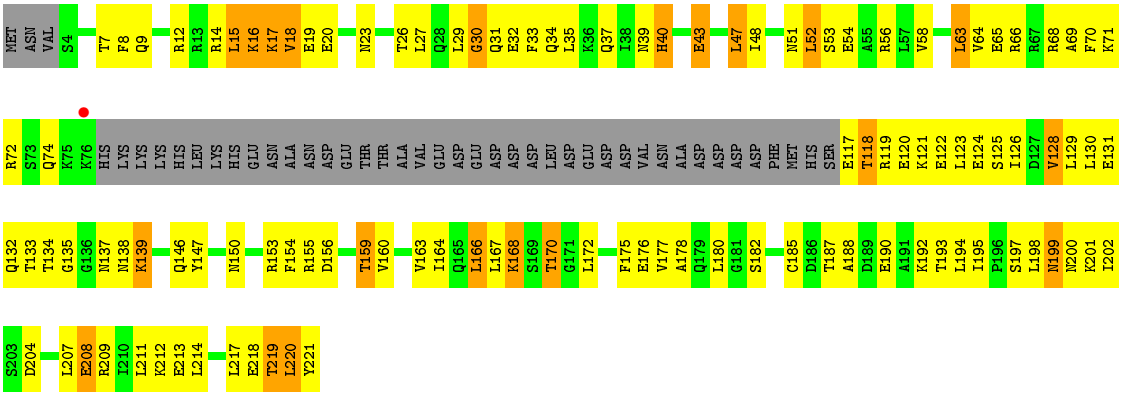
Chain C:



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

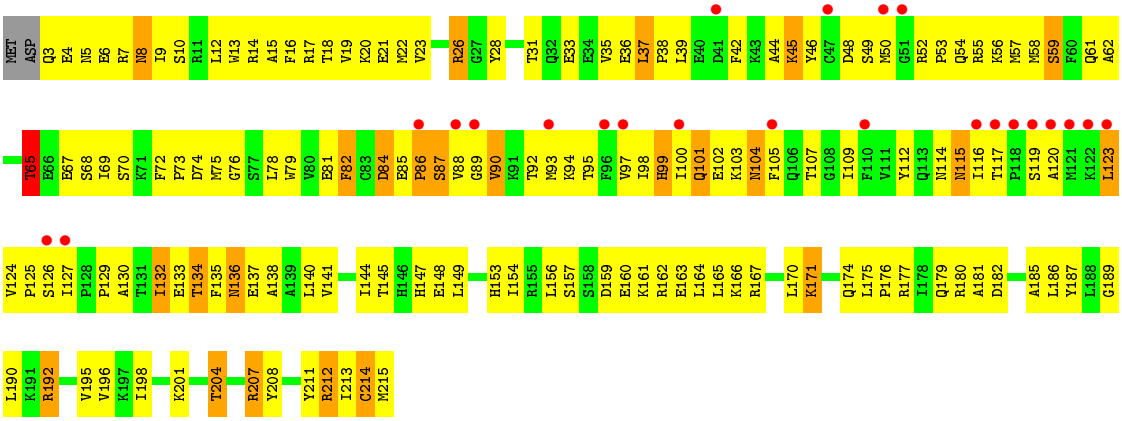
Chain D:





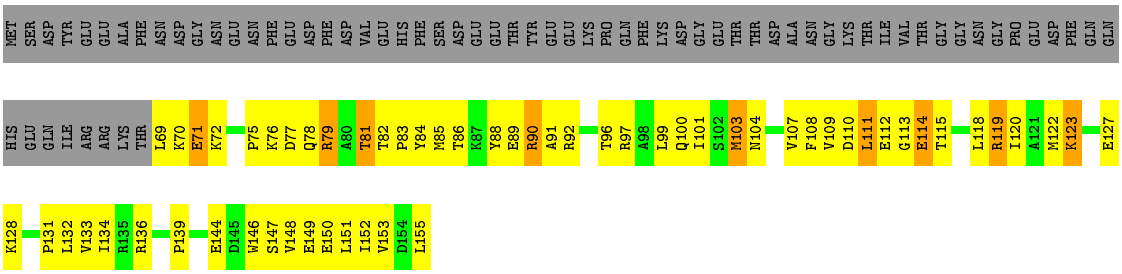
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



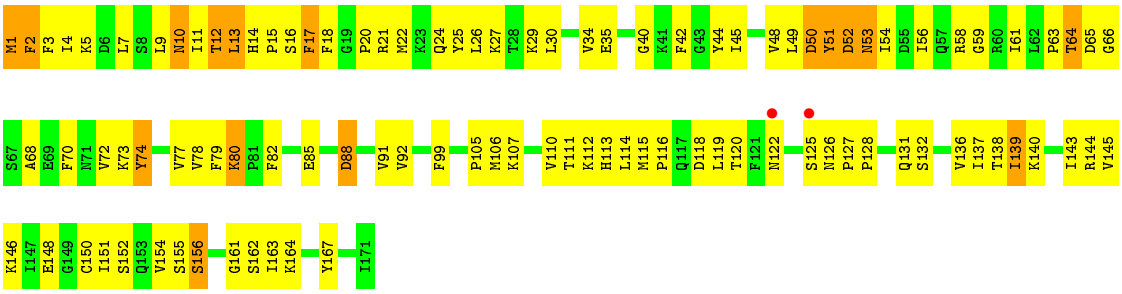
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



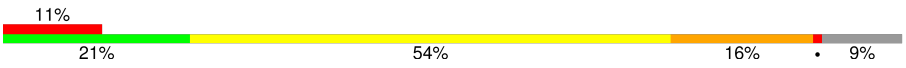
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

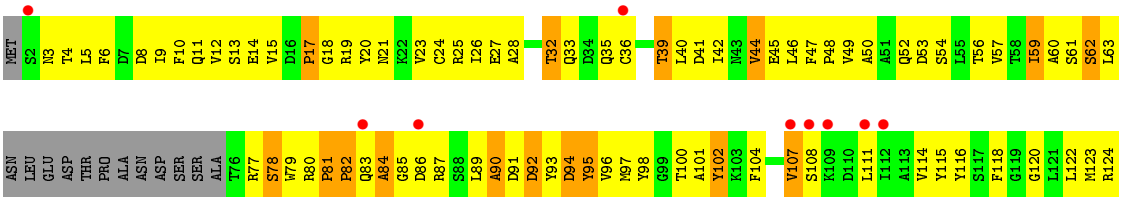
Chain G:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

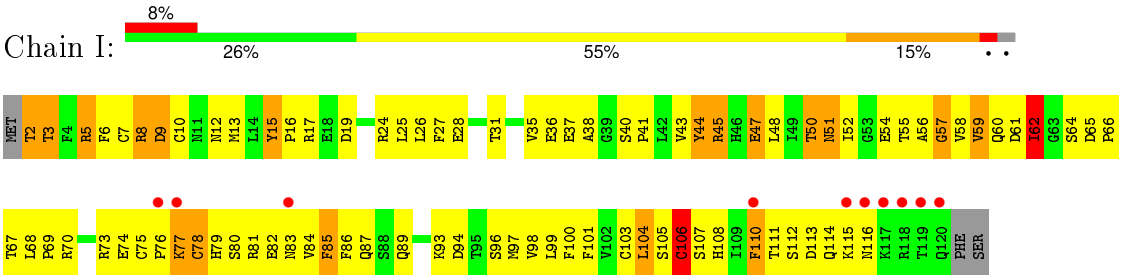
Chain H:





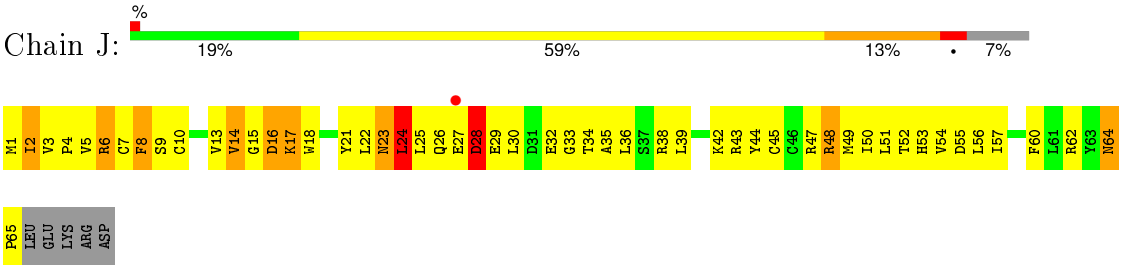
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



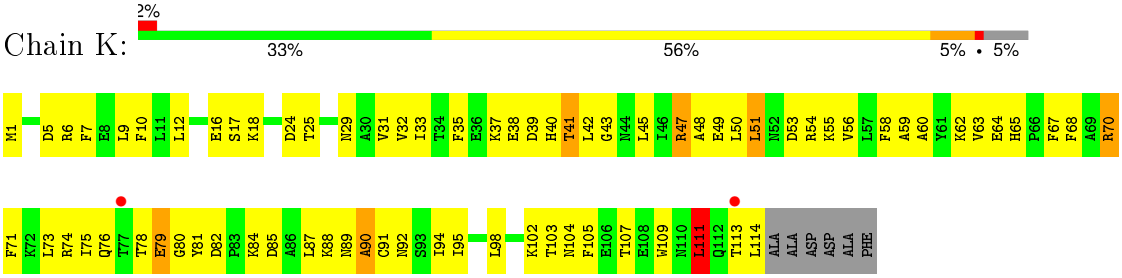
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



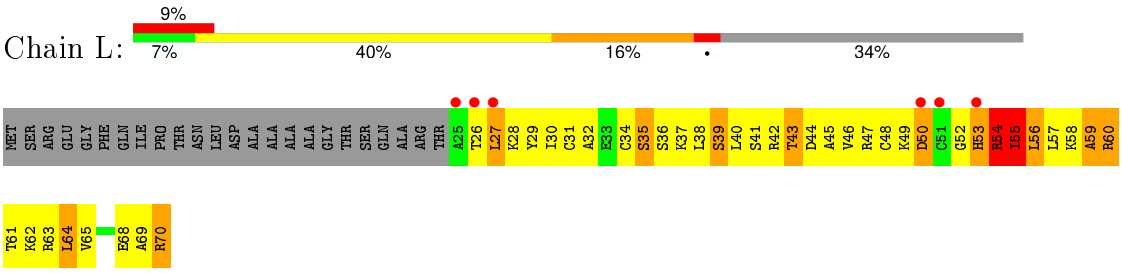
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



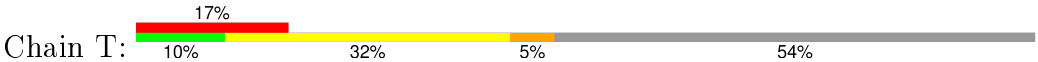
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

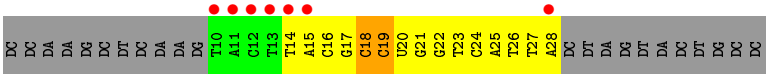
Chain L:



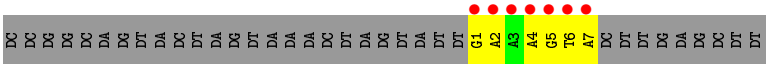
• Molecule 13: 5'-D(*CP*CP*AP*AP*GP*CP*TP*CP*AP*AP*G*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*TP*AP*CP*TP*AP*GP*TP*AP*CP*TP*GP*CP*C)-3'

Chain T:

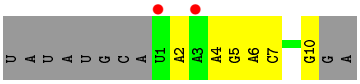




• Molecule 14: 5'-D(*CP*CP*GP*GP*CP*AP*GP*TP*AP*CP*TP*AP*GP*TP*AP*AP*AP*CP*TP*AP*GP*TP*AP*TP*T*GP*AP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP*T)-3'



• Molecule 15: 5'-R(*UP*AP*UP*AP*UP*GP*CP*A*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*A)-3'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.14Å 392.69Å 282.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.09 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (49.09-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.254 0.217 , 0.260	Depositor DCC
R_{free} test set	3325 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.5	EDS
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 168339 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/11365	0.78	7/15367 (0.0%)
2	B	0.49	0/8957	0.74	1/12078 (0.0%)
3	C	0.51	0/2133	0.75	1/2891 (0.0%)
4	D	0.46	0/1374	0.74	1/1849 (0.1%)
5	E	0.46	0/1780	0.68	1/2395 (0.0%)
6	F	0.57	0/717	0.86	1/967 (0.1%)
7	G	0.52	0/1368	0.80	0/1844
8	H	0.47	0/1086	0.76	0/1470
9	I	0.45	0/989	0.68	0/1331
10	J	0.50	0/541	0.88	0/727
11	K	0.49	0/937	0.72	0/1265
12	L	0.60	0/365	0.84	0/485
13	T	0.56	0/403	0.82	0/617
14	N	0.79	0/164	0.77	0/252
15	P	0.58	0/239	0.80	0/371
All	All	0.50	0/32418	0.76	12/43909 (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
13	T	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	26	THR	N-CA-C	-8.03	89.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	39	ALA	N-CA-C	6.23	127.81	111.00
5	E	171	LYS	N-CA-C	-6.18	94.32	111.00
1	A	56	PRO	N-CA-C	-6.06	96.34	112.10
1	A	1445	ILE	CB-CA-C	-5.83	99.94	111.60
6	F	71	GLU	N-CA-C	-5.61	95.85	111.00
1	A	219	PHE	CB-CA-C	-5.61	99.18	110.40
1	A	311	GLN	N-CA-C	5.59	126.10	111.00
1	A	567	LYS	C-N-CD	5.47	139.88	128.40
1	A	331	GLY	N-CA-C	5.44	126.71	113.10
2	B	1130	PHE	N-CA-C	-5.39	96.46	111.00
1	A	452	LYS	N-CA-C	-5.38	96.48	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	T	18	DC	Sidechain
13	T	19	DC	Sidechain
13	T	21	DG	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	11166	0	11248	1160	0
2	B	8786	0	8819	1073	0
3	C	2095	0	2051	275	0
4	D	1365	0	1325	116	0
5	E	1744	0	1772	190	0
6	F	705	0	731	72	0
7	G	1340	0	1357	149	0
8	H	1068	0	1040	174	0
9	I	971	0	929	128	0
10	J	532	0	542	84	0
11	K	919	0	929	97	0
12	L	363	0	388	74	0
13	T	382	0	215	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	145	0	80	9	0
15	P	213	0	111	4	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31803	0	31537	3317	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 52.

All (3317) 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)
14:N:5:DG:H2"	14:N:6:DT:H71	1.17	1.15
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.22	1.14
2:B:345:LYS:HE2	2:B:349:ILE:HD11	1.30	1.14
3:C:189:THR:HG22	3:C:190:ASP:H	1.11	1.14
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.83	1.14
1:A:1386:ARG:HB2	1:A:1403:GLU:HG3	1.26	1.13
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.22	1.12
2:B:559:SER:HA	2:B:563:MET:HB3	1.26	1.10
6:F:111:LEU:H	6:F:111:LEU:HD12	1.05	1.10
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.27	1.09
8:H:59:ILE:HG22	8:H:60:ALA:H	1.12	1.09
2:B:505:ASP:HB3	13:T:17:DG:H22	1.17	1.09
2:B:806:THR:HG22	2:B:808:ALA:H	1.18	1.09
1:A:53:LEU:HD23	1:A:54:ASN:N	1.65	1.09
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.25	1.08
2:B:542:MET:HE3	2:B:747:MET:HG3	1.37	1.07
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.33	1.06
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.37	1.06
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.37	1.06
2:B:664:THR:HA	2:B:667:GLN:HE21	1.15	1.06
2:B:593:PRO:HG2	2:B:617:ARG:HH21	1.10	1.05
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.30	1.04
2:B:815:ARG:HH11	2:B:815:ARG:HB2	1.15	1.04
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.37	1.04
2:B:882:THR:HG23	2:B:884:ARG:H	1.15	1.03
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.37	1.03
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.17	1.03
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.18	1.02
2:B:654:ARG:H	2:B:657:HIS:HD2	1.02	1.02
1:A:567:LYS:HB3	8:H:96:VAL:H	1.22	1.02
1:A:63:ARG:H	1:A:74:MET:HE1	1.21	1.01
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.25	1.01
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.42	1.01
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.23	1.01
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.23	1.01
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.43	1.01
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.90	1.01
2:B:505:ASP:HB3	13:T:17:DG:N2	1.75	1.00
1:A:53:LEU:CD2	1:A:54:ASN:H	1.72	1.00
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.27	1.00
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.91	0.99
1:A:858:ASN:ND2	1:A:860:LEU:H	1.58	0.99
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.43	0.99
4:D:40:HIS:HA	7:G:73:LYS:HZ1	1.23	0.99
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.93	0.99
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.46	0.98
8:H:104:PHE:CZ	8:H:136:LYS:HA	1.99	0.98
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.46	0.97
2:B:295:GLY:H	2:B:298:LEU:HD23	1.27	0.97
2:B:955:THR:HG22	2:B:956:THR:H	1.30	0.97
2:B:531:GLN:HG3	2:B:532:ALA:H	1.30	0.97
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.09	0.97
9:I:111:THR:HG22	9:I:113:ASP:H	1.29	0.96
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.47	0.96
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.48	0.96
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.96
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.21	0.96
5:E:22:MET:O	5:E:26:ARG:HG2	1.66	0.95
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.31	0.95
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.48	0.95
6:F:119:ARG:HG3	6:F:119:ARG:HH11	1.29	0.95
1:A:53:LEU:HD23	1:A:54:ASN:H	0.81	0.95
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.47	0.95
3:C:73:GLN:HE22	3:C:75:MET:HB2	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.49	0.94
1:A:901:LEU:N	1:A:926:GLN:HE21	1.64	0.94
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.48	0.94
12:L:28:LYS:HB2	12:L:39:SER:HA	1.50	0.94
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.83	0.93
7:G:52:ASP:C	7:G:53:ASN:HD22	1.70	0.93
2:B:123:THR:HG23	2:B:205:ILE:HA	1.48	0.93
9:I:50:THR:HG22	9:I:51:ASN:H	1.33	0.93
1:A:900:ASP:HA	1:A:926:GLN:NE2	1.83	0.93
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.09	0.93
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.46	0.93
2:B:882:THR:HG23	2:B:884:ARG:N	1.84	0.93
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.34	0.93
6:F:111:LEU:N	6:F:111:LEU:HD12	1.84	0.92
2:B:884:ARG:O	2:B:936:ASP:HB2	1.69	0.92
3:C:189:THR:HG22	3:C:190:ASP:N	1.80	0.92
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.05	0.92
1:A:71:GLN:HG3	1:A:72:GLU:H	1.35	0.92
1:A:350:ARG:HH11	1:A:488:ASN:HD21	1.15	0.92
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.01	0.92
9:I:105:SER:O	9:I:106:CYS:HB3	1.65	0.91
2:B:315:LYS:HG2	9:I:13:MET:HE1	1.51	0.91
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.51	0.91
6:F:111:LEU:H	6:F:111:LEU:CD1	1.83	0.91
8:H:135:LEU:HD13	8:H:137:GLN:HB2	1.53	0.91
2:B:955:THR:HG22	2:B:956:THR:N	1.84	0.91
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.36	0.91
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.35	0.91
1:A:1385:THR:HG22	1:A:1387:HIS:H	1.33	0.91
8:H:59:ILE:HG22	8:H:60:ALA:N	1.84	0.90
1:A:903:ASN:HD22	1:A:906:HIS:H	1.12	0.90
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.69	0.90
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.01	0.90
4:D:40:HIS:HA	7:G:73:LYS:NZ	1.88	0.89
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.36	0.89
10:J:1:MET:H1	10:J:57:ILE:N	1.71	0.89
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.38	0.89
11:K:113:THR:O	11:K:114:LEU:HB2	1.69	0.89
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.55	0.89
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.55	0.88
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.54	0.88
3:C:189:THR:CG2	3:C:190:ASP:H	1.86	0.88
4:D:220:LEU:HD22	4:D:221:TYR:H	1.37	0.88
4:D:156:ASP:HB2	4:D:159:THR:OG1	1.73	0.88
1:A:399:HIS:O	1:A:401:GLY:N	2.07	0.88
1:A:901:LEU:H	1:A:926:GLN:HE21	1.15	0.88
9:I:77:LYS:HG2	9:I:78:CYS:H	1.38	0.87
4:D:220:LEU:HD13	4:D:221:TYR:N	1.89	0.87
10:J:1:MET:N	10:J:57:ILE:H	1.72	0.87
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.10	0.87
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.90	0.87
2:B:168:GLY:N	2:B:450:ALA:HB1	1.89	0.87
1:A:90:VAL:HG12	1:A:297:GLN:NE2	1.88	0.87
5:E:120:ALA:O	5:E:123:LEU:HG	1.74	0.87
3:C:22:LEU:HD21	3:C:25:VAL:HG11	1.56	0.87
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.55	0.86
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.56	0.86
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.03	0.86
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.24	0.86
1:A:225:ASN:ND2	1:A:228:PHE:H	1.73	0.86
2:B:345:LYS:HG2	2:B:346:GLU:H	1.39	0.86
2:B:882:THR:HG21	2:B:934:LYS:O	1.76	0.86
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.75	0.86
6:F:99:LEU:O	6:F:103:MET:HG3	1.75	0.86
1:A:34:LYS:NZ	1:A:57:ARG:HH12	1.72	0.86
1:A:855:THR:HG21	1:A:857:ARG:HE	1.41	0.86
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.56	0.85
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.58	0.85
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.57	0.85
1:A:567:LYS:HB3	8:H:96:VAL:N	1.91	0.85
7:G:111:THR:HB	7:G:114:LEU:HD13	1.58	0.85
2:B:25:ILE:HD11	2:B:653:VAL:HG12	1.57	0.85
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.57	0.85
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.57	0.85
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.11	0.85
14:N:5:DG:C2'	14:N:6:DT:H71	2.05	0.84
2:B:261:ARG:NH1	2:B:261:ARG:HB3	1.92	0.84
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.58	0.84
1:A:858:ASN:HD22	1:A:858:ASN:C	1.80	0.84
5:E:22:MET:CE	5:E:26:ARG:HE	1.90	0.84
1:A:71:GLN:HG3	1:A:72:GLU:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.38	0.84
1:A:982:THR:HG22	1:A:984:LYS:H	1.38	0.84
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.57	0.84
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.41	0.84
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.59	0.84
2:B:642:ASP:HA	2:B:649:LYS:HA	1.58	0.84
3:C:99:LEU:HD23	3:C:99:LEU:N	1.93	0.84
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.60	0.84
7:G:1:MET:SD	7:G:2:PHE:N	2.51	0.84
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.42	0.84
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.75	0.84
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.92	0.84
2:B:218:SER:HB2	2:B:241:ARG:NH1	1.92	0.84
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.12	0.83
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.21	0.83
6:F:103:MET:CE	7:G:66:GLY:H	1.91	0.83
2:B:806:THR:HG22	2:B:808:ALA:N	1.93	0.83
5:E:90:VAL:N	5:E:120:ALA:HB2	1.93	0.83
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.43	0.83
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.42	0.83
1:A:63:ARG:H	1:A:74:MET:CE	1.90	0.83
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.12	0.83
1:A:534:LEU:O	1:A:574:GLY:HA3	1.78	0.83
1:A:62:ASP:HB3	1:A:64:ASN:HB2	1.59	0.83
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.59	0.83
2:B:549:THR:HG22	2:B:550:ASP:N	1.94	0.83
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.94	0.83
1:A:698:GLN:HA	9:I:97:MET:O	1.79	0.83
7:G:111:THR:HG22	7:G:113:HIS:H	1.42	0.83
3:C:11:ARG:NH2	3:C:229:TYR:HD2	1.77	0.82
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.59	0.82
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.60	0.82
9:I:111:THR:HG22	9:I:112:SER:N	1.93	0.82
7:G:1:MET:SD	7:G:79:PHE:CD1	2.73	0.82
1:A:140:THR:HA	1:A:143:LYS:HE2	1.61	0.82
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.61	0.82
7:G:1:MET:HE3	7:G:80:LYS:N	1.94	0.82
1:A:913:LEU:HD12	1:A:914:GLU:H	1.44	0.82
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.14	0.82
2:B:654:ARG:H	2:B:657:HIS:CD2	1.94	0.82
1:A:535:THR:HG21	1:A:616:VAL:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.44	0.82
1:A:901:LEU:H	1:A:926:GLN:NE2	1.77	0.82
2:B:601:ARG:O	2:B:605:ARG:HG3	1.79	0.82
2:B:504:ARG:HG3	2:B:505:ASP:H	1.42	0.81
2:B:955:THR:CG2	2:B:956:THR:H	1.91	0.81
8:H:4:THR:HA	8:H:60:ALA:HB2	1.61	0.81
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.45	0.81
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.62	0.81
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.62	0.81
2:B:801:LYS:O	10:J:52:THR:HG23	1.80	0.81
1:A:710:LEU:H	1:A:710:LEU:HD12	1.45	0.81
2:B:211:VAL:O	2:B:480:SER:HA	1.81	0.81
2:B:1072:MET:HE2	2:B:1087:PHE:HD1	1.45	0.81
9:I:111:THR:HG22	9:I:112:SER:H	1.46	0.81
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.79	0.81
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.61	0.81
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.81	0.81
1:A:754:SER:H	1:A:757:ASN:HD22	1.28	0.81
1:A:344:ARG:NH1	1:A:344:ARG:HB3	1.95	0.81
10:J:1:MET:H1	10:J:57:ILE:H	0.85	0.81
3:C:128:ASN:O	3:C:129:ILE:HG13	1.81	0.81
3:C:238:ILE:HD11	3:C:246:ARG:CZ	2.11	0.80
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.63	0.80
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.63	0.80
7:G:79:PHE:CE2	7:G:106:MET:HE2	2.17	0.80
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.62	0.80
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.61	0.80
11:K:1:MET:HG2	11:K:1:MET:O	1.80	0.80
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.10	0.80
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.63	0.80
5:E:165:LEU:HD21	5:E:175:LEU:HD11	1.62	0.80
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.80	0.80
2:B:126:SER:OG	2:B:172:ILE:HD11	1.82	0.80
2:B:641:GLU:HB3	2:B:643:ASP:OD2	1.82	0.80
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.79	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.63	0.80
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.17	0.80
2:B:172:ILE:HG12	2:B:178:ASN:HD22	1.47	0.80
3:C:50:GLU:HB3	12:L:64:LEU:CD1	2.12	0.80
1:A:596:THR:O	1:A:598:LEU:N	2.15	0.80
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:THR:O	1:A:679:ILE:HG13	1.81	0.80
3:C:115:SER:HB3	3:C:141:GLY:O	1.82	0.80
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.64	0.80
1:A:488:ASN:HD22	2:B:1128:LEU:HD13	1.47	0.79
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.64	0.79
1:A:71:GLN:CG	1:A:72:GLU:H	1.92	0.79
2:B:245:GLU:O	2:B:246:LYS:HG3	1.82	0.79
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.11	0.79
8:H:135:LEU:HD22	8:H:137:GLN:HG3	1.64	0.79
1:A:780:VAL:O	1:A:782:ARG:HG2	1.81	0.79
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.81	0.79
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.98	0.79
1:A:254:GLU:HB2	2:B:935:ARG:NH2	1.98	0.79
2:B:101:MET:HG2	2:B:111:ALA:HA	1.64	0.79
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.63	0.79
9:I:50:THR:HG22	9:I:51:ASN:N	1.96	0.79
3:C:32:SER:O	3:C:36:VAL:HG23	1.83	0.79
3:C:253:LYS:O	3:C:256:ALA:HB3	1.82	0.79
2:B:345:LYS:HA	2:B:348:ARG:HE	1.47	0.79
1:A:22:PHE:HB2	2:B:1211:ASN:ND2	1.98	0.79
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.65	0.78
2:B:559:SER:CA	2:B:563:MET:HB3	2.12	0.78
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.62	0.78
11:K:79:GLU:HG3	11:K:80:GLY:N	1.98	0.78
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.17	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.65	0.78
1:A:34:LYS:HZ1	1:A:57:ARG:HH12	1.32	0.78
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.62	0.78
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.19	0.78
2:B:664:THR:HA	2:B:667:GLN:NE2	1.96	0.78
5:E:180:ARG:NH2	5:E:192:ARG:HB2	1.97	0.78
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.98	0.78
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.64	0.78
2:B:605:ARG:NH1	2:B:639:ILE:HG21	1.98	0.78
2:B:345:LYS:HE2	2:B:349:ILE:CD1	2.13	0.78
2:B:277:LYS:HE3	2:B:336:ARG:HD2	1.66	0.78
1:A:601:LYS:HB2	1:A:603:ASN:ND2	1.99	0.78
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.66	0.78
2:B:115:GLN:O	2:B:119:LEU:HD12	1.83	0.77
1:A:567:LYS:CB	8:H:95:TYR:HA	2.14	0.77
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ALA:O	5:E:19:VAL:HG23	1.83	0.77
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.66	0.77
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.13	0.77
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.19	0.77
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.98	0.77
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.49	0.77
7:G:126:ASN:ND2	7:G:127:PRO:HA	1.99	0.77
1:A:886:ILE:HG22	1:A:887:GLY:N	1.99	0.77
2:B:295:GLY:N	2:B:298:LEU:HD23	2.00	0.77
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.14	0.77
3:C:124:LEU:O	3:C:127:ARG:HG2	1.83	0.77
7:G:14:HIS:HD2	7:G:16:SER:CB	1.98	0.77
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.82	0.77
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.65	0.77
2:B:345:LYS:N	2:B:347:LYS:HE2	2.00	0.77
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.66	0.77
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.24	0.77
2:B:292:ILE:HD11	2:B:327:ARG:H	1.48	0.77
5:E:17:ARG:HH21	5:E:35:VAL:HG12	1.49	0.77
3:C:165:LYS:O	11:K:6:ARG:NH1	2.18	0.77
1:A:1329:THR:HG22	1:A:1331:SER:N	1.99	0.77
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.66	0.76
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.68	0.76
2:B:359:GLU:O	2:B:362:PRO:HD3	1.84	0.76
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.66	0.76
12:L:38:LEU:O	12:L:39:SER:HB3	1.83	0.76
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.85	0.76
6:F:77:ASP:O	6:F:78:GLN:HB2	1.84	0.76
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.15	0.76
1:A:151:ASP:OD1	1:A:163:SER:HA	1.85	0.76
2:B:873:THR:O	2:B:914:LYS:HA	1.84	0.76
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.65	0.76
2:B:274:PRO:O	2:B:275:TYR:HB2	1.83	0.76
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.66	0.76
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.00	0.76
1:A:1114:PRO:O	1:A:1311:VAL:HG23	1.86	0.76
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.21	0.76
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.11	0.76
1:A:55:ASP:N	1:A:56:PRO:HD3	1.98	0.76
8:H:104:PHE:HZ	8:H:136:LYS:HA	1.49	0.76
9:I:70:ARG:NH1	9:I:84:VAL:HB	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:ARG:HG2	12:L:61:THR:H	1.51	0.76
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.67	0.76
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.66	0.76
2:B:549:THR:CG2	2:B:550:ASP:H	1.98	0.76
8:H:93:TYR:HB3	8:H:144:ILE:O	1.85	0.76
1:A:1171:GLN:O	1:A:1174:PHE:HB2	1.86	0.76
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	1.86	0.75
3:C:76:ASP:OD2	3:C:128:ASN:N	2.19	0.75
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.16	0.75
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.49	0.75
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.66	0.75
4:D:34:GLN:O	4:D:47:LEU:HD23	1.85	0.75
1:A:326:ARG:HD3	1:A:330:LYS:NZ	2.01	0.75
2:B:43:LEU:HD13	2:B:492:LEU:HD13	1.68	0.75
5:E:22:MET:HE3	5:E:26:ARG:HE	1.51	0.75
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.22	0.75
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.67	0.75
1:A:524:VAL:HG12	1:A:525:GLN:H	1.51	0.75
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.67	0.75
11:K:63:VAL:HG23	11:K:63:VAL:O	1.86	0.75
1:A:225:ASN:ND2	1:A:227:VAL:H	1.85	0.75
1:A:215:SER:OG	1:A:218:ASP:HB2	1.86	0.75
12:L:49:LYS:O	12:L:50:ASP:HB2	1.86	0.75
1:A:903:ASN:HD22	1:A:906:HIS:N	1.82	0.75
2:B:902:GLY:O	12:L:65:VAL:HG11	1.87	0.75
14:N:5:DG:H2"	14:N:6:DT:C7	2.08	0.75
4:D:220:LEU:HD22	4:D:221:TYR:N	2.01	0.75
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.22	0.74
8:H:127:GLY:O	8:H:128:ASN:HB2	1.87	0.74
4:D:220:LEU:CD2	4:D:221:TYR:H	2.01	0.74
2:B:345:LYS:CE	2:B:349:ILE:HD11	2.15	0.74
2:B:296:GLU:O	2:B:299:GLU:HB2	1.87	0.74
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.69	0.74
1:A:56:PRO:O	1:A:57:ARG:CD	2.36	0.74
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.87	0.74
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.51	0.74
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.67	0.74
1:A:1386:ARG:NH1	13:T:16:DC:H5"	2.03	0.74
2:B:815:ARG:HB2	2:B:815:ARG:NH1	1.99	0.74
2:B:871:THR:HG22	2:B:872:GLU:N	2.02	0.74
1:A:37:PHE:HD1	1:A:37:PHE:N	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:HD3	11:K:59:ALA:O	1.87	0.74
1:A:252:PHE:O	1:A:253:ASN:HB2	1.87	0.74
3:C:123:ASN:HD21	3:C:125:MET:HG2	1.50	0.74
14:N:1:DG:H2"	14:N:2:DA:OP2	1.87	0.74
2:B:273:LEU:HB2	2:B:276:ILE:CD1	2.11	0.74
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.70	0.74
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.69	0.74
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.70	0.74
1:A:774:ARG:HE	1:A:797:LYS:HB2	1.52	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.70	0.74
2:B:815:ARG:HH11	2:B:815:ARG:CB	1.98	0.74
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.16	0.74
1:A:51:GLY:O	1:A:56:PRO:HB3	1.88	0.74
3:C:147:LEU:N	3:C:147:LEU:HD23	2.03	0.74
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.70	0.74
5:E:19:VAL:O	5:E:23:VAL:HG23	1.88	0.74
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.05	0.74
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.53	0.73
2:B:842:ASN:HD22	2:B:845:SER:H	1.36	0.73
2:B:1159:ARG:HD2	2:B:1159:ARG:O	1.88	0.73
2:B:504:ARG:O	2:B:506:GLY:N	2.22	0.73
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.88	0.73
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.68	0.73
2:B:652:LYS:HD3	2:B:688:GLY:O	1.88	0.73
2:B:332:ASP:O	2:B:334:ILE:N	2.20	0.73
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.18	0.73
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.24	0.73
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.71	0.73
4:D:118:THR:HB	4:D:121:LYS:HB2	1.70	0.73
2:B:549:THR:HG22	2:B:550:ASP:H	1.50	0.73
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.52	0.73
1:A:12:ARG:HB2	2:B:1218:THR:CG2	2.18	0.73
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.03	0.73
7:G:1:MET:HE3	7:G:80:LYS:H	1.53	0.73
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.16	0.73
12:L:55:ILE:H	12:L:55:ILE:HD13	1.54	0.73
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.70	0.73
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.73
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.09	0.73
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.71	0.73
2:B:1099:VAL:O	2:B:1101:ASP:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:LYS:O	6:F:79:ARG:HD3	1.89	0.73
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.16	0.73
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.03	0.73
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.71	0.73
2:B:424:LEU:HA	2:B:427:ASP:OD2	1.89	0.73
1:A:42:ASP:HA	1:A:46:THR:O	1.88	0.73
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.54	0.72
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.02	0.72
1:A:751:SER:O	1:A:752:LYS:HG2	1.89	0.72
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.89	0.72
9:I:77:LYS:HB3	9:I:77:LYS:NZ	2.03	0.72
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.19	0.72
1:A:134:ARG:HD2	1:A:221:SER:O	1.89	0.72
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.10	0.72
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.25	0.72
1:A:590:ARG:O	1:A:591:PHE:HB2	1.89	0.72
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.70	0.72
13:T:19:DC:C5	13:T:20:BRU:BR	2.98	0.72
2:B:345:LYS:C	2:B:347:LYS:H	1.92	0.72
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.20	0.72
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.70	0.72
3:C:196:ASP:OD2	3:C:199:LYS:HE3	1.89	0.72
14:N:6:DT:H2"	14:N:7:DA:C8	2.25	0.72
1:A:69:THR:O	1:A:71:GLN:N	2.22	0.72
2:B:390:LEU:O	2:B:391:ASP:HB2	1.88	0.72
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.19	0.72
7:G:106:MET:HG2	7:G:107:LYS:N	2.03	0.72
1:A:974:ASP:HB2	1:A:976:THR:HG23	1.71	0.72
2:B:593:PRO:CG	2:B:617:ARG:HH21	1.97	0.72
3:C:7:GLN:HG2	11:K:104:ASN:ND2	2.05	0.72
2:B:65:GLU:HG3	2:B:66:ASP:OD1	1.90	0.72
1:A:222:LEU:O	1:A:224:PHE:HD1	1.72	0.72
1:A:858:ASN:HD22	1:A:860:LEU:H	1.37	0.72
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.25	0.72
1:A:1242:VAL:O	1:A:1243:VAL:HG23	1.90	0.72
1:A:646:PHE:O	1:A:650:GLN:HG3	1.90	0.72
9:I:111:THR:CG2	9:I:112:SER:H	2.02	0.71
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.72	0.71
1:A:35:ILE:HG22	1:A:35:ILE:O	1.90	0.71
6:F:119:ARG:CG	6:F:119:ARG:HH11	2.04	0.71
2:B:165:VAL:HG11	2:B:448:ILE:HD12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:O	2:B:759:PRO:HD3	1.90	0.71
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.19	0.71
2:B:185:THR:H	2:B:188:ASP:HB2	1.53	0.71
8:H:5:LEU:HD13	8:H:134:ASN:HA	1.71	0.71
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.03	0.71
11:K:37:LYS:O	11:K:38:GLU:HG2	1.91	0.71
1:A:129:LYS:O	1:A:130:ASP:HB2	1.89	0.71
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.24	0.71
4:D:220:LEU:HD13	4:D:221:TYR:H	1.52	0.71
6:F:103:MET:HE1	7:G:66:GLY:H	1.54	0.71
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.26	0.71
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.72	0.71
11:K:65:HIS:CD2	11:K:67:PHE:H	2.08	0.71
2:B:1172:ILE:O	2:B:1172:ILE:HG22	1.91	0.71
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.26	0.71
7:G:1:MET:SD	7:G:79:PHE:HD1	2.11	0.71
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.72	0.71
2:B:425:THR:HA	2:B:428:ILE:HD12	1.71	0.71
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.71	0.71
5:E:153:HIS:O	5:E:154:ILE:HG13	1.90	0.71
4:D:185:CYS:O	4:D:211:LEU:HD22	1.91	0.71
1:A:975:HIS:HA	1:A:1036:ARG:HG3	1.72	0.71
8:H:12:VAL:HG11	8:H:26:ILE:HD11	1.73	0.71
5:E:159:ASP:HA	5:E:162:ARG:NH2	2.05	0.71
2:B:616:ILE:N	2:B:616:ILE:HD12	2.05	0.71
2:B:172:ILE:HD12	2:B:172:ILE:N	2.06	0.71
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.21	0.71
2:B:408:LEU:HD21	2:B:545:ILE:HD12	1.70	0.71
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.26	0.70
1:A:66:LYS:O	1:A:67:CYS:HB2	1.90	0.70
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.21	0.70
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.21	0.70
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.73	0.70
8:H:130:ARG:H	8:H:130:ARG:HD2	1.54	0.70
10:J:23:ASN:C	10:J:25:LEU:H	1.94	0.70
1:A:1120:LEU:HD13	1:A:1304:TRP:O	1.90	0.70
1:A:864:ILE:HD12	1:A:864:ILE:N	2.05	0.70
6:F:97:ARG:O	6:F:101:ILE:HG13	1.91	0.70
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.19	0.70
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.21	0.70
9:I:5:ARG:HG2	9:I:6:PHE:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:HB2	2:B:1099:VAL:HG11	1.72	0.70
8:H:4:THR:HA	8:H:60:ALA:CB	2.21	0.70
8:H:4:THR:HG22	8:H:5:LEU:N	2.07	0.70
2:B:549:THR:CG2	2:B:550:ASP:N	2.54	0.70
11:K:6:ARG:O	11:K:9:LEU:HG	1.90	0.70
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.72	0.70
14:N:1:DG:H1'	14:N:2:DA:O5'	1.92	0.70
7:G:14:HIS:HD2	7:G:16:SER:HB3	1.54	0.70
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.56	0.70
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.73	0.70
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.74	0.70
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.26	0.70
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.74	0.70
9:I:111:THR:HG22	9:I:113:ASP:N	2.06	0.70
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.73	0.70
9:I:93:LYS:HD2	9:I:93:LYS:H	1.55	0.70
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.27	0.69
8:H:100:THR:HG23	8:H:138:GLU:HA	1.73	0.69
7:G:17:PHE:N	7:G:17:PHE:CD2	2.59	0.69
2:B:806:THR:HB	2:B:809:MET:HG3	1.75	0.69
1:A:710:LEU:H	1:A:710:LEU:CD1	2.05	0.69
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.22	0.69
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.41	0.69
3:C:57:VAL:CG1	10:J:60:PHE:HB3	2.13	0.69
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.56	0.69
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.57	0.69
2:B:345:LYS:O	2:B:347:LYS:HG2	1.91	0.69
2:B:278:GLN:HG2	2:B:279:ASP:H	1.57	0.69
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.24	0.69
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.72	0.69
1:A:549:MET:SD	1:A:577:ILE:HD11	2.32	0.69
3:C:152:GLU:HG2	3:C:153:LEU:H	1.56	0.69
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.19	0.69
2:B:642:ASP:HA	2:B:649:LYS:HG3	1.74	0.69
5:E:12:LEU:HD21	5:E:58:MET:SD	2.32	0.69
3:C:258:ILE:O	3:C:262:LEU:HB2	1.92	0.69
2:B:505:ASP:O	2:B:507:LYS:HG3	1.93	0.69
10:J:65:PRO:HG3	12:L:32:ALA:O	1.92	0.69
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.74	0.69
2:B:708:GLU:O	2:B:710:LEU:N	2.26	0.69
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:GLU:HA	1:A:1171:GLN:NE2	2.08	0.69
1:A:1236:LEU:O	1:A:1237:ILE:HG13	1.92	0.69
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.26	0.69
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.73	0.69
1:A:34:LYS:CE	1:A:57:ARG:HH12	2.05	0.69
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.23	0.69
9:I:50:THR:CG2	9:I:51:ASN:H	2.05	0.69
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.57	0.69
1:A:350:ARG:HH11	1:A:488:ASN:ND2	1.90	0.69
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.75	0.69
1:A:326:ARG:HH11	1:A:330:LYS:HZ1	1.41	0.69
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.28	0.69
8:H:135:LEU:HD21	8:H:137:GLN:HE21	1.58	0.69
1:A:37:PHE:CD1	1:A:37:PHE:N	2.58	0.69
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.08	0.69
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.27	0.69
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.75	0.69
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.58	0.69
2:B:507:LYS:HA	2:B:512:ARG:HH21	1.54	0.69
2:B:254:LEU:HD23	2:B:381:MET:CE	2.22	0.69
5:E:116:ILE:HG22	5:E:120:ALA:HB3	1.75	0.69
6:F:75:PRO:O	6:F:77:ASP:O	2.11	0.69
1:A:362:ASP:OD1	1:A:459:ARG:HD3	1.93	0.68
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.75	0.68
2:B:654:ARG:N	2:B:657:HIS:HD2	1.86	0.68
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.76	0.68
2:B:364:ILE:O	2:B:365:THR:HB	1.93	0.68
8:H:139:ASN:O	8:H:140:ALA:HB2	1.91	0.68
1:A:388:LEU:O	1:A:392:VAL:HG23	1.94	0.68
2:B:216:GLU:OE1	2:B:537:LYS:HE2	1.94	0.68
2:B:197:PHE:CE2	2:B:816:GLU:HG2	2.28	0.68
9:I:82:GLU:O	9:I:104:LEU:HG	1.92	0.68
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.24	0.68
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.74	0.68
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.91	0.68
2:B:659:ALA:HA	2:B:662:MET:HE2	1.74	0.68
1:A:70:CYS:O	1:A:72:GLU:HG2	1.93	0.68
2:B:423:LYS:O	2:B:423:LYS:HD3	1.93	0.68
1:A:67:CYS:C	1:A:68:GLN:HG3	2.14	0.68
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.08	0.68
6:F:109:VAL:CG1	6:F:123:LYS:HD3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.75	0.68
7:G:17:PHE:N	7:G:17:PHE:HD2	1.91	0.68
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.76	0.68
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	1.74	0.68
1:A:832:ALA:O	13:T:18:DC:H5'	1.93	0.68
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.24	0.68
2:B:605:ARG:HH12	2:B:639:ILE:HG21	1.57	0.68
2:B:916:THR:O	2:B:935:ARG:HG2	1.93	0.68
2:B:41:LYS:HE2	2:B:41:LYS:HA	1.76	0.68
2:B:531:GLN:CG	2:B:532:ALA:H	2.05	0.68
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.77	0.68
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.24	0.68
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.76	0.68
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.24	0.68
1:A:270:LEU:O	1:A:274:ILE:HG13	1.94	0.68
1:A:150:THR:HG23	1:A:166:GLY:HA3	1.74	0.67
2:B:461:LEU:H	2:B:461:LEU:HD12	1.59	0.67
2:B:294:ASP:O	2:B:296:GLU:N	2.26	0.67
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.05	0.67
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.75	0.67
1:A:942:PHE:CE1	5:E:207:ARG:HD3	2.28	0.67
1:A:535:THR:CG2	1:A:616:VAL:HA	2.25	0.67
2:B:90:ILE:HD12	2:B:432:MET:SD	2.34	0.67
13:T:19:DC:C6	13:T:20:BRU:BR	3.03	0.67
2:B:705:MET:H	2:B:710:LEU:CD1	2.07	0.67
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.07	0.67
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.75	0.67
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.41	0.67
1:A:858:ASN:ND2	1:A:860:LEU:N	2.39	0.67
9:I:74:GLU:HA	9:I:80:SER:O	1.93	0.67
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.21	0.67
3:C:50:GLU:HB3	12:L:64:LEU:HD11	1.75	0.67
3:C:203:GLN:HG3	3:C:207:CYS:SG	2.34	0.67
2:B:906:SER:O	2:B:941:LEU:HD23	1.94	0.67
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.76	0.67
2:B:871:THR:HG22	2:B:872:GLU:H	1.60	0.67
5:E:207:ARG:HH11	5:E:207:ARG:CB	2.06	0.67
1:A:1276:VAL:HG11	1:A:1315:GLU:HB3	1.76	0.67
2:B:324:ILE:HG23	2:B:329:THR:HG22	1.77	0.67
1:A:1032:LEU:O	1:A:1036:ARG:HD3	1.94	0.67
2:B:90:ILE:CD1	2:B:432:MET:SD	2.83	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:HB3	1:A:45:GLN:N	2.10	0.67
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.75	0.67
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.34	0.67
9:I:35:VAL:HG12	9:I:36:GLU:N	2.10	0.67
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.58	0.67
1:A:869:GLY:O	5:E:204:THR:HG21	1.95	0.67
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.23	0.67
7:G:27:LYS:HD3	7:G:51:TYR:HE2	1.56	0.67
2:B:942:ARG:NH2	13:T:24:DC:OP2	2.28	0.67
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.77	0.67
2:B:377:PHE:O	2:B:380:TYR:N	2.28	0.67
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.25	0.67
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.77	0.67
2:B:976:ILE:O	2:B:990:ILE:HB	1.95	0.67
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.75	0.67
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.25	0.67
1:A:1006:ILE:HG22	1:A:1007:ILE:N	2.08	0.67
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.25	0.67
1:A:219:PHE:O	1:A:222:LEU:N	2.27	0.67
2:B:705:MET:HB3	2:B:706:GLN:OE1	1.95	0.67
1:A:593:GLU:HA	1:A:593:GLU:OE1	1.93	0.67
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.29	0.66
12:L:58:LYS:O	12:L:59:ALA:O	2.13	0.66
2:B:90:ILE:HG22	2:B:90:ILE:O	1.95	0.66
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.24	0.66
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.66
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.25	0.66
2:B:991:GLY:O	2:B:992:ILE:HB	1.94	0.66
1:A:1002:GLY:H	1:A:1007:ILE:HG21	1.60	0.66
4:D:170:THR:CG2	4:D:172:LEU:HG	2.25	0.66
2:B:185:THR:O	2:B:188:ASP:HB2	1.95	0.66
4:D:159:THR:O	4:D:163:VAL:HG23	1.96	0.66
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.77	0.66
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.76	0.66
10:J:27:GLU:O	10:J:29:GLU:N	2.28	0.66
4:D:164:ILE:O	4:D:168:LYS:HG2	1.95	0.66
2:B:637:LEU:HD22	2:B:741:CYS:O	1.94	0.66
2:B:863:GLU:OE2	2:B:873:THR:HA	1.95	0.66
9:I:111:THR:CG2	9:I:112:SER:N	2.58	0.66
9:I:77:LYS:HG2	9:I:78:CYS:N	2.10	0.66
1:A:982:THR:HB	1:A:985:ASP:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:ASP:HB3	2:B:632:ARG:NE	2.11	0.66
5:E:56:LYS:HG3	5:E:84:ASP:HB2	1.78	0.66
12:L:55:ILE:O	12:L:56:LEU:HB2	1.95	0.66
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.44	0.66
2:B:175:ARG:HG3	2:B:175:ARG:HH11	1.60	0.66
5:E:85:GLU:C	5:E:87:SER:H	1.99	0.66
1:A:855:THR:HG21	1:A:857:ARG:NE	2.11	0.66
1:A:783:THR:HG21	1:A:796:SER:O	1.95	0.66
2:B:603:LEU:HB3	2:B:609:ILE:CG1	2.24	0.66
1:A:350:ARG:HD2	1:A:488:ASN:ND2	2.10	0.66
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.78	0.66
1:A:326:ARG:HD3	1:A:330:LYS:HZ2	1.61	0.66
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.26	0.66
8:H:100:THR:HG22	8:H:101:ALA:N	2.10	0.66
1:A:787:PHE:HE1	1:A:796:SER:HA	1.59	0.66
1:A:1048:ASN:O	1:A:1049:ILE:C	2.33	0.66
1:A:335:ARG:HH12	2:B:1206:GLU:CD	1.99	0.66
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.96	0.66
7:G:106:MET:CG	7:G:107:LYS:N	2.58	0.66
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.78	0.66
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.61	0.66
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.77	0.66
1:A:855:THR:HA	1:A:866:PHE:O	1.95	0.66
1:A:182:VAL:CG2	1:A:201:VAL:HG22	2.26	0.66
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	1.95	0.66
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.95	0.66
7:G:126:ASN:HD22	7:G:128:PRO:HD3	1.60	0.66
4:D:204:ASP:O	4:D:208:GLU:HB2	1.96	0.66
2:B:255:GLN:HB2	2:B:272:THR:HB	1.78	0.66
2:B:345:LYS:HG2	2:B:346:GLU:N	2.11	0.65
9:I:16:PRO:HB3	9:I:27:PHE:HE2	1.61	0.65
5:E:7:ARG:HG3	5:E:8:ASN:H	1.61	0.65
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.31	0.65
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.11	0.65
5:E:93:MET:O	5:E:97:VAL:HG23	1.96	0.65
2:B:273:LEU:O	2:B:276:ILE:HB	1.97	0.65
2:B:806:THR:CG2	2:B:808:ALA:H	2.03	0.65
2:B:951:GLN:HE21	12:L:57:LEU:HD13	1.61	0.65
2:B:576:ASP:HA	2:B:622:LYS:NZ	2.10	0.65
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.78	0.65
13:T:18:DC:OP1	13:T:18:DC:H3'	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:42:ARG:O	12:L:43:THR:HB	1.96	0.65
2:B:276:ILE:HD13	2:B:280:ILE:HD11	1.79	0.65
1:A:710:LEU:N	1:A:710:LEU:HD12	2.10	0.65
1:A:224:PHE:HD2	1:A:229:SER:O	1.80	0.65
1:A:787:PHE:CE1	1:A:796:SER:HA	2.31	0.65
2:B:848:ARG:HD2	10:J:8:PHE:O	1.96	0.65
2:B:897:GLY:O	2:B:898:LEU:HD23	1.96	0.65
1:A:809:THR:HG23	1:A:812:GLU:OE1	1.96	0.65
2:B:378:LEU:O	2:B:382:ILE:HG13	1.95	0.65
2:B:890:TYR:O	2:B:893:LEU:HB2	1.95	0.65
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.27	0.65
6:F:119:ARG:NH1	6:F:119:ARG:HG3	2.06	0.65
12:L:30:ILE:O	12:L:56:LEU:HA	1.96	0.65
7:G:138:THR:HG22	7:G:139:ILE:N	2.11	0.65
4:D:71:LYS:HG2	4:D:74:GLN:NE2	2.12	0.65
4:D:130:LEU:O	4:D:132:GLN:N	2.30	0.65
2:B:589:VAL:HG12	2:B:590:HIS:N	2.12	0.65
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.11	0.65
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.78	0.65
1:A:50:ILE:C	1:A:52:GLY:H	2.00	0.65
1:A:167:CYS:O	1:A:169:ASN:N	2.29	0.65
6:F:153:VAL:O	6:F:153:VAL:HG12	1.97	0.65
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.32	0.65
8:H:59:ILE:O	8:H:60:ALA:HB3	1.97	0.65
1:A:903:ASN:ND2	1:A:906:HIS:H	1.90	0.65
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.29	0.65
2:B:879:ARG:HD2	2:B:883:LEU:HD23	1.79	0.65
2:B:417:PHE:HE1	2:B:453:ILE:HD13	1.61	0.65
1:A:903:ASN:ND2	1:A:906:HIS:N	2.45	0.65
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.97	0.65
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.61	0.65
1:A:108:MET:SD	1:A:210:ILE:HD13	2.37	0.65
7:G:53:ASN:HD22	7:G:53:ASN:N	1.94	0.64
1:A:914:GLU:HB2	1:A:979:SER:O	1.97	0.64
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.79	0.64
1:A:332:LYS:H	1:A:337:ARG:HB3	1.60	0.64
2:B:39:ARG:NH1	2:B:665:GLU:HG2	2.12	0.64
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.96	0.64
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.62	0.64
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.12	0.64
2:B:44:VAL:HG21	2:B:199:MET:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:ASN:ND2	1:A:858:ASN:C	2.49	0.64
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.27	0.64
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.78	0.64
8:H:83:GLN:H	11:K:54:ARG:HD3	1.62	0.64
1:A:705:LYS:HD2	1:A:708:MET:CE	2.27	0.64
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.33	0.64
3:C:52:GLU:OE2	3:C:154:LYS:HD2	1.97	0.64
1:A:668:ASP:CB	1:A:741:ASN:HD21	2.07	0.64
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.79	0.64
4:D:190:GLU:O	4:D:194:LEU:HG	1.98	0.64
1:A:853:ASP:O	1:A:854:ASN:HB2	1.97	0.64
6:F:107:VAL:HG12	6:F:109:VAL:H	1.62	0.64
1:A:707:GLY:HA3	1:A:1281:ARG:HD3	1.79	0.64
9:I:110:PHE:HD2	9:I:110:PHE:H	1.44	0.64
2:B:313:MET:O	2:B:316:PRO:HD2	1.97	0.64
1:A:42:ASP:HB3	1:A:45:GLN:H	1.63	0.64
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.33	0.64
2:B:351:TYR:O	2:B:355:ILE:HG13	1.97	0.64
7:G:14:HIS:CD2	7:G:16:SER:H	2.16	0.64
2:B:882:THR:HG22	2:B:883:LEU:N	2.13	0.64
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.62	0.64
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.27	0.64
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.80	0.64
1:A:513:SER:OG	1:A:515:GLN:HB3	1.97	0.64
1:A:666:ILE:HD12	1:A:667:GLY:H	1.62	0.64
1:A:335:ARG:HH12	2:B:1202:LEU:HD22	1.63	0.64
2:B:865:LYS:NZ	2:B:869:SER:HA	2.12	0.64
8:H:47:PHE:HD2	8:H:95:TYR:HD1	1.43	0.64
3:C:179:GLU:HG2	3:C:180:TYR:N	2.13	0.64
1:A:69:THR:HG21	2:B:1174:LYS:NZ	2.12	0.64
1:A:709:THR:HB	1:A:712:GLU:HG3	1.78	0.64
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.27	0.64
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.79	0.64
1:A:830:LYS:CE	1:A:1081:LEU:HD12	2.28	0.64
2:B:882:THR:CG2	2:B:883:LEU:N	2.61	0.63
1:A:41:MET:O	1:A:50:ILE:HG13	1.98	0.63
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.38	0.63
4:D:220:LEU:CD1	4:D:221:TYR:H	2.11	0.63
1:A:866:PHE:C	1:A:867:ILE:HD12	2.18	0.63
2:B:20:ASP:O	2:B:22:SER:N	2.31	0.63
2:B:176:SER:O	2:B:182:SER:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H3	10:J:56:LEU:N	1.94	0.63
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.98	0.63
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.34	0.63
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.13	0.63
7:G:150:CYS:C	7:G:151:ILE:HG13	2.18	0.63
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.80	0.63
2:B:731:VAL:HG12	2:B:732:SER:N	2.11	0.63
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.81	0.63
7:G:74:TYR:HD2	7:G:74:TYR:H	1.46	0.63
7:G:79:PHE:HE2	7:G:106:MET:HE2	1.61	0.63
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.28	0.63
2:B:705:MET:H	2:B:710:LEU:HD12	1.62	0.63
1:A:1438:THR:HG22	6:F:92:ARG:HD2	1.80	0.63
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.28	0.63
5:E:22:MET:HE2	5:E:26:ARG:HE	1.61	0.63
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.81	0.63
1:A:1195:LEU:HD11	1:A:1267:MET:HE2	1.79	0.63
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.63	0.63
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.79	0.63
1:A:545:GLN:O	1:A:548:ASN:N	2.31	0.63
2:B:57:TYR:HD1	2:B:57:TYR:N	1.97	0.63
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.13	0.63
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.80	0.63
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.99	0.63
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.17	0.63
5:E:55:ARG:HA	5:E:58:MET:HG3	1.81	0.63
2:B:842:ASN:ND2	2:B:845:SER:H	1.95	0.63
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.28	0.63
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.13	0.63
1:A:68:GLN:O	1:A:68:GLN:OE1	2.15	0.63
3:C:3:GLU:HB3	11:K:104:ASN:HD21	1.63	0.63
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.32	0.63
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.13	0.63
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.13	0.63
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.79	0.63
1:A:728:LYS:O	1:A:732:LEU:HG	1.99	0.63
3:C:50:GLU:HB3	12:L:64:LEU:HD12	1.80	0.63
1:A:1161:THR:C	1:A:1163:ILE:H	2.00	0.63
2:B:347:LYS:HG3	2:B:348:ARG:H	1.64	0.63
2:B:711:GLU:H	2:B:712:PRO:HD2	1.64	0.63
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:O	1:A:460:VAL:HG23	1.99	0.63
1:A:447:GLN:NE2	13:T:20:BRU:H4'	2.13	0.63
2:B:1074:ASN:OD1	2:B:1076:HIS:HB2	1.99	0.63
5:E:140:LEU:HD12	5:E:140:LEU:N	2.14	0.62
3:C:213:PRO:O	3:C:214:ASN:HB2	1.99	0.62
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.34	0.62
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.04	0.62
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.14	0.62
1:A:399:HIS:O	1:A:400:PRO:C	2.36	0.62
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.79	0.62
9:I:70:ARG:HH11	9:I:84:VAL:HB	1.61	0.62
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.03	0.62
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.31	0.62
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.82	0.62
2:B:187:SER:O	2:B:191:LYS:HG3	1.99	0.62
6:F:89:GLU:HB3	6:F:134:ILE:HD13	1.79	0.62
1:A:1386:ARG:HB2	1:A:1403:GLU:CG	2.18	0.62
1:A:822:GLU:HA	2:B:513:GLN:HE22	1.64	0.62
2:B:881:ASN:HD22	2:B:933:SER:N	1.96	0.62
1:A:901:LEU:N	1:A:926:GLN:NE2	2.41	0.62
2:B:707:PRO:HG2	2:B:708:GLU:H	1.63	0.62
2:B:865:LYS:O	2:B:866:TYR:HD1	1.81	0.62
1:A:967:ALA:O	1:A:971:PHE:HD1	1.82	0.62
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.34	0.62
1:A:311:GLN:O	1:A:312:PRO:C	2.37	0.62
2:B:110:HIS:CB	12:L:54:ARG:HH22	2.12	0.62
1:A:61:ILE:O	1:A:62:ASP:CB	2.48	0.62
2:B:57:TYR:CD1	2:B:57:TYR:N	2.66	0.62
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.33	0.62
7:G:145:VAL:HG12	7:G:146:LYS:N	2.14	0.62
10:J:53:HIS:CD2	10:J:54:VAL:N	2.67	0.62
8:H:8:ASP:OD2	8:H:9:ILE:N	2.26	0.62
1:A:107:CYS:N	1:A:114:LEU:HD21	2.14	0.62
7:G:112:LYS:NZ	7:G:120:THR:HA	2.14	0.62
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.34	0.62
2:B:502:ILE:HD13	2:B:502:ILE:H	1.64	0.62
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.28	0.62
3:C:173:ALA:O	3:C:174:ALA:HB3	1.98	0.62
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.29	0.62
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.35	0.62
1:A:105:CYS:O	1:A:114:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.99	0.62
1:A:598:LEU:HD11	8:H:124:ARG:HB2	1.81	0.62
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.64	0.62
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.82	0.62
1:A:974:ASP:C	1:A:976:THR:H	2.02	0.62
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.18	0.62
2:B:770:GLN:HG2	2:B:983:ARG:O	1.99	0.62
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.30	0.62
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.82	0.62
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.64	0.62
9:I:104:LEU:HD23	9:I:104:LEU:N	2.13	0.62
1:A:913:LEU:HG	1:A:915:SER:H	1.63	0.62
10:J:23:ASN:C	10:J:25:LEU:N	2.51	0.62
4:D:39:ASN:HD22	4:D:43:GLU:HG3	1.65	0.62
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.15	0.61
3:C:242:GLN:OE1	3:C:245:VAL:HG21	2.00	0.61
2:B:560:GLU:O	2:B:561:TRP:CD1	2.52	0.61
6:F:132:LEU:O	6:F:148:VAL:HG23	2.00	0.61
8:H:36:CYS:HA	8:H:126:GLU:O	2.01	0.61
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.30	0.61
1:A:767:GLN:NE2	1:A:774:ARG:HD2	2.15	0.61
6:F:109:VAL:HG12	6:F:110:ASP:H	1.65	0.61
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.80	0.61
1:A:741:ASN:HD22	1:A:742:ASN:N	1.97	0.61
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.15	0.61
6:F:109:VAL:HG12	6:F:110:ASP:N	2.16	0.61
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.65	0.61
6:F:111:LEU:O	6:F:113:GLY:N	2.33	0.61
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.65	0.61
9:I:80:SER:OG	9:I:105:SER:HB2	2.00	0.61
1:A:326:ARG:HH11	1:A:330:LYS:NZ	1.98	0.61
1:A:1079:MET:HG2	1:A:1359:ASP:OD1	2.00	0.61
8:H:33:GLN:HG2	8:H:129:TYR:HE2	1.65	0.61
3:C:166:GLU:CG	11:K:10:PHE:HZ	2.07	0.61
2:B:642:ASP:O	2:B:644:GLU:N	2.29	0.61
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.00	0.61
2:B:839:MET:HE2	2:B:980:PHE:HB2	1.81	0.61
1:A:298:PHE:O	1:A:302:THR:HB	2.00	0.61
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.81	0.61
5:E:98:ILE:HA	5:E:101:GLN:HB2	1.83	0.61
2:B:780:VAL:HG21	10:J:56:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:936:ASP:OD1	2:B:937:ALA:N	2.34	0.61
1:A:709:THR:HG23	9:I:94:ASP:HA	1.82	0.61
8:H:89:LEU:C	8:H:91:ASP:H	2.04	0.61
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.35	0.61
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.00	0.61
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.33	0.61
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.36	0.61
2:B:296:GLU:C	2:B:299:GLU:HB2	2.20	0.61
1:A:709:THR:HG22	1:A:711:ARG:H	1.66	0.61
3:C:58:LEU:HD11	10:J:2:ILE:HG13	1.82	0.61
1:A:1436:ILE:O	1:A:1437:GLY:C	2.39	0.61
2:B:579:ARG:NH1	2:B:579:ARG:HG2	2.16	0.61
2:B:464:GLY:HA2	2:B:479:VAL:O	2.01	0.61
9:I:55:THR:O	9:I:55:THR:HG22	1.99	0.61
10:J:27:GLU:C	10:J:29:GLU:H	2.04	0.61
4:D:208:GLU:O	4:D:212:LYS:HG3	2.00	0.61
1:A:567:LYS:CD	8:H:95:TYR:HA	2.31	0.61
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.00	0.61
4:D:217:LEU:O	4:D:219:THR:N	2.34	0.61
1:A:1000:LEU:N	1:A:1000:LEU:HD12	2.16	0.61
7:G:51:TYR:HD2	7:G:51:TYR:C	2.04	0.61
2:B:583:ASN:HD21	2:B:628:THR:HG23	1.64	0.61
5:E:7:ARG:HG3	5:E:8:ASN:N	2.16	0.61
1:A:385:ILE:HG22	1:A:386:ASP:N	2.16	0.61
1:A:773:LYS:H	1:A:773:LYS:HD2	1.66	0.61
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.83	0.60
2:B:839:MET:CE	2:B:980:PHE:HB2	2.31	0.60
13:T:19:DC:H2"	13:T:20:BRU:H6	1.82	0.60
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.83	0.60
3:C:208:GLU:O	3:C:210:GLU:N	2.34	0.60
1:A:208:LEU:HD23	1:A:208:LEU:O	2.02	0.60
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.47	0.60
2:B:506:GLY:HA2	2:B:508:LEU:HG	1.84	0.60
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.28	0.60
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.36	0.60
1:A:628:GLY:O	1:A:632:VAL:HG23	2.00	0.60
2:B:755:ILE:HG22	2:B:755:ILE:O	2.00	0.60
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.36	0.60
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.64	0.60
2:B:235:SER:O	2:B:236:HIS:HD2	1.84	0.60
13:T:16:DC:H2"	13:T:17:DG:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:HE2	5:E:26:ARG:NE	2.16	0.60
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.67	0.60
2:B:502:ILE:N	2:B:502:ILE:HD13	2.15	0.60
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.83	0.60
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.01	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.83	0.60
10:J:1:MET:N	10:J:56:LEU:N	2.49	0.60
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.31	0.60
1:A:903:ASN:ND2	1:A:905:ASP:N	2.48	0.60
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.83	0.60
1:A:803:SER:H	1:A:806:ARG:HG3	1.66	0.60
1:A:1080:THR:O	1:A:1080:THR:HG22	2.02	0.60
2:B:96:TYR:N	2:B:129:PHE:O	2.29	0.60
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.63	0.60
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.82	0.60
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.84	0.60
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.83	0.60
5:E:114:ASN:O	5:E:115:ASN:HB3	2.01	0.60
11:K:82:ASP:OD1	11:K:84:LYS:N	2.33	0.60
1:A:393:ARG:NH1	1:A:393:ARG:HG3	2.17	0.60
1:A:1092:LYS:O	1:A:1094:VAL:HG23	2.02	0.60
5:E:136:ASN:OD1	5:E:138:ALA:N	2.35	0.60
1:A:304:MET:O	1:A:324:SER:HB2	2.02	0.60
2:B:882:THR:CG2	2:B:934:LYS:O	2.47	0.60
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.67	0.60
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.32	0.60
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.37	0.60
2:B:705:MET:N	2:B:710:LEU:HD12	2.17	0.60
1:A:393:ARG:HG3	1:A:393:ARG:HH11	1.67	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HE3	1.84	0.60
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.67	0.60
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.65	0.60
1:A:821:ARG:O	1:A:825:ILE:HG13	2.02	0.59
1:A:899:VAL:O	1:A:929:LEU:HD12	2.02	0.59
1:A:225:ASN:HD22	1:A:228:PHE:H	1.49	0.59
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.16	0.59
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.02	0.59
2:B:244:LEU:HG	2:B:250:PHE:H	1.67	0.59
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.83	0.59
2:B:287:ARG:HG3	2:B:292:ILE:HG12	1.83	0.59
7:G:51:TYR:C	7:G:51:TYR:CD2	2.74	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:ARG:HH11	13:T:16:DC:H5"	1.66	0.59
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.36	0.59
3:C:22:LEU:HD13	3:C:230:MET:CE	2.32	0.59
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.82	0.59
1:A:774:ARG:HE	1:A:797:LYS:CB	2.15	0.59
3:C:186:LEU:HD12	3:C:186:LEU:N	2.17	0.59
1:A:962:ARG:HA	1:A:965:GLN:HG3	1.82	0.59
12:L:55:ILE:O	12:L:56:LEU:CB	2.50	0.59
2:B:98:THR:O	2:B:126:SER:HB2	2.02	0.59
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.17	0.59
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.03	0.59
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.15	0.59
3:C:89:GLU:O	3:C:90:ASP:HB3	2.02	0.59
2:B:956:THR:HA	2:B:961:LEU:O	2.02	0.59
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.32	0.59
2:B:218:SER:HB2	2:B:241:ARG:HH11	1.61	0.59
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.84	0.59
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.32	0.59
4:D:71:LYS:HG2	4:D:74:GLN:HE21	1.68	0.59
1:A:260:ASP:OD1	1:A:261:ASP:N	2.36	0.59
2:B:454:THR:HG22	2:B:455:SER:N	2.18	0.59
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.66	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.83	0.59
2:B:424:LEU:O	2:B:428:ILE:HG13	2.03	0.59
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.17	0.59
1:A:133:LYS:O	1:A:136:ALA:HB3	2.02	0.59
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.85	0.59
8:H:18:GLY:O	8:H:19:ARG:HB2	2.01	0.59
1:A:287:HIS:HA	1:A:290:GLU:CD	2.23	0.59
5:E:176:PRO:O	5:E:212:ARG:HA	2.02	0.59
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.85	0.59
9:I:78:CYS:SG	9:I:103:CYS:SG	3.00	0.59
4:D:121:LYS:O	4:D:124:GLU:HB3	2.01	0.59
1:A:1025:ARG:HA	1:A:1030:ARG:NH1	2.17	0.59
1:A:1205:LYS:O	1:A:1207:LEU:HG	2.03	0.59
1:A:322:VAL:O	1:A:322:VAL:HG12	2.01	0.59
2:B:847:ASP:O	3:C:65:HIS:HE1	1.86	0.59
2:B:604:ARG:C	2:B:606:LYS:H	2.06	0.59
2:B:1099:VAL:C	2:B:1101:ASP:H	2.05	0.59
5:E:5:ASN:O	5:E:9:ILE:HG13	2.03	0.59
13:T:25:DA:H2"	13:T:26:DT:OP2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:LEU:HD11	4:D:150:ASN:HD21	1.68	0.59
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.84	0.59
2:B:882:THR:CG2	2:B:884:ARG:H	2.04	0.59
2:B:215:GLN:HE21	2:B:215:GLN:HA	1.68	0.59
2:B:1181:GLU:HG2	2:B:1188:LYS:CG	2.33	0.59
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.83	0.59
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.37	0.59
1:A:284:ALA:O	1:A:286:HIS:N	2.31	0.59
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.85	0.59
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.01	0.59
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.33	0.59
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.65	0.59
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.33	0.59
1:A:144:THR:O	1:A:146:MET:HG3	2.03	0.59
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.85	0.59
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.83	0.59
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.03	0.59
2:B:507:LYS:HA	2:B:512:ARG:NH2	2.17	0.58
2:B:944:THR:HG21	2:B:1122:ARG:HH21	1.64	0.58
5:E:119:SER:O	5:E:123:LEU:HD21	2.03	0.58
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.83	0.58
7:G:106:MET:CG	7:G:107:LYS:H	2.16	0.58
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.38	0.58
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.67	0.58
11:K:111:LEU:HD23	11:K:111:LEU:N	2.18	0.58
2:B:880:THR:HB	2:B:934:LYS:HD2	1.85	0.58
1:A:62:ASP:O	1:A:63:ARG:C	2.42	0.58
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.03	0.58
9:I:62:ILE:HG12	9:I:62:ILE:O	2.03	0.58
1:A:337:ARG:HD3	2:B:1132:GLU:CD	2.23	0.58
4:D:69:ALA:HB2	4:D:72:ARG:NH1	2.17	0.58
2:B:557:PHE:CD2	2:B:557:PHE:C	2.76	0.58
1:A:933:TYR:O	1:A:937:VAL:HG23	2.03	0.58
1:A:297:GLN:O	1:A:297:GLN:HG3	2.00	0.58
11:K:60:ALA:O	11:K:73:LEU:HD12	2.03	0.58
2:B:486:TYR:CE1	2:B:1096:ARG:NH2	2.71	0.58
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.16	0.58
10:J:30:LEU:HD21	10:J:38:ARG:NH1	2.18	0.58
2:B:345:LYS:O	2:B:347:LYS:N	2.30	0.58
13:T:14:DT:H2"	13:T:15:DA:C2	2.38	0.58
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.85	0.58
2:B:101:MET:CG	2:B:111:ALA:HA	2.33	0.58
2:B:959:ASP:HB2	2:B:961:LEU:HG	1.86	0.58
2:B:215:GLN:NE2	2:B:499:ASN:HB3	2.18	0.58
5:E:85:GLU:O	5:E:87:SER:N	2.34	0.58
8:H:130:ARG:N	8:H:130:ARG:HD2	2.17	0.58
2:B:110:HIS:HB2	12:L:54:ARG:HH22	1.68	0.58
7:G:1:MET:HE3	7:G:79:PHE:HA	1.86	0.58
13:T:19:DC:H2'	13:T:20:BRU:BR	2.58	0.58
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.39	0.58
3:C:138:GLU:OE1	3:C:138:GLU:N	2.36	0.58
8:H:32:THR:HG22	8:H:33:GLN:N	2.17	0.58
8:H:59:ILE:CG2	8:H:60:ALA:N	2.58	0.58
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.38	0.58
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.03	0.58
1:A:567:LYS:CB	1:A:568:PRO:CD	2.82	0.58
12:L:52:GLY:O	12:L:53:HIS:C	2.42	0.58
9:I:50:THR:CG2	9:I:51:ASN:N	2.66	0.58
4:D:155:ARG:O	4:D:155:ARG:HG2	2.02	0.58
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.68	0.58
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.39	0.58
2:B:610:ASN:OD1	2:B:611:PRO:HD2	2.04	0.58
2:B:737:THR:HG21	9:I:66:PRO:HA	1.84	0.58
10:J:52:THR:O	10:J:52:THR:HG22	2.03	0.58
1:A:768:GLN:CG	1:A:816:HIS:HA	2.27	0.58
3:C:244:VAL:HG12	3:C:248:ILE:HD11	1.86	0.58
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.85	0.58
10:J:14:VAL:HG12	10:J:14:VAL:O	2.04	0.58
2:B:292:ILE:CD1	2:B:327:ARG:H	2.17	0.58
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.85	0.58
5:E:67:GLU:O	5:E:70:SER:N	2.29	0.58
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.33	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.37	0.58
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.02	0.58
12:L:27:LEU:HB3	12:L:37:LYS:HD3	1.84	0.58
1:A:1285:MET:HE3	1:A:1286:LYS:H	1.68	0.58
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.39	0.58
1:A:351:THR:HG22	1:A:468:PHE:CE1	2.38	0.58
1:A:984:LYS:HB3	1:A:988:LEU:HD12	1.86	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.03	0.58
1:A:830:LYS:HE2	1:A:1081:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:40:SER:OG	9:I:41:PRO:HD2	2.04	0.58
3:C:226:ASP:O	3:C:227:THR:HB	2.03	0.58
1:A:825:ILE:O	1:A:829:VAL:HG23	2.03	0.58
8:H:5:LEU:HD22	8:H:133:ASN:O	2.04	0.58
2:B:294:ASP:C	2:B:296:GLU:H	2.06	0.58
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.02	0.58
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.27	0.57
1:A:168:GLY:O	1:A:169:ASN:C	2.41	0.57
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.69	0.57
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.38	0.57
6:F:118:LEU:O	6:F:122:MET:HG3	2.04	0.57
14:N:6:DT:H2"	14:N:7:DA:N7	2.19	0.57
1:A:1115:SER:OG	1:A:1116:LEU:N	2.37	0.57
1:A:853:ASP:C	1:A:853:ASP:OD1	2.42	0.57
1:A:1171:GLN:HG3	1:A:1172:LEU:H	1.68	0.57
1:A:1215:ARG:HA	1:A:1218:GLN:CG	2.34	0.57
8:H:61:SER:O	8:H:62:SER:HB2	2.04	0.57
1:A:998:LEU:N	1:A:998:LEU:HD12	2.19	0.57
2:B:29:ASP:OD1	2:B:658:ILE:HG21	2.04	0.57
1:A:50:ILE:HG22	1:A:52:GLY:H	1.70	0.57
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.25	0.57
2:B:209:GLU:OE2	2:B:483:LEU:HD23	2.04	0.57
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.85	0.57
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.39	0.57
1:A:666:ILE:N	1:A:666:ILE:HD12	2.20	0.57
4:D:51:ASN:O	4:D:52:LEU:O	2.21	0.57
2:B:303:TYR:HD2	2:B:303:TYR:N	2.01	0.57
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.04	0.57
2:B:970:THR:HG22	2:B:971:THR:N	2.19	0.57
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.86	0.57
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.86	0.57
1:A:866:PHE:O	1:A:867:ILE:HD12	2.05	0.57
8:H:82:PRO:HB2	11:K:54:ARG:NH1	2.19	0.57
2:B:710:LEU:HD22	2:B:733:HIS:HB3	1.87	0.57
1:A:714:PHE:O	1:A:718:VAL:HG23	2.05	0.57
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.40	0.57
5:E:98:ILE:HA	5:E:101:GLN:HE21	1.70	0.57
2:B:912:ILE:O	2:B:938:SER:HB3	2.04	0.57
1:A:1332:PHE:HE1	1:A:1381:LEU:HD13	1.69	0.57
1:A:475:THR:HG22	1:A:476:SER:N	2.19	0.57
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:LEU:CD2	8:H:137:GLN:HE21	2.17	0.57
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.34	0.57
3:C:244:VAL:O	3:C:248:ILE:HG13	2.03	0.57
1:A:1095:THR:HG23	1:A:1112:LYS:HD2	1.86	0.57
5:E:90:VAL:HG22	5:E:90:VAL:O	2.04	0.57
8:H:61:SER:CB	8:H:139:ASN:HB3	2.35	0.57
2:B:525:ALA:O	2:B:768:THR:HG23	2.05	0.57
1:A:1035:TYR:O	1:A:1037:LEU:N	2.37	0.57
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.33	0.57
2:B:303:TYR:N	2:B:303:TYR:CD2	2.73	0.57
1:A:535:THR:HG21	1:A:617:VAL:H	1.68	0.57
2:B:1096:ARG:HB3	2:B:1096:ARG:HH11	1.70	0.57
5:E:84:ASP:O	5:E:86:PRO:HD3	2.05	0.57
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.87	0.57
3:C:184:ASN:HD21	3:C:189:THR:HB	1.69	0.57
2:B:604:ARG:O	2:B:606:LYS:N	2.37	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.39	0.57
1:A:1277:GLU:C	1:A:1279:ILE:H	2.08	0.57
1:A:84:ILE:HG23	1:A:84:ILE:O	2.04	0.57
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.87	0.57
2:B:776:GLN:O	2:B:1095:LEU:HA	2.05	0.57
2:B:433:GLN:O	2:B:434:ARG:HG3	2.05	0.57
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.87	0.57
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.04	0.57
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.85	0.57
1:A:1161:THR:C	1:A:1163:ILE:N	2.56	0.57
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.87	0.57
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.87	0.57
1:A:567:LYS:HZ2	8:H:47:PHE:HB3	1.70	0.57
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.85	0.57
12:L:38:LEU:O	12:L:39:SER:CB	2.53	0.57
8:H:82:PRO:O	8:H:84:ALA:N	2.32	0.57
1:A:650:GLN:O	1:A:654:ASN:HB2	2.05	0.57
2:B:446:LEU:HG	2:B:448:ILE:HG13	1.87	0.57
2:B:728:ARG:O	2:B:729:ILE:HG13	2.05	0.57
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.57
2:B:167:ILE:N	2:B:167:ILE:HD12	2.20	0.56
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.34	0.56
10:J:8:PHE:N	10:J:49:MET:HE3	2.20	0.56
12:L:27:LEU:HD23	12:L:27:LEU:N	2.20	0.56
7:G:9:LEU:HG	7:G:10:ASN:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:TYR:CD1	9:I:15:TYR:N	2.72	0.56
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.05	0.56
2:B:903:VAL:O	2:B:949:VAL:HG23	2.05	0.56
1:A:567:LYS:NZ	8:H:47:PHE:HB3	2.20	0.56
1:A:66:LYS:O	1:A:67:CYS:CB	2.52	0.56
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.62	0.56
1:A:903:ASN:ND2	1:A:905:ASP:H	2.04	0.56
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.49	0.56
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.20	0.56
1:A:863:VAL:C	1:A:864:ILE:HD12	2.25	0.56
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.34	0.56
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.35	0.56
2:B:638:PHE:HA	2:B:690:VAL:HG23	1.86	0.56
2:B:871:THR:CG2	2:B:872:GLU:N	2.67	0.56
1:A:60:SER:OG	1:A:61:ILE:N	2.38	0.56
3:C:39:ALA:HA	3:C:164:ALA:CB	2.34	0.56
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.85	0.56
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.40	0.56
2:B:582:VAL:O	2:B:582:VAL:HG12	2.05	0.56
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.40	0.56
1:A:326:ARG:HH11	1:A:330:LYS:HE3	1.70	0.56
3:C:203:GLN:CG	3:C:207:CYS:SG	2.93	0.56
1:A:286:HIS:O	1:A:288:ALA:N	2.36	0.56
1:A:1256:GLU:HA	1:A:1259:MET:HB2	1.86	0.56
1:A:713:SER:O	1:A:717:ASN:ND2	2.38	0.56
1:A:844:ALA:O	1:A:845:LEU:HD23	2.05	0.56
2:B:871:THR:CG2	2:B:872:GLU:H	2.17	0.56
1:A:40:THR:HG23	1:A:41:MET:N	2.21	0.56
2:B:185:THR:N	2:B:188:ASP:HB2	2.20	0.56
12:L:29:TYR:O	12:L:30:ILE:HG13	2.05	0.56
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.35	0.56
8:H:111:LEU:HA	8:H:127:GLY:O	2.05	0.56
2:B:53:GLN:NE2	2:B:57:TYR:HB2	2.21	0.56
1:A:310:GLY:O	1:A:312:PRO:HD2	2.06	0.56
1:A:96:ILE:HG21	1:A:176:LYS:HE3	1.86	0.56
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.41	0.56
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.15	0.56
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.87	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.87	0.56
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.71	0.56
4:D:52:LEU:O	4:D:54:GLU:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:O	1:A:546:VAL:C	2.44	0.56
6:F:147:SER:OG	6:F:150:GLU:HG3	2.05	0.56
1:A:326:ARG:HH11	1:A:330:LYS:CE	2.18	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.87	0.56
4:D:198:LEU:O	4:D:200:ASN:N	2.39	0.56
1:A:337:ARG:HD3	2:B:1132:GLU:OE2	2.05	0.56
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.36	0.56
1:A:591:PHE:HD2	1:A:595:THR:HB	1.71	0.56
1:A:774:ARG:NH2	1:A:797:LYS:HG3	2.21	0.56
2:B:434:ARG:O	2:B:436:VAL:HG23	2.06	0.56
5:E:48:ASP:CG	5:E:49:SER:H	2.09	0.56
3:C:186:LEU:CD1	3:C:186:LEU:N	2.69	0.56
8:H:100:THR:CG2	8:H:101:ALA:N	2.68	0.56
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.40	0.56
3:C:43:THR:HG22	3:C:44:LEU:N	2.19	0.56
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.06	0.56
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.36	0.56
10:J:8:PHE:H	10:J:49:MET:HE3	1.71	0.56
5:E:124:VAL:C	5:E:126:SER:H	2.10	0.56
1:A:801:GLU:OE1	2:B:729:ILE:HG21	2.06	0.56
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.06	0.56
2:B:1072:MET:CE	2:B:1087:PHE:HD1	2.17	0.56
1:A:786:HIS:CD2	1:A:786:HIS:N	2.74	0.56
3:C:184:ASN:ND2	3:C:189:THR:HB	2.21	0.56
7:G:14:HIS:CD2	7:G:16:SER:CB	2.85	0.56
2:B:589:VAL:HG12	2:B:590:HIS:H	1.71	0.56
2:B:679:TYR:CE1	2:B:683:SER:HB3	2.41	0.56
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.36	0.56
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.88	0.56
4:D:219:THR:HG22	4:D:220:LEU:O	2.06	0.56
1:A:1224:LEU:HD11	1:A:1240:CYS:CB	2.34	0.56
2:B:226:PHE:HA	2:B:395:GLN:CG	2.36	0.56
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.41	0.56
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.88	0.56
4:D:123:LEU:HD11	4:D:150:ASN:ND2	2.21	0.56
2:B:737:THR:HB	9:I:66:PRO:CB	2.36	0.56
4:D:220:LEU:CG	4:D:221:TYR:H	2.19	0.55
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.40	0.55
2:B:405:ARG:O	2:B:406:LEU:HD23	2.06	0.55
2:B:522:VAL:HG12	2:B:523:CYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:LEU:O	1:A:927:VAL:HG23	2.06	0.55
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.40	0.55
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.37	0.55
1:A:71:GLN:CG	1:A:72:GLU:N	2.58	0.55
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.70	0.55
1:A:732:LEU:O	1:A:735:VAL:HG23	2.06	0.55
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.55
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.88	0.55
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.89	0.55
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.88	0.55
6:F:82:THR:HG22	6:F:84:TYR:H	1.70	0.55
8:H:4:THR:CG2	8:H:5:LEU:N	2.69	0.55
1:A:567:LYS:HE3	8:H:46:LEU:CB	2.36	0.55
2:B:128:LEU:N	2:B:128:LEU:HD12	2.22	0.55
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.89	0.55
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.87	0.55
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.53	0.55
2:B:508:LEU:O	2:B:509:ALA:HB3	2.06	0.55
13:T:15:DA:H2"	13:T:16:DC:H5'	1.88	0.55
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.37	0.55
2:B:181:LEU:HD22	2:B:189:LEU:HD22	1.88	0.55
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.87	0.55
2:B:390:LEU:HD13	2:B:392:ARG:HH21	1.70	0.55
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.07	0.55
5:E:19:VAL:HG22	5:E:140:LEU:HD23	1.87	0.55
8:H:89:LEU:O	8:H:91:ASP:N	2.40	0.55
1:A:79:GLY:N	2:B:1205:GLN:HE22	2.05	0.55
1:A:864:ILE:CD1	1:A:864:ILE:N	2.70	0.55
1:A:699:ALA:O	1:A:700:ASN:HB3	2.07	0.55
1:A:470:LEU:C	1:A:470:LEU:HD12	2.27	0.55
13:T:15:DA:H2"	13:T:16:DC:OP2	2.06	0.55
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.32	0.55
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.06	0.55
1:A:55:ASP:C	1:A:57:ARG:H	2.10	0.55
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.89	0.55
3:C:229:TYR:CD1	3:C:229:TYR:N	2.73	0.55
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.39	0.55
4:D:130:LEU:C	4:D:132:GLN:H	2.10	0.55
1:A:622:VAL:HG22	1:A:622:VAL:O	2.06	0.55
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.38	0.55
8:H:63:LEU:C	8:H:90:ALA:HB3	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.06	0.55
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.88	0.55
3:C:223:ALA:O	3:C:224:GLN:HG2	2.07	0.55
1:A:538:ASP:O	1:A:540:PHE:HD1	1.90	0.55
3:C:183:TRP:O	3:C:185:LYS:N	2.40	0.55
2:B:276:ILE:HD13	2:B:280:ILE:CD1	2.36	0.55
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.06	0.55
1:A:913:LEU:HD12	1:A:914:GLU:N	2.19	0.55
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.88	0.55
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.35	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.55
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.88	0.55
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.88	0.55
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.42	0.55
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.70	0.55
2:B:128:LEU:HD11	2:B:170:LEU:N	2.22	0.55
2:B:59:LEU:CD1	2:B:417:PHE:CE2	2.90	0.55
5:E:165:LEU:CD2	5:E:175:LEU:HD11	2.33	0.55
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.72	0.55
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.40	0.55
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.06	0.55
1:A:879:GLU:O	1:A:955:PRO:HA	2.06	0.55
1:A:567:LYS:CG	1:A:568:PRO:CD	2.75	0.55
2:B:710:LEU:HA	2:B:733:HIS:CG	2.42	0.55
3:C:254:LYS:HB3	11:K:42:LEU:HD12	1.89	0.55
3:C:121:VAL:HG12	3:C:121:VAL:O	2.07	0.55
1:A:60:SER:C	1:A:61:ILE:HG13	2.28	0.55
4:D:40:HIS:CA	7:G:73:LYS:NZ	2.67	0.55
1:A:399:HIS:CB	1:A:400:PRO:CD	2.85	0.55
1:A:1030:ARG:HA	1:A:1034:GLU:HG3	1.88	0.55
1:A:740:LEU:HD12	1:A:740:LEU:C	2.27	0.55
1:A:417:TYR:O	1:A:418:SER:C	2.45	0.55
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.37	0.54
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.88	0.54
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.42	0.54
7:G:126:ASN:ND2	7:G:128:PRO:HD3	2.22	0.54
2:B:966:VAL:HG12	2:B:967:ARG:N	2.21	0.54
1:A:1207:LEU:HD13	1:A:1273:LEU:HD23	1.89	0.54
1:A:738:LYS:H	1:A:738:LYS:HD2	1.72	0.54
1:A:814:PHE:CD2	1:A:814:PHE:O	2.60	0.54
3:C:187:LYS:HG3	3:C:219:PHE:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:MET:O	6:F:104:ASN:HB2	2.08	0.54
2:B:287:ARG:HD2	2:B:324:ILE:HG22	1.90	0.54
5:E:17:ARG:HG3	5:E:18:THR:N	2.21	0.54
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.43	0.54
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.38	0.54
1:A:1356:ILE:HG21	1:A:1363:VAL:CG2	2.37	0.54
7:G:9:LEU:HG	7:G:10:ASN:H	1.72	0.54
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.34	0.54
2:B:273:LEU:HD22	2:B:360:PHE:HD1	1.73	0.54
5:E:212:ARG:NH1	5:E:212:ARG:HG3	2.18	0.54
1:A:668:ASP:HB3	1:A:741:ASN:ND2	2.11	0.54
3:C:66:ARG:NH2	10:J:3:VAL:O	2.41	0.54
1:A:92:HIS:O	1:A:94:GLY:N	2.40	0.54
1:A:1205:LYS:C	1:A:1274:ARG:HH12	2.10	0.54
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.89	0.54
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.89	0.54
1:A:202:LEU:HD23	1:A:202:LEU:N	2.23	0.54
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.22	0.54
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.75	0.54
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.89	0.54
1:A:56:PRO:O	1:A:57:ARG:HD2	2.08	0.54
2:B:274:PRO:HG2	2:B:359:GLU:CB	2.37	0.54
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.22	0.54
2:B:497:ARG:NH2	2:B:775:LYS:HZ2	2.05	0.54
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.89	0.54
3:C:99:LEU:CD2	3:C:99:LEU:N	2.65	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.54	0.54
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.66	0.54
5:E:13:TRP:O	5:E:16:PHE:HB3	2.07	0.54
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.42	0.54
2:B:408:LEU:N	2:B:408:LEU:HD12	2.23	0.54
1:A:946:VAL:HG12	1:A:947:PHE:N	2.21	0.54
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.37	0.54
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.88	0.54
10:J:52:THR:CG2	10:J:52:THR:O	2.56	0.54
2:B:128:LEU:HD13	2:B:168:GLY:O	2.07	0.54
1:A:1215:ARG:HB2	1:A:1215:ARG:HH11	1.71	0.54
1:A:130:ASP:O	1:A:131:SER:C	2.46	0.54
1:A:1438:THR:CG2	6:F:92:ARG:HB2	2.37	0.54
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.48	0.54
2:B:260:GLY:O	2:B:267:ARG:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.89	0.54
1:A:855:THR:CG2	1:A:857:ARG:HE	2.18	0.54
4:D:66:ARG:HG3	7:G:51:TYR:CD1	2.43	0.54
2:B:917:PRO:O	2:B:918:ILE:HG13	2.08	0.54
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.37	0.54
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.72	0.54
2:B:235:SER:OG	2:B:236:HIS:CD2	2.61	0.54
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.07	0.54
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.08	0.54
2:B:878:GLN:O	2:B:879:ARG:C	2.46	0.54
8:H:44:VAL:O	8:H:44:VAL:HG12	2.08	0.54
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.71	0.54
9:I:50:THR:HG22	9:I:52:ILE:H	1.73	0.54
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.90	0.54
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.88	0.54
2:B:1182:CYS:O	2:B:1183:LYS:C	2.47	0.54
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.90	0.54
1:A:1164:PRO:HA	1:A:1167:GLU:HG2	1.90	0.54
2:B:258:LEU:O	2:B:258:LEU:HG	2.07	0.54
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.90	0.54
2:B:383:ASN:O	2:B:387:LEU:HD13	2.08	0.54
3:C:148:ARG:CZ	3:C:149:LYS:HE3	2.38	0.54
12:L:31:CYS:SG	12:L:34:CYS:SG	3.05	0.54
1:A:767:GLN:CD	1:A:774:ARG:HD2	2.29	0.54
1:A:738:LYS:C	1:A:740:LEU:H	2.11	0.54
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.07	0.54
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.70	0.54
1:A:33:ALA:HB1	1:A:56:PRO:HB2	1.90	0.54
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.54
1:A:1036:ARG:NH1	1:A:1036:ARG:HG2	2.17	0.54
1:A:731:ARG:O	1:A:735:VAL:HG22	2.08	0.54
12:L:60:ARG:HG2	12:L:61:THR:N	2.21	0.54
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.38	0.54
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.72	0.54
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.72	0.54
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.43	0.53
2:B:417:PHE:CE1	2:B:453:ILE:HD13	2.43	0.53
2:B:245:GLU:C	2:B:246:LYS:HG3	2.28	0.53
1:A:549:MET:SD	1:A:577:ILE:CD1	2.97	0.53
1:A:763:ALA:O	1:A:803:SER:HB3	2.08	0.53
1:A:321:PRO:O	1:A:322:VAL:HB	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:TYR:HD1	2:B:259:TYR:H	1.55	0.53
8:H:11:GLN:HA	8:H:53:ASP:O	2.08	0.53
2:B:345:LYS:HA	2:B:348:ARG:NE	2.21	0.53
2:B:95:ILE:HG13	2:B:129:PHE:O	2.08	0.53
3:C:39:ALA:O	3:C:164:ALA:HB3	2.09	0.53
2:B:390:LEU:HD13	2:B:392:ARG:NH2	2.23	0.53
3:C:22:LEU:HD21	3:C:25:VAL:CG1	2.35	0.53
3:C:115:SER:HB2	3:C:142:VAL:HB	1.89	0.53
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.91	0.53
1:A:1454:MET:O	1:A:1454:MET:HG3	2.07	0.53
1:A:512:VAL:HA	1:A:519:PRO:HA	1.90	0.53
6:F:133:VAL:HG13	6:F:146:TRP:O	2.08	0.53
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.09	0.53
2:B:638:PHE:HB2	2:B:741:CYS:O	2.09	0.53
1:A:12:ARG:HD2	2:B:1218:THR:CG2	2.38	0.53
1:A:590:ARG:NH1	1:A:590:ARG:HG3	2.21	0.53
5:E:28:TYR:C	5:E:65:THR:HG22	2.28	0.53
11:K:54:ARG:O	11:K:54:ARG:HG2	2.07	0.53
8:H:15:VAL:HA	8:H:26:ILE:HG13	1.89	0.53
3:C:6:PRO:O	3:C:7:GLN:HG3	2.08	0.53
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.71	0.53
8:H:127:GLY:O	8:H:128:ASN:CB	2.55	0.53
1:A:1208:THR:O	1:A:1211:GLN:HB2	2.09	0.53
1:A:786:HIS:O	1:A:787:PHE:HD2	1.92	0.53
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.08	0.53
2:B:247:GLY:C	2:B:249:ARG:H	2.10	0.53
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.43	0.53
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.90	0.53
2:B:185:THR:H	2:B:188:ASP:CB	2.21	0.53
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.09	0.53
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.44	0.53
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.90	0.53
9:I:59:VAL:O	9:I:61:ASP:N	2.41	0.53
2:B:744:HIS:CD2	2:B:746:SER:OG	2.58	0.53
2:B:707:PRO:HG2	2:B:708:GLU:N	2.24	0.53
3:C:31:ASN:O	3:C:34:ARG:HB3	2.08	0.53
2:B:63:ILE:HG22	2:B:64:CYS:SG	2.48	0.53
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.74	0.53
2:B:781:PHE:O	2:B:782:LEU:HG	2.08	0.53
5:E:99:HIS:C	5:E:99:HIS:HD1	2.12	0.53
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.35	0.53
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.90	0.53
2:B:906:SER:O	2:B:907:GLY:O	2.27	0.53
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.91	0.53
1:A:963:ILE:HG22	1:A:1045:VAL:HG13	1.91	0.53
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.08	0.53
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.90	0.53
2:B:295:GLY:O	2:B:299:GLU:HG2	2.09	0.53
2:B:653:VAL:HA	2:B:689:LEU:HD22	1.91	0.53
4:D:156:ASP:HB2	4:D:159:THR:HG1	1.74	0.53
2:B:486:TYR:N	2:B:486:TYR:CD2	2.75	0.53
1:A:528:LEU:O	1:A:531:ILE:HG22	2.09	0.53
2:B:792:MET:HE2	13:T:24:DC:OP1	2.09	0.53
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.24	0.53
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.39	0.53
2:B:487:THR:CG2	2:B:488:TYR:N	2.72	0.53
9:I:17:ARG:HD2	9:I:28:GLU:OE1	2.08	0.53
1:A:1404:GLU:O	1:A:1408:ILE:HG13	2.08	0.53
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.26	0.53
2:B:638:PHE:HB3	2:B:651:LEU:CD2	2.39	0.53
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.88	0.53
4:D:122:GLU:HG2	4:D:126:ILE:HG13	1.91	0.53
1:A:12:ARG:HD2	2:B:1218:THR:HG21	1.91	0.53
11:K:59:ALA:HA	11:K:74:ARG:O	2.09	0.53
1:A:252:PHE:O	1:A:256:GLN:NE2	2.42	0.53
5:E:17:ARG:HH21	5:E:35:VAL:CG1	2.21	0.53
5:E:157:SER:C	5:E:159:ASP:H	2.10	0.53
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.91	0.53
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.39	0.53
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.22	0.53
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.90	0.53
12:L:53:HIS:O	12:L:55:ILE:HD13	2.08	0.53
5:E:46:TYR:CE2	5:E:58:MET:HA	2.44	0.53
2:B:576:ASP:HA	2:B:622:LYS:HZ1	1.73	0.53
5:E:190:LEU:HD11	5:E:196:VAL:HG21	1.91	0.53
8:H:15:VAL:HG21	8:H:49:VAL:O	2.09	0.53
2:B:857:ARG:NH2	13:T:24:DC:OP1	2.42	0.53
13:T:15:DA:H1'	13:T:16:DC:C5'	2.39	0.53
2:B:891:ASP:C	2:B:893:LEU:H	2.12	0.53
8:H:57:VAL:HG13	8:H:142:LEU:HD11	1.91	0.53
1:A:58:LEU:O	1:A:59:GLY:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:VAL:O	3:C:18:VAL:HG12	2.08	0.53
3:C:146:LYS:C	3:C:147:LEU:HD23	2.28	0.53
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.74	0.53
1:A:1323:ASP:C	1:A:1325:THR:H	2.13	0.53
1:A:22:PHE:CB	2:B:1211:ASN:ND2	2.69	0.53
4:D:15:LEU:O	4:D:17:LYS:N	2.38	0.53
2:B:850:LEU:HD12	2:B:851:PHE:N	2.24	0.53
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.26	0.52
3:C:105:GLY:HA3	3:C:149:LYS:O	2.09	0.52
4:D:220:LEU:CD1	4:D:221:TYR:N	2.67	0.52
2:B:215:GLN:NE2	2:B:215:GLN:HA	2.23	0.52
2:B:464:GLY:CA	2:B:479:VAL:O	2.57	0.52
8:H:81:PRO:CB	8:H:82:PRO:CD	2.86	0.52
4:D:193:THR:HG22	4:D:194:LEU:HD23	1.91	0.52
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.73	0.52
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.72	0.52
1:A:696:GLU:O	1:A:696:GLU:HG2	2.09	0.52
2:B:345:LYS:C	2:B:347:LYS:N	2.61	0.52
2:B:294:ASP:H	9:I:12:ASN:ND2	2.07	0.52
2:B:110:HIS:ND1	2:B:111:ALA:N	2.57	0.52
1:A:50:ILE:HG22	1:A:52:GLY:N	2.23	0.52
1:A:901:LEU:HB2	1:A:926:GLN:CG	2.38	0.52
12:L:40:LEU:HB3	12:L:44:ASP:OD2	2.09	0.52
4:D:70:PHE:HE1	7:G:51:TYR:CE1	2.27	0.52
2:B:227:LYS:HG3	2:B:395:GLN:OE1	2.10	0.52
8:H:111:LEU:HD23	8:H:127:GLY:O	2.09	0.52
1:A:920:LEU:HD23	1:A:921:GLY:N	2.24	0.52
1:A:486:GLU:OE2	2:B:1102:LYS:HD3	2.09	0.52
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.89	0.52
2:B:654:ARG:O	2:B:656:GLY:N	2.43	0.52
3:C:239:PRO:O	3:C:242:GLN:N	2.42	0.52
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.90	0.52
2:B:313:MET:CE	2:B:386:LEU:HD22	2.40	0.52
1:A:331:GLY:O	1:A:332:LYS:HB3	2.09	0.52
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.08	0.52
1:A:208:LEU:HA	1:A:235:ILE:HD12	1.90	0.52
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.91	0.52
12:L:54:ARG:HG3	12:L:54:ARG:HH11	1.74	0.52
1:A:50:ILE:C	1:A:52:GLY:N	2.63	0.52
2:B:531:GLN:HG3	2:B:532:ALA:N	2.12	0.52
4:D:155:ARG:HB2	4:D:221:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:ARG:HH11	6:F:79:ARG:HB2	1.74	0.52
2:B:575:PRO:HG2	2:B:576:ASP:H	1.73	0.52
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.09	0.52
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.93	0.52
4:D:29:LEU:HD23	7:G:82:PHE:CZ	2.45	0.52
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.91	0.52
8:H:4:THR:HG22	8:H:5:LEU:H	1.73	0.52
2:B:805:THR:HB	2:B:809:MET:SD	2.50	0.52
3:C:66:ARG:NH1	3:C:144:ILE:O	2.42	0.52
8:H:13:SER:O	8:H:14:GLU:HB2	2.09	0.52
2:B:521:LEU:HD13	2:B:633:VAL:HG12	1.92	0.52
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.44	0.52
13:T:15:DA:H1'	13:T:16:DC:H5"	1.92	0.52
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.25	0.52
1:A:900:ASP:CA	1:A:926:GLN:NE2	2.65	0.52
6:F:76:LYS:O	6:F:79:ARG:HB2	2.09	0.52
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.25	0.52
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.63	0.52
1:A:89:PRO:C	1:A:204:THR:HG21	2.30	0.52
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.09	0.52
5:E:179:GLN:O	5:E:182:ASP:HB2	2.10	0.52
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.09	0.52
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.10	0.52
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.42	0.52
1:A:567:LYS:HZ2	8:H:47:PHE:CB	2.21	0.52
1:A:62:ASP:HB3	1:A:64:ASN:CB	2.36	0.52
4:D:40:HIS:CA	7:G:73:LYS:HZ1	2.10	0.52
3:C:133:ILE:HD13	3:C:236:GLY:C	2.30	0.52
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.45	0.52
2:B:128:LEU:O	2:B:167:ILE:HD12	2.09	0.52
1:A:350:ARG:HD2	1:A:488:ASN:HD21	1.74	0.52
4:D:117:GLU:HG3	4:D:155:ARG:NH1	2.24	0.52
7:G:1:MET:SD	7:G:79:PHE:CE1	3.03	0.52
8:H:91:ASP:C	8:H:93:TYR:H	2.12	0.52
2:B:1224:PHE:CZ	5:E:174:GLN:NE2	2.78	0.52
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.25	0.52
1:A:105:CYS:SG	1:A:139:TRP:HA	2.50	0.52
1:A:1376:THR:HG23	5:E:212:ARG:NH2	2.25	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.10	0.52
2:B:170:LEU:O	2:B:172:ILE:HD12	2.09	0.52
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.74	0.52
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.75	0.52
1:A:1225:PHE:CZ	1:A:1227:ILE:HD11	2.45	0.52
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.92	0.52
7:G:155:SER:O	7:G:156:SER:HB3	2.09	0.52
1:A:1147:THR:HG22	9:I:48:LEU:HD12	1.92	0.52
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.92	0.52
1:A:283:GLY:O	1:A:285:PRO:CD	2.58	0.52
2:B:299:GLU:OE1	2:B:572:HIS:CE1	2.62	0.52
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.40	0.52
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.45	0.52
5:E:26:ARG:HD3	5:E:187:TYR:O	2.09	0.52
3:C:133:ILE:HD12	3:C:237:SER:HA	1.91	0.52
2:B:479:VAL:O	2:B:480:SER:HB3	2.10	0.52
8:H:62:SER:O	8:H:63:LEU:O	2.28	0.52
1:A:322:VAL:CG1	1:A:322:VAL:O	2.58	0.52
1:A:283:GLY:O	1:A:285:PRO:HD2	2.09	0.52
11:K:29:ASN:O	11:K:76:GLN:HG3	2.10	0.52
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.24	0.52
7:G:110:VAL:HG22	7:G:161:GLY:O	2.10	0.52
2:B:25:ILE:CD1	2:B:653:VAL:HG12	2.35	0.52
1:A:710:LEU:HD22	9:I:96:SER:HB3	1.92	0.52
9:I:50:THR:HG23	9:I:52:ILE:HG12	1.91	0.52
1:A:91:PHE:H	1:A:297:GLN:HE22	1.57	0.52
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.74	0.52
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.42	0.52
1:A:341:MET:CE	1:A:843:LYS:HZ1	2.23	0.52
11:K:31:VAL:HG12	11:K:32:VAL:H	1.75	0.52
2:B:220:GLY:O	2:B:222:ILE:HG13	2.10	0.52
3:C:8:VAL:HG21	11:K:105:PHE:HA	1.92	0.52
4:D:32:GLU:HG2	7:G:42:PHE:CE2	2.45	0.52
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.91	0.51
9:I:85:PHE:HD1	9:I:99:LEU:CD2	2.23	0.51
2:B:168:GLY:H	2:B:450:ALA:HB1	1.72	0.51
3:C:124:LEU:O	3:C:125:MET:C	2.49	0.51
5:E:54:GLN:HA	5:E:84:ASP:OD1	2.10	0.51
1:A:974:ASP:O	1:A:976:THR:N	2.43	0.51
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.92	0.51
2:B:44:VAL:CG1	2:B:199:MET:HG2	2.40	0.51
1:A:1206:ASP:O	1:A:1274:ARG:CZ	2.58	0.51
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:ASP:O	3:C:27:LEU:C	2.48	0.51
4:D:128:VAL:HG12	4:D:129:LEU:N	2.25	0.51
1:A:559:VAL:HG12	1:A:559:VAL:O	2.10	0.51
2:B:347:LYS:HG3	2:B:348:ARG:N	2.26	0.51
8:H:33:GLN:OE1	8:H:33:GLN:HA	2.10	0.51
2:B:33:VAL:O	2:B:36:ALA:HB3	2.10	0.51
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.10	0.51
10:J:16:ASP:O	10:J:18:TRP:N	2.44	0.51
1:A:445:ASN:CB	1:A:455:MET:HG2	2.35	0.51
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.21	0.51
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.51
1:A:42:ASP:O	1:A:44:THR:N	2.41	0.51
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.24	0.51
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.92	0.51
1:A:332:LYS:C	1:A:334:GLY:H	2.14	0.51
2:B:63:ILE:O	2:B:67:SER:HB3	2.10	0.51
4:D:207:LEU:HD12	4:D:207:LEU:O	2.11	0.51
8:H:134:ASN:O	8:H:135:LEU:O	2.27	0.51
2:B:298:LEU:H	2:B:298:LEU:HD22	1.75	0.51
2:B:637:LEU:O	2:B:690:VAL:HG22	2.10	0.51
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.92	0.51
13:T:19:DC:C2'	13:T:20:BRU:H6	2.41	0.51
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.43	0.51
1:A:839:ARG:HG2	1:A:839:ARG:HH11	1.76	0.51
2:B:298:LEU:N	2:B:298:LEU:HD22	2.25	0.51
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.76	0.51
1:A:225:ASN:C	1:A:225:ASN:ND2	2.64	0.51
2:B:287:ARG:NH1	2:B:324:ILE:O	2.39	0.51
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.92	0.51
1:A:699:ALA:O	1:A:700:ASN:CB	2.58	0.51
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.93	0.51
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.46	0.51
1:A:873:MET:C	1:A:1058:VAL:HG23	2.30	0.51
2:B:283:VAL:HG21	2:B:317:CYS:O	2.10	0.51
1:A:34:LYS:HB3	1:A:36:ARG:NH1	2.25	0.51
2:B:847:ASP:C	2:B:849:GLY:H	2.14	0.51
3:C:239:PRO:O	3:C:240:VAL:C	2.49	0.51
1:A:1435:PRO:O	1:A:1436:ILE:HD12	2.11	0.51
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.93	0.51
5:E:23:VAL:HG13	5:E:28:TYR:HD1	1.75	0.51
2:B:1096:ARG:CB	2:B:1096:ARG:HH11	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1028:GLU:OE1	2:B:1090:THR:HG23	2.10	0.51
2:B:408:LEU:O	2:B:411:PRO:HD2	2.11	0.51
1:A:286:HIS:C	1:A:288:ALA:H	2.13	0.51
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.40	0.51
2:B:254:LEU:CD2	2:B:361:LEU:HD11	2.39	0.51
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.45	0.51
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.51
1:A:71:GLN:O	1:A:73:GLY:N	2.37	0.51
5:E:212:ARG:CG	5:E:212:ARG:HH11	2.17	0.51
7:G:88:ASP:CB	7:G:144:ARG:HA	2.36	0.51
1:A:1036:ARG:HH11	1:A:1036:ARG:CG	2.16	0.51
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.46	0.51
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.91	0.51
7:G:138:THR:CG2	7:G:139:ILE:N	2.74	0.51
5:E:58:MET:O	5:E:59:SER:O	2.27	0.51
9:I:62:ILE:O	9:I:62:ILE:CG1	2.58	0.51
8:H:138:GLU:O	8:H:139:ASN:C	2.49	0.51
2:B:380:TYR:O	2:B:383:ASN:HB3	2.11	0.51
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.75	0.51
1:A:34:LYS:O	1:A:35:ILE:HB	2.11	0.51
5:E:186:LEU:O	5:E:189:GLY:N	2.38	0.51
12:L:34:CYS:O	12:L:36:SER:N	2.44	0.51
12:L:46:VAL:HG12	12:L:56:LEU:HD12	1.93	0.51
2:B:172:ILE:HG22	2:B:173:MET:N	2.25	0.51
2:B:830:TYR:C	2:B:832:GLY:N	2.64	0.51
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.39	0.51
1:A:545:GLN:O	1:A:547:LEU:N	2.42	0.51
10:J:53:HIS:HD2	10:J:54:VAL:N	2.09	0.51
2:B:235:SER:C	2:B:236:HIS:HD2	2.13	0.51
1:A:998:LEU:CD1	1:A:998:LEU:N	2.74	0.51
6:F:81:THR:HG23	6:F:144:GLU:OE1	2.10	0.51
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.40	0.51
5:E:127:ILE:O	5:E:127:ILE:HG13	2.10	0.51
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.27	0.51
2:B:1176:ASN:C	2:B:1178:ASN:H	2.13	0.51
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.44	0.51
2:B:604:ARG:HA	2:B:609:ILE:O	2.10	0.51
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.11	0.51
1:A:225:ASN:C	1:A:225:ASN:HD22	2.13	0.51
1:A:447:GLN:HE22	13:T:20:BRU:H4'	1.75	0.51
1:A:1226:VAL:C	1:A:1227:ILE:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.41	0.51
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.57	0.51
4:D:134:THR:HG22	4:D:135:GLY:N	2.25	0.51
1:A:364:VAL:O	1:A:364:VAL:HG13	2.11	0.51
2:B:504:ARG:O	2:B:505:ASP:C	2.49	0.51
2:B:505:ASP:O	2:B:507:LYS:N	2.44	0.51
12:L:47:ARG:NE	12:L:54:ARG:HG2	2.26	0.51
2:B:114:PRO:O	2:B:116:GLU:N	2.44	0.51
4:D:122:GLU:C	4:D:124:GLU:N	2.62	0.51
12:L:49:LYS:O	12:L:50:ASP:CB	2.57	0.51
2:B:446:LEU:HD21	2:B:448:ILE:HD11	1.93	0.51
2:B:970:THR:HG22	2:B:971:THR:H	1.74	0.51
1:A:250:ILE:O	1:A:258:GLY:HA3	2.11	0.51
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.46	0.51
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.40	0.51
3:C:236:GLY:C	3:C:238:ILE:N	2.64	0.51
2:B:48:LEU:O	2:B:51:PHE:N	2.43	0.51
1:A:1170:ILE:N	1:A:1170:ILE:HD12	2.18	0.51
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.92	0.51
1:A:596:THR:C	1:A:598:LEU:N	2.62	0.51
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.31	0.51
1:A:1356:ILE:HD13	1:A:1363:VAL:HG21	1.93	0.51
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.59	0.50
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.50
2:B:763:GLN:CG	2:B:765:PRO:HD2	2.26	0.50
2:B:640:VAL:HG12	2:B:649:LYS:HG2	1.92	0.50
2:B:842:ASN:HB2	2:B:1009:ASP:HA	1.93	0.50
2:B:175:ARG:HB2	2:B:200:GLY:HA3	1.92	0.50
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.11	0.50
10:J:28:ASP:O	10:J:30:LEU:HD12	2.11	0.50
3:C:191:TYR:HB3	3:C:201:TRP:CD1	2.47	0.50
2:B:661:LEU:HD23	2:B:679:TYR:O	2.11	0.50
1:A:34:LYS:H	1:A:34:LYS:HD3	1.75	0.50
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.50
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.26	0.50
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.42	0.50
1:A:91:PHE:N	1:A:297:GLN:HE22	2.09	0.50
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.75	0.50
2:B:217:ARG:HG2	2:B:217:ARG:NH1	2.27	0.50
2:B:850:LEU:HD12	2:B:851:PHE:H	1.76	0.50
7:G:91:VAL:HG12	7:G:92:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:O	1:A:149:GLU:OE1	2.29	0.50
1:A:423:ASP:O	1:A:424:ILE:HB	2.10	0.50
1:A:567:LYS:HD3	8:H:95:TYR:CA	2.39	0.50
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.29	0.50
3:C:144:ILE:O	3:C:145:CYS:HB3	2.12	0.50
2:B:189:LEU:O	2:B:192:LEU:N	2.45	0.50
1:A:1159:ARG:NH2	1:A:1187:GLN:NE2	2.60	0.50
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.47	0.50
8:H:80:ARG:O	8:H:81:PRO:O	2.28	0.50
1:A:1155:ASP:OD2	1:A:1162:VAL:HG23	2.11	0.50
5:E:44:ALA:O	5:E:45:LYS:HB2	2.11	0.50
7:G:22:MET:O	7:G:25:TYR:N	2.45	0.50
3:C:233:GLU:OE2	10:J:43:ARG:NH2	2.39	0.50
1:A:471:ASN:O	1:A:474:VAL:HG12	2.11	0.50
2:B:276:ILE:HG22	2:B:278:GLN:O	2.11	0.50
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.93	0.50
1:A:53:LEU:O	1:A:54:ASN:C	2.50	0.50
3:C:133:ILE:CD1	3:C:237:SER:HA	2.41	0.50
2:B:791:THR:O	2:B:792:MET:O	2.29	0.50
1:A:1002:GLY:N	1:A:1007:ILE:HG21	2.24	0.50
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.93	0.50
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.93	0.50
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.60	0.50
2:B:860:MET:HE2	2:B:963:PHE:CE1	2.46	0.50
1:A:990:VAL:O	1:A:994:GLN:HG3	2.12	0.50
3:C:83:SER:OG	3:C:160:LYS:HD3	2.11	0.50
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.26	0.50
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.12	0.50
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.93	0.50
3:C:56:THR:HG22	3:C:57:VAL:N	2.27	0.50
2:B:333:PHE:O	2:B:334:ILE:HG12	2.12	0.50
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.11	0.50
1:A:335:ARG:NH1	2:B:1202:LEU:HD22	2.25	0.50
2:B:861:ASP:OD1	2:B:862:GLN:N	2.45	0.50
1:A:552:TRP:O	1:A:554:PRO:HD3	2.11	0.50
2:B:957:ASN:O	2:B:958:GLN:C	2.49	0.50
2:B:882:THR:CB	2:B:934:LYS:O	2.60	0.50
1:A:63:ARG:N	1:A:74:MET:CE	2.69	0.50
1:A:1376:THR:HG23	5:E:212:ARG:HH21	1.76	0.50
2:B:128:LEU:HD11	2:B:170:LEU:HB3	1.94	0.50
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.12	0.50
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.94	0.50
1:A:979:SER:OG	1:A:980:ASP:N	2.45	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.11	0.50
1:A:1407:GLU:CD	1:A:1407:GLU:N	2.65	0.50
11:K:18:LYS:HZ2	11:K:38:GLU:HG2	1.74	0.50
8:H:63:LEU:C	8:H:90:ALA:CB	2.80	0.50
2:B:859:TYR:CD1	2:B:859:TYR:N	2.80	0.50
1:A:316:GLN:O	1:A:318:SER:N	2.44	0.50
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.46	0.50
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.29	0.50
1:A:35:ILE:HA	1:A:52:GLY:O	2.12	0.50
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.92	0.50
1:A:72:GLU:OE2	2:B:1175:LEU:HG	2.11	0.50
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.94	0.50
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.31	0.50
9:I:106:CYS:O	9:I:107:SER:HB2	2.12	0.50
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	1.94	0.50
8:H:143:LEU:N	8:H:143:LEU:HD12	2.26	0.50
2:B:745:PRO:O	2:B:748:ILE:HG12	2.12	0.50
2:B:174:LEU:O	2:B:175:ARG:HB2	2.11	0.50
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.45	0.50
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.94	0.50
11:K:42:LEU:O	11:K:42:LEU:HD23	2.10	0.50
9:I:8:ARG:O	9:I:10:CYS:N	2.41	0.50
1:A:40:THR:HG23	1:A:41:MET:H	1.76	0.50
2:B:205:ILE:N	2:B:205:ILE:HD12	2.27	0.50
7:G:4:ILE:CG1	7:G:77:VAL:HG22	2.41	0.50
2:B:221:ASN:N	2:B:241:ARG:O	2.26	0.50
1:A:913:LEU:HD11	1:A:981:LEU:O	2.12	0.50
3:C:208:GLU:C	3:C:210:GLU:H	2.14	0.50
11:K:68:PHE:CD2	11:K:68:PHE:N	2.78	0.50
2:B:504:ARG:CG	2:B:505:ASP:H	2.19	0.50
2:B:1087:PHE:CD2	2:B:1087:PHE:C	2.85	0.50
2:B:128:LEU:HD11	2:B:170:LEU:CB	2.42	0.50
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.42	0.50
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.42	0.50
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.93	0.50
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.60	0.50
8:H:91:ASP:O	8:H:93:TYR:N	2.39	0.50
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:PHE:HE2	2:B:816:GLU:HG2	1.73	0.50
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.41	0.50
1:A:720:ARG:O	1:A:724:GLU:HG3	2.12	0.50
1:A:27:VAL:O	1:A:30:ILE:HG22	2.11	0.50
3:C:56:THR:HG22	3:C:57:VAL:H	1.77	0.49
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.94	0.49
2:B:261:ARG:HH11	2:B:261:ARG:CB	2.07	0.49
3:C:166:GLU:C	11:K:6:ARG:NH1	2.65	0.49
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.90	0.49
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.93	0.49
1:A:731:ARG:HG3	1:A:734:GLU:OE1	2.11	0.49
5:E:65:THR:O	5:E:69:ILE:HG13	2.12	0.49
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.42	0.49
2:B:237:VAL:HG12	2:B:239:GLU:HG3	1.94	0.49
1:A:1126:ALA:O	1:A:1128:GLN:N	2.40	0.49
7:G:26:LEU:HD11	7:G:70:PHE:CE1	2.47	0.49
2:B:100:PRO:O	2:B:101:MET:HG3	2.11	0.49
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.76	0.49
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.15	0.49
2:B:315:LYS:HG2	9:I:13:MET:CE	2.33	0.49
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.42	0.49
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.21	0.49
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.12	0.49
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.42	0.49
1:A:100:LYS:O	1:A:104:GLU:HG3	2.12	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.57	0.49
2:B:104:GLU:CD	12:L:54:ARG:HE	2.15	0.49
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.43	0.49
2:B:123:THR:O	2:B:125:SER:N	2.44	0.49
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.46	0.49
9:I:83:ASN:HA	9:I:104:LEU:HD21	1.94	0.49
2:B:412:LEU:CD2	2:B:479:VAL:HG11	2.43	0.49
1:A:1345:ARG:HH11	1:A:1373:ASP:CG	2.16	0.49
3:C:73:GLN:HE22	3:C:75:MET:CB	2.12	0.49
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.94	0.49
4:D:122:GLU:C	4:D:124:GLU:H	2.15	0.49
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.47	0.49
1:A:409:SER:O	1:A:410:GLY:C	2.51	0.49
3:C:259:LEU:HD12	11:K:88:LYS:HG2	1.93	0.49
2:B:422:LYS:HA	2:B:425:THR:HB	1.93	0.49
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ALA:C	1:A:845:LEU:HD23	2.33	0.49
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.93	0.49
2:B:803:LEU:O	2:B:805:THR:HG23	2.11	0.49
1:A:567:LYS:CD	8:H:95:TYR:CD2	2.94	0.49
1:A:69:THR:O	1:A:70:CYS:C	2.50	0.49
9:I:103:CYS:HB3	9:I:107:SER:H	1.78	0.49
9:I:78:CYS:SG	9:I:105:SER:O	2.70	0.49
2:B:640:VAL:O	2:B:641:GLU:C	2.49	0.49
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.12	0.49
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.66	0.49
1:A:332:LYS:H	1:A:337:ARG:CB	2.25	0.49
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.43	0.49
15:P:4:A:O2'	15:P:5:G:H5'	2.13	0.49
7:G:116:PRO:HB2	7:G:118:ASP:OD1	2.12	0.49
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.12	0.49
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.47	0.49
2:B:664:THR:HG23	2:B:678:GLU:N	2.26	0.49
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.49
1:A:65:LEU:O	1:A:66:LYS:O	2.31	0.49
1:A:401:GLY:C	1:A:435:HIS:HD2	2.15	0.49
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.94	0.49
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.95	0.49
9:I:70:ARG:HA	9:I:83:ASN:O	2.12	0.49
2:B:578:THR:HG23	2:B:622:LYS:C	2.33	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.41	0.49
2:B:429:PHE:HA	2:B:432:MET:CE	2.42	0.49
1:A:332:LYS:O	1:A:334:GLY:N	2.45	0.49
13:T:26:DT:H2"	13:T:27:DT:OP2	2.12	0.49
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.74	0.49
1:A:920:LEU:HD23	1:A:920:LEU:C	2.33	0.49
1:A:619:LYS:HD2	1:A:750:GLY:O	2.12	0.49
1:A:276:LEU:O	1:A:279:LEU:HB2	2.12	0.49
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.94	0.49
1:A:446:ARG:HB2	1:A:487:MET:SD	2.52	0.49
8:H:6:PHE:HE1	8:H:129:TYR:HE1	1.61	0.49
3:C:101:LEU:C	3:C:102:GLN:HG3	2.31	0.49
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.95	0.49
4:D:51:ASN:C	4:D:52:LEU:O	2.51	0.49
1:A:1265:ASN:C	1:A:1267:MET:N	2.65	0.49
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.47	0.49
2:B:408:LEU:CD2	2:B:545:ILE:HD12	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.46	0.49
2:B:1221:SER:O	2:B:1223:ASP:N	2.45	0.49
1:A:555:ASP:O	1:A:556:TRP:C	2.51	0.49
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.47	0.49
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.46	0.49
8:H:59:ILE:O	8:H:60:ALA:CB	2.61	0.49
2:B:661:LEU:C	2:B:663:ALA:N	2.65	0.49
2:B:880:THR:O	2:B:881:ASN:HB2	2.12	0.49
1:A:399:HIS:CG	1:A:400:PRO:N	2.79	0.49
9:I:105:SER:O	9:I:106:CYS:CB	2.49	0.49
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.43	0.49
12:L:59:ALA:O	12:L:60:ARG:O	2.31	0.49
2:B:1001:PHE:C	2:B:1001:PHE:CD1	2.85	0.49
1:A:869:GLY:O	1:A:870:GLU:HB2	2.11	0.49
1:A:738:LYS:HB3	8:H:19:ARG:HH12	1.77	0.49
2:B:860:MET:HE2	2:B:963:PHE:HE1	1.77	0.49
2:B:134:LYS:O	2:B:135:ARG:C	2.51	0.49
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.95	0.49
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.28	0.49
8:H:129:TYR:H	8:H:130:ARG:HD2	1.78	0.49
8:H:4:THR:CG2	8:H:5:LEU:H	2.25	0.49
2:B:880:THR:O	2:B:880:THR:HG22	2.13	0.49
4:D:40:HIS:CD2	4:D:40:HIS:C	2.86	0.49
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.13	0.49
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.95	0.49
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.74	0.49
1:A:1265:ASN:O	1:A:1268:LEU:N	2.46	0.49
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.42	0.49
7:G:138:THR:O	7:G:140:LYS:N	2.46	0.49
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.95	0.49
1:A:208:LEU:HD23	1:A:208:LEU:C	2.34	0.49
2:B:305:VAL:O	2:B:305:VAL:HG12	2.12	0.49
2:B:29:ASP:HB3	2:B:658:ILE:HD11	1.95	0.49
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.48	0.49
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.13	0.49
9:I:15:TYR:HD1	9:I:15:TYR:N	2.11	0.49
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.95	0.49
3:C:82:TYR:O	3:C:85:ASP:N	2.46	0.49
2:B:597:MET:SD	2:B:624:LEU:HD11	2.53	0.48
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.94	0.48
2:B:298:LEU:H	2:B:298:LEU:CD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HA	2:B:129:PHE:O	2.13	0.48
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.28	0.48
2:B:114:PRO:O	2:B:115:GLN:C	2.51	0.48
4:D:154:PHE:CD2	4:D:163:VAL:HG21	2.47	0.48
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.25	0.48
1:A:103:CYS:HB3	1:A:108:MET:HE1	1.95	0.48
4:D:39:ASN:HB3	4:D:43:GLU:HG3	1.94	0.48
2:B:491:THR:O	2:B:495:LEU:HD12	2.13	0.48
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.94	0.48
1:A:814:PHE:O	1:A:818:MET:HG3	2.13	0.48
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.48	0.48
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.95	0.48
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.81	0.48
1:A:1329:THR:CG2	1:A:1331:SER:H	2.15	0.48
1:A:1437:GLY:O	1:A:1439:GLY:N	2.46	0.48
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.78	0.48
4:D:58:VAL:HG11	7:G:4:ILE:HD11	1.95	0.48
1:A:782:ARG:NH2	2:B:699:GLU:O	2.42	0.48
1:A:549:MET:CE	1:A:656:TRP:HD1	2.26	0.48
1:A:1215:ARG:CA	1:A:1218:GLN:HG2	2.40	0.48
8:H:116:TYR:HE2	8:H:140:ALA:HB2	1.78	0.48
1:A:1450:LEU:HG	1:A:1450:LEU:O	2.13	0.48
5:E:171:LYS:HD3	5:E:171:LYS:N	2.27	0.48
8:H:126:GLU:C	8:H:130:ARG:HH22	2.16	0.48
2:B:882:THR:C	2:B:884:ARG:H	2.17	0.48
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.48
2:B:1087:PHE:C	2:B:1087:PHE:HD2	2.16	0.48
1:A:1158:PRO:HG2	1:A:1159:ARG:HE	1.78	0.48
1:A:134:ARG:NH1	1:A:220:THR:O	2.47	0.48
2:B:831:SER:HG	2:B:994:TYR:HE1	1.62	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.95	0.48
3:C:261:ALA:C	3:C:263:THR:H	2.17	0.48
2:B:388:CYS:C	2:B:390:LEU:N	2.66	0.48
3:C:124:LEU:HD12	3:C:124:LEU:N	2.27	0.48
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.96	0.48
4:D:170:THR:HG21	4:D:172:LEU:HG	1.95	0.48
5:E:10:SER:O	5:E:14:ARG:HG3	2.13	0.48
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.79	0.48
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.96	0.48
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.48	0.48
2:B:100:PRO:O	2:B:180:TYR:OH	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:CG2	2:B:884:ARG:N	2.68	0.48
7:G:40:GLY:O	7:G:80:LYS:HE2	2.14	0.48
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.58	0.48
11:K:89:ASN:O	11:K:91:CYS:N	2.46	0.48
11:K:53:ASP:O	11:K:56:VAL:HB	2.13	0.48
1:A:229:SER:HA	1:A:233:TRP:CE3	2.48	0.48
5:E:159:ASP:HA	5:E:162:ARG:CZ	2.42	0.48
4:D:188:ALA:N	4:D:208:GLU:OE2	2.47	0.48
5:E:124:VAL:HB	5:E:125:PRO:CD	2.43	0.48
2:B:418:LYS:O	2:B:420:LEU:N	2.47	0.48
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.95	0.48
4:D:137:ASN:O	4:D:139:LYS:N	2.43	0.48
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.48
2:B:34:ILE:O	2:B:37:PHE:N	2.45	0.48
4:D:154:PHE:CD1	4:D:154:PHE:N	2.81	0.48
2:B:711:GLU:H	2:B:712:PRO:CD	2.26	0.48
1:A:1048:ASN:O	1:A:1050:GLU:N	2.47	0.48
2:B:1003:ALA:HB1	3:C:179:GLU:HB2	1.94	0.48
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.95	0.48
15:P:6:A:H2'	15:P:7:C:O4'	2.12	0.48
10:J:34:THR:O	10:J:35:ALA:C	2.52	0.48
2:B:346:GLU:HA	2:B:349:ILE:HD12	1.96	0.48
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.49	0.48
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.43	0.48
6:F:147:SER:C	6:F:149:GLU:N	2.65	0.48
8:H:12:VAL:HA	8:H:28:ALA:CB	2.44	0.48
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.96	0.48
2:B:55:VAL:HG12	2:B:97:VAL:HG21	1.96	0.48
2:B:519:TRP:C	2:B:519:TRP:CD1	2.87	0.48
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.31	0.48
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	1.96	0.48
4:D:160:VAL:HG12	4:D:160:VAL:O	2.14	0.48
7:G:1:MET:O	7:G:2:PHE:C	2.52	0.48
1:A:913:LEU:CD1	1:A:914:GLU:H	2.21	0.48
1:A:1277:GLU:O	1:A:1279:ILE:N	2.44	0.48
1:A:326:ARG:NH2	1:A:1407:GLU:OE2	2.47	0.48
9:I:110:PHE:CD2	9:I:110:PHE:N	2.78	0.48
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.48	0.48
1:A:818:MET:HG2	2:B:514:LEU:HG	1.95	0.48
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.95	0.48
2:B:1072:MET:HE3	2:B:1085:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1085:ILE:HG22	2:B:1086:PHE:O	2.13	0.48
1:A:711:ARG:HH21	9:I:87:GLN:CD	2.16	0.48
2:B:48:LEU:HD23	2:B:173:MET:SD	2.54	0.48
2:B:388:CYS:C	2:B:390:LEU:H	2.15	0.48
1:A:22:PHE:CB	2:B:1211:ASN:HD21	2.27	0.48
5:E:19:VAL:HG22	5:E:140:LEU:CD2	2.43	0.48
1:A:92:HIS:O	1:A:93:VAL:C	2.52	0.48
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.43	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.95	0.48
1:A:306:ASN:CB	1:A:324:SER:HB3	2.44	0.48
2:B:225:VAL:HG12	2:B:238:ALA:HA	1.95	0.48
1:A:684:ALA:O	1:A:687:LYS:HB2	2.14	0.48
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.14	0.48
1:A:663:SER:OG	1:A:664:THR:N	2.46	0.48
1:A:1385:THR:C	1:A:1387:HIS:N	2.67	0.48
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.49	0.48
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.48
1:A:401:GLY:C	1:A:435:HIS:CD2	2.87	0.48
11:K:88:LYS:O	11:K:91:CYS:HB2	2.14	0.48
1:A:229:SER:HA	1:A:233:TRP:HE3	1.79	0.48
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.96	0.48
1:A:635:ARG:NH1	1:A:635:ARG:HA	2.29	0.48
2:B:37:PHE:HE2	2:B:542:MET:HA	1.79	0.47
1:A:1445:ILE:HD13	7:G:70:PHE:CZ	2.49	0.47
2:B:914:LYS:HD3	2:B:937:ALA:O	2.13	0.47
3:C:164:ALA:HA	3:C:167:HIS:O	2.14	0.47
10:J:36:LEU:HD13	10:J:47:ARG:HG3	1.96	0.47
12:L:55:ILE:CG1	12:L:56:LEU:H	2.26	0.47
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.44	0.47
2:B:583:ASN:ND2	2:B:628:THR:CG2	2.74	0.47
1:A:1030:ARG:HG3	1:A:1034:GLU:HG3	1.96	0.47
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.43	0.47
1:A:343:LYS:HB2	2:B:1117:GLN:OE1	2.14	0.47
1:A:418:SER:C	1:A:420:ARG:H	2.18	0.47
5:E:88:VAL:HG12	5:E:89:GLY:N	2.28	0.47
1:A:2:VAL:C	1:A:4:GLN:H	2.17	0.47
2:B:516:ASN:HD22	2:B:516:ASN:H	1.63	0.47
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.50	0.47
9:I:5:ARG:CD	9:I:36:GLU:OE2	2.63	0.47
2:B:604:ARG:C	2:B:606:LYS:N	2.67	0.47
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:951:GLN:HE21	12:L:57:LEU:CD1	2.25	0.47
2:B:778:MET:CE	2:B:1094:ARG:CD	2.83	0.47
1:A:1313:LEU:O	1:A:1315:GLU:N	2.47	0.47
1:A:1020:CYS:O	1:A:1024:SER:HB2	2.15	0.47
1:A:596:THR:C	1:A:598:LEU:H	2.17	0.47
2:B:56:ASP:C	2:B:57:TYR:HD1	2.18	0.47
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.96	0.47
5:E:159:ASP:HA	5:E:162:ARG:HH22	1.78	0.47
4:D:194:LEU:HD21	7:G:167:TYR:HB2	1.95	0.47
1:A:317:LYS:O	1:A:318:SER:HB3	2.14	0.47
2:B:727:LYS:HD3	2:B:1049:ASP:OD1	2.15	0.47
1:A:1390:ASN:OD1	1:A:1399:ARG:HA	2.14	0.47
3:C:249:ASP:HB2	11:K:102:LYS:NZ	2.28	0.47
1:A:1451:VAL:HG22	7:G:20:PRO:O	2.14	0.47
1:A:308:ILE:HG22	1:A:309:ALA:N	2.28	0.47
1:A:53:LEU:CD2	1:A:54:ASN:N	2.51	0.47
2:B:34:ILE:O	2:B:35:SER:C	2.52	0.47
2:B:881:ASN:CB	2:B:933:SER:N	2.77	0.47
3:C:173:ALA:O	3:C:174:ALA:CB	2.63	0.47
10:J:13:VAL:HG12	10:J:14:VAL:N	2.30	0.47
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.14	0.47
2:B:365:THR:OG1	2:B:367:LEU:HG	2.15	0.47
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.77	0.47
5:E:59:SER:OG	5:E:81:GLU:HG3	2.14	0.47
6:F:76:LYS:O	6:F:79:ARG:NH1	2.46	0.47
5:E:157:SER:C	5:E:159:ASP:N	2.67	0.47
2:B:1073:TYR:CD1	2:B:1073:TYR:N	2.83	0.47
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.97	0.47
5:E:93:MET:HG3	5:E:97:VAL:CG2	2.44	0.47
4:D:192:LYS:HE3	4:D:207:LEU:HD23	1.95	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.97	0.47
11:K:48:ALA:O	11:K:51:LEU:HB2	2.14	0.47
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.59	0.47
5:E:50:MET:HG3	5:E:50:MET:O	2.15	0.47
9:I:56:ALA:O	9:I:57:GLY:C	2.52	0.47
1:A:1385:THR:O	1:A:1387:HIS:N	2.48	0.47
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.50	0.47
2:B:390:LEU:O	2:B:391:ASP:CB	2.60	0.47
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.44	0.47
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.14	0.47
2:B:705:MET:H	2:B:710:LEU:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HD3	1:A:302:THR:CG2	2.44	0.47
1:A:324:SER:O	1:A:327:ALA:HB3	2.15	0.47
1:A:961:ARG:O	1:A:965:GLN:HG3	2.15	0.47
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.29	0.47
1:A:523:ILE:HG21	1:A:527:THR:HG22	1.95	0.47
8:H:145:ARG:O	8:H:146:ARG:HB2	2.15	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.95	0.47
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.66	0.47
2:B:803:LEU:HG	2:B:822:ASN:OD1	2.14	0.47
2:B:637:LEU:O	2:B:690:VAL:CG2	2.62	0.47
3:C:98:VAL:C	3:C:99:LEU:HD23	2.34	0.47
3:C:147:LEU:CB	3:C:151:GLN:HB2	2.42	0.47
2:B:364:ILE:HG22	2:B:365:THR:N	2.29	0.47
5:E:134:THR:C	5:E:135:PHE:HD1	2.17	0.47
5:E:55:ARG:HH11	5:E:55:ARG:HG3	1.80	0.47
11:K:65:HIS:HD2	11:K:67:PHE:H	1.56	0.47
2:B:1001:PHE:HD2	3:C:34:ARG:NH2	2.12	0.47
2:B:235:SER:C	2:B:236:HIS:CD2	2.88	0.47
1:A:261:ASP:OD1	1:A:322:VAL:HA	2.14	0.47
1:A:1364:ASN:HD22	1:A:1365:TYR:H	1.62	0.47
1:A:518:LYS:HE2	1:A:624:SER:O	2.15	0.47
11:K:62:LYS:O	11:K:71:PHE:HB2	2.15	0.47
2:B:465:ASN:HA	2:B:477:ALA:N	2.29	0.47
9:I:2:THR:O	9:I:3:THR:C	2.53	0.47
1:A:829:VAL:C	1:A:831:THR:H	2.16	0.47
9:I:35:VAL:CG1	9:I:36:GLU:N	2.77	0.47
1:A:567:LYS:HE3	8:H:46:LEU:HB3	1.96	0.47
12:L:40:LEU:HD22	12:L:44:ASP:OD2	2.15	0.47
2:B:373:ARG:NH2	2:B:587:HIS:ND1	2.62	0.47
1:A:705:LYS:HB2	1:A:708:MET:CE	2.43	0.47
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.83	0.47
3:C:31:ASN:O	3:C:35:ARG:HG3	2.14	0.47
1:A:1007:ILE:O	1:A:1010:ALA:HB3	2.15	0.47
4:D:170:THR:HB	4:D:172:LEU:HG	1.95	0.47
1:A:206:GLU:O	1:A:210:ILE:HG13	2.15	0.47
1:A:966:ASN:O	1:A:967:ALA:C	2.52	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.77	0.47
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.62	0.47
2:B:1223:ASP:OD1	2:B:1224:PHE:N	2.36	0.47
10:J:9:SER:OG	10:J:48:ARG:NH2	2.47	0.47
3:C:33:LEU:O	3:C:37:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:ASN:ND2	2:B:387:LEU:HD11	2.29	0.47
2:B:651:LEU:HD21	2:B:741:CYS:CB	2.41	0.47
2:B:661:LEU:O	2:B:664:THR:N	2.47	0.47
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.96	0.47
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.43	0.47
1:A:533:LYS:NZ	1:A:745:GLN:HE22	2.12	0.47
1:A:858:ASN:HD21	1:A:860:LEU:H	1.53	0.47
4:D:153:ARG:C	4:D:154:PHE:CD1	2.88	0.47
8:H:82:PRO:HB2	11:K:54:ARG:CZ	2.44	0.47
5:E:56:LYS:HE3	5:E:84:ASP:CB	2.44	0.47
1:A:528:LEU:HD23	1:A:751:SER:HA	1.95	0.47
2:B:758:PHE:O	2:B:761:HIS:HB2	2.15	0.47
7:G:17:PHE:HD2	7:G:17:PHE:H	1.59	0.47
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.78	0.47
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.15	0.47
2:B:792:MET:HE1	13:T:23:DT:O3'	2.14	0.47
2:B:174:LEU:HD12	2:B:174:LEU:N	2.29	0.47
1:A:961:ARG:HD3	1:A:965:GLN:CD	2.35	0.47
1:A:717:ASN:HB3	1:A:721:PHE:CZ	2.48	0.47
2:B:860:MET:SD	2:B:861:ASP:N	2.87	0.47
7:G:44:TYR:CE2	7:G:105:PRO:HB2	2.50	0.47
2:B:953:LEU:C	2:B:953:LEU:HD23	2.35	0.47
2:B:874:PHE:HD1	2:B:962:LYS:HD3	1.79	0.47
10:J:24:LEU:HD23	10:J:24:LEU:N	2.30	0.47
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.80	0.47
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.27	0.47
2:B:531:GLN:CG	2:B:532:ALA:N	2.76	0.47
3:C:147:LEU:CD2	3:C:147:LEU:N	2.75	0.47
12:L:30:ILE:HG22	12:L:31:CYS:N	2.29	0.47
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.96	0.47
2:B:125:SER:HA	2:B:172:ILE:CD1	2.45	0.47
2:B:128:LEU:HD13	2:B:169:ARG:HA	1.97	0.47
4:D:66:ARG:HG3	7:G:51:TYR:HD1	1.79	0.47
2:B:842:ASN:ND2	2:B:844:SER:HB2	2.30	0.47
2:B:407:ASP:C	2:B:408:LEU:HD12	2.34	0.47
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.45	0.47
2:B:906:SER:O	2:B:907:GLY:C	2.53	0.47
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.96	0.47
1:A:321:PRO:O	1:A:322:VAL:CB	2.63	0.47
1:A:1285:MET:CE	1:A:1286:LYS:H	2.28	0.47
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:O	1:A:71:GLN:HA	2.14	0.47
1:A:1094:VAL:O	1:A:1095:THR:C	2.52	0.47
9:I:77:LYS:HB3	9:I:77:LYS:HZ2	1.77	0.47
7:G:1:MET:HE1	7:G:2:PHE:HA	1.96	0.47
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.79	0.47
3:C:123:ASN:CG	3:C:125:MET:H	2.18	0.47
5:E:17:ARG:NH2	5:E:35:VAL:HG12	2.24	0.47
2:B:842:ASN:HD22	2:B:845:SER:N	2.08	0.47
5:E:48:ASP:CG	5:E:49:SER:N	2.68	0.47
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.15	0.47
1:A:726:ARG:O	1:A:729:ALA:HB3	2.14	0.47
5:E:92:THR:HG22	5:E:92:THR:O	2.13	0.47
8:H:107:VAL:HG21	8:H:126:GLU:OE2	2.15	0.47
1:A:54:ASN:OD1	1:A:54:ASN:O	2.32	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.07	0.47
12:L:38:LEU:HD22	12:L:56:LEU:HD21	1.96	0.47
4:D:118:THR:HB	4:D:121:LYS:HD2	1.97	0.47
2:B:649:LYS:HD3	2:B:736:THR:O	2.15	0.47
7:G:49:LEU:HD11	7:G:77:VAL:HG23	1.96	0.47
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.50	0.47
8:H:84:ALA:C	8:H:86:ASP:N	2.66	0.47
2:B:733:HIS:C	2:B:735:ALA:H	2.18	0.47
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.55	0.47
1:A:1227:ILE:N	1:A:1227:ILE:HD12	2.30	0.47
5:E:114:ASN:O	5:E:115:ASN:CB	2.63	0.47
1:A:308:ILE:HG22	1:A:309:ALA:H	1.79	0.47
5:E:102:GLU:C	5:E:104:ASN:N	2.68	0.47
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.97	0.47
1:A:56:PRO:O	1:A:57:ARG:CG	2.63	0.46
5:E:61:GLN:HG2	5:E:62:ALA:N	2.31	0.46
5:E:23:VAL:O	5:E:28:TYR:HB2	2.15	0.46
2:B:743:ILE:O	2:B:744:HIS:HB2	2.14	0.46
2:B:68:THR:O	2:B:69:LEU:HD23	2.14	0.46
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.96	0.46
5:E:124:VAL:H	5:E:125:PRO:HD2	1.80	0.46
4:D:29:LEU:O	4:D:30:GLY:O	2.32	0.46
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.96	0.46
3:C:263:THR:C	3:C:265:MET:H	2.18	0.46
2:B:55:VAL:CG1	2:B:97:VAL:HG21	2.45	0.46
5:E:92:THR:CG2	5:E:92:THR:O	2.62	0.46
2:B:377:PHE:C	2:B:379:GLY:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:ARG:HH11	9:I:5:ARG:HB2	1.80	0.46
1:A:90:VAL:CG1	1:A:297:GLN:NE2	2.72	0.46
1:A:255:SER:OG	2:B:918:ILE:HG21	2.14	0.46
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.49	0.46
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.15	0.46
2:B:610:ASN:OD1	2:B:611:PRO:CD	2.63	0.46
2:B:225:VAL:HG12	2:B:238:ALA:HB2	1.97	0.46
1:A:390:GLN:O	1:A:394:ASN:HB2	2.16	0.46
4:D:16:LYS:O	4:D:18:VAL:N	2.49	0.46
2:B:571:PRO:HG2	2:B:572:HIS:CE1	2.51	0.46
12:L:54:ARG:HG3	12:L:54:ARG:H	1.36	0.46
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.98	0.46
1:A:34:LYS:N	1:A:34:LYS:HD3	2.29	0.46
9:I:101:PHE:N	9:I:101:PHE:CD1	2.84	0.46
9:I:85:PHE:HD2	9:I:85:PHE:H	1.59	0.46
10:J:14:VAL:HG11	10:J:50:ILE:HG12	1.96	0.46
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.41	0.46
1:A:1265:ASN:O	1:A:1267:MET:N	2.48	0.46
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.97	0.46
2:B:242:SER:HB2	2:B:362:PRO:HG2	1.96	0.46
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.62	0.46
9:I:93:LYS:H	9:I:93:LYS:CD	2.27	0.46
6:F:109:VAL:HG11	6:F:123:LYS:CD	2.43	0.46
1:A:1006:ILE:CG2	1:A:1007:ILE:N	2.73	0.46
5:E:85:GLU:C	5:E:87:SER:N	2.68	0.46
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.45	0.46
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.97	0.46
1:A:320:ARG:HB2	1:A:320:ARG:NH1	2.31	0.46
2:B:34:ILE:HG12	2:B:542:MET:CE	2.46	0.46
2:B:35:SER:HA	2:B:811:TYR:HE2	1.80	0.46
10:J:5:VAL:O	10:J:6:ARG:O	2.34	0.46
3:C:6:PRO:CB	3:C:25:VAL:HG12	2.41	0.46
2:B:641:GLU:HB3	2:B:643:ASP:CG	2.36	0.46
4:D:31:GLN:O	4:D:34:GLN:HG3	2.15	0.46
1:A:1157:ASP:O	1:A:1159:ARG:N	2.45	0.46
2:B:1004:GLU:HA	3:C:177:GLU:HG2	1.97	0.46
5:E:165:LEU:HD21	5:E:175:LEU:CD1	2.39	0.46
5:E:135:PHE:N	5:E:135:PHE:CD1	2.83	0.46
1:A:707:GLY:CA	1:A:1281:ARG:HD3	2.43	0.46
1:A:384:ASN:O	1:A:385:ILE:C	2.54	0.46
2:B:1031:LEU:HD12	2:B:1031:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.97	0.46
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.03	0.46
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.30	0.46
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.46	0.46
2:B:412:LEU:HD22	2:B:479:VAL:HG11	1.96	0.46
2:B:636:PRO:HG2	2:B:743:ILE:HD12	1.97	0.46
3:C:186:LEU:CD1	3:C:186:LEU:H	2.29	0.46
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.30	0.46
2:B:175:ARG:CG	2:B:175:ARG:HH11	2.26	0.46
1:A:311:GLN:O	1:A:313:GLN:N	2.48	0.46
5:E:170:LEU:C	5:E:171:LYS:HD3	2.35	0.46
3:C:263:THR:C	3:C:265:MET:N	2.66	0.46
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.98	0.46
2:B:794:ASN:C	2:B:795:ILE:HD12	2.36	0.46
8:H:98:TYR:C	8:H:118:PHE:HD2	2.19	0.46
2:B:347:LYS:HG3	2:B:348:ARG:HG2	1.97	0.46
2:B:31:TRP:HA	2:B:31:TRP:CE3	2.49	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.98	0.46
1:A:56:PRO:O	1:A:57:ARG:HD3	2.14	0.46
1:A:61:ILE:O	1:A:62:ASP:HB2	2.15	0.46
1:A:67:CYS:O	1:A:68:GLN:HG3	2.15	0.46
1:A:67:CYS:O	1:A:70:CYS:HB3	2.16	0.46
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.97	0.46
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.46	0.46
11:K:50:LEU:HD13	11:K:75:ILE:HG12	1.98	0.46
11:K:89:ASN:O	11:K:90:ALA:C	2.53	0.46
2:B:68:THR:HG22	2:B:69:LEU:N	2.31	0.46
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.46
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.76	0.46
2:B:758:PHE:N	2:B:759:PRO:CD	2.78	0.46
2:B:707:PRO:CG	2:B:708:GLU:H	2.27	0.46
12:L:42:ARG:O	12:L:43:THR:CB	2.63	0.46
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.51	0.46
5:E:147:HIS:CD2	5:E:149:LEU:H	2.34	0.46
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.49	0.46
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.97	0.46
3:C:260:LEU:O	3:C:263:THR:HB	2.15	0.46
4:D:14:ARG:O	4:D:16:LYS:N	2.49	0.46
1:A:1327:ILE:O	1:A:1327:ILE:HG23	2.15	0.46
3:C:57:VAL:O	3:C:57:VAL:HG12	2.16	0.46
2:B:597:MET:SD	2:B:617:ARG:HB2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.97	0.46
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.98	0.46
3:C:148:ARG:H	3:C:151:GLN:HG3	1.80	0.46
1:A:12:ARG:CZ	2:B:1192:TYR:CE2	2.98	0.46
1:A:1124:HIS:CB	1:A:1130:GLN:HG2	2.46	0.46
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.16	0.46
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.51	0.46
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.95	0.46
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.31	0.46
2:B:714:GLU:HG2	2:B:715:ALA:N	2.29	0.46
9:I:19:ASP:HB3	9:I:24:ARG:HG3	1.98	0.46
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.31	0.46
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.97	0.46
9:I:85:PHE:N	9:I:85:PHE:CD2	2.82	0.46
3:C:238:ILE:HD11	3:C:246:ARG:HD2	1.97	0.46
12:L:34:CYS:O	12:L:35:SER:C	2.54	0.46
1:A:488:ASN:HB3	2:B:1128:LEU:CD1	2.44	0.46
1:A:1166:ASP:O	1:A:1170:ILE:HD12	2.16	0.46
3:C:22:LEU:C	3:C:22:LEU:HD23	2.35	0.46
4:D:47:LEU:HD13	4:D:48:ILE:N	2.30	0.46
1:A:84:ILE:O	1:A:84:ILE:CG2	2.64	0.46
1:A:596:THR:O	1:A:597:LEU:C	2.54	0.46
2:B:629:ASP:HB3	2:B:632:ARG:CD	2.46	0.46
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.31	0.46
1:A:332:LYS:C	1:A:334:GLY:N	2.68	0.46
8:H:54:SER:O	8:H:146:ARG:HD2	2.15	0.46
2:B:874:PHE:HA	2:B:913:GLY:O	2.16	0.46
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.81	0.46
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.97	0.46
3:C:58:LEU:HD23	3:C:58:LEU:N	2.30	0.46
1:A:225:ASN:HD22	1:A:227:VAL:H	1.63	0.46
2:B:842:ASN:ND2	2:B:845:SER:OG	2.47	0.46
5:E:56:LYS:HE3	5:E:84:ASP:HB3	1.97	0.46
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.46	0.46
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.51	0.46
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.16	0.46
9:I:8:ARG:C	9:I:10:CYS:H	2.19	0.46
4:D:27:LEU:HD11	4:D:197:SER:HB3	1.97	0.46
8:H:25:ARG:HA	8:H:41:ASP:HA	1.98	0.46
3:C:209:TYR:HD1	3:C:209:TYR:H	1.64	0.46
1:A:825:ILE:HG21	2:B:509:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:HIS:NE2	2:B:592:ASN:O	2.48	0.46
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.49	0.46
3:C:174:ALA:O	10:J:10:CYS:O	2.34	0.46
1:A:1166:ASP:O	1:A:1170:ILE:CD1	2.64	0.46
1:A:428:TYR:H	1:A:428:TYR:HD1	1.63	0.46
1:A:1325:THR:O	5:E:148:GLU:HB2	2.16	0.46
5:E:39:LEU:O	5:E:42:PHE:HB3	2.15	0.46
5:E:56:LYS:CG	5:E:84:ASP:HB2	2.46	0.46
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.50	0.46
7:G:145:VAL:HG12	7:G:146:LYS:H	1.80	0.46
2:B:236:HIS:HE1	2:B:389:ALA:HA	1.80	0.46
1:A:208:LEU:C	1:A:208:LEU:CD2	2.84	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.74	0.45
2:B:101:MET:HA	2:B:112:LEU:H	1.81	0.45
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.51	0.45
2:B:48:LEU:O	2:B:49:ASP:C	2.54	0.45
6:F:90:ARG:HG3	6:F:91:ALA:N	2.30	0.45
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.50	0.45
5:E:135:PHE:N	5:E:135:PHE:HD1	2.13	0.45
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.42	0.45
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.97	0.45
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.42	0.45
3:C:152:GLU:HG2	3:C:153:LEU:N	2.28	0.45
2:B:792:MET:H	2:B:857:ARG:HA	1.80	0.45
10:J:27:GLU:O	10:J:29:GLU:HG3	2.16	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.45	0.45
1:A:1280:GLU:OE1	1:A:1280:GLU:HA	2.14	0.45
1:A:658:LEU:HD13	2:B:831:SER:HA	1.99	0.45
1:A:346:ASP:OD1	2:B:1106:ARG:NH2	2.48	0.45
1:A:320:ARG:CB	1:A:320:ARG:HH11	2.29	0.45
4:D:7:THR:O	4:D:9:GLN:N	2.41	0.45
1:A:1156:PRO:HA	1:A:1190:PRO:HA	1.96	0.45
2:B:511:PRO:O	2:B:513:GLN:N	2.49	0.45
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.97	0.45
2:B:681:TRP:C	2:B:683:SER:N	2.69	0.45
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.98	0.45
2:B:113:TYR:O	2:B:114:PRO:C	2.55	0.45
2:B:47:GLN:O	2:B:173:MET:SD	2.75	0.45
1:A:598:LEU:HD12	8:H:115:TYR:CE2	2.51	0.45
1:A:1407:GLU:O	1:A:1411:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:PRO:HG2	2:B:708:GLU:HG2	1.98	0.45
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.98	0.45
2:B:737:THR:CG2	9:I:66:PRO:HA	2.46	0.45
2:B:737:THR:HB	9:I:66:PRO:HB2	1.99	0.45
4:D:197:SER:O	4:D:201:LYS:HE2	2.16	0.45
1:A:1230:GLU:O	1:A:1233:ASP:N	2.48	0.45
1:A:1349:TYR:O	1:A:1350:LYS:C	2.55	0.45
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.16	0.45
2:B:663:ALA:O	2:B:667:GLN:HG3	2.17	0.45
2:B:185:THR:O	2:B:186:GLU:C	2.53	0.45
4:D:118:THR:HG21	4:D:121:LYS:HG3	1.98	0.45
1:A:252:PHE:HB2	1:A:256:GLN:OE1	2.16	0.45
2:B:696:GLU:O	2:B:699:GLU:HB2	2.16	0.45
5:E:42:PHE:CZ	5:E:58:MET:CE	2.99	0.45
9:I:58:VAL:O	9:I:59:VAL:C	2.55	0.45
1:A:767:GLN:HE22	1:A:774:ARG:HB3	1.80	0.45
1:A:974:ASP:CB	1:A:976:THR:HG23	2.43	0.45
2:B:710:LEU:O	2:B:711:GLU:OE2	2.34	0.45
11:K:40:HIS:O	11:K:43:GLY:N	2.49	0.45
1:A:476:SER:O	1:A:477:PRO:C	2.55	0.45
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.81	0.45
2:B:487:THR:O	2:B:490:SER:HB3	2.16	0.45
2:B:953:LEU:O	2:B:953:LEU:HD23	2.17	0.45
2:B:1059:LEU:CD2	2:B:1065:GLN:O	2.65	0.45
2:B:661:LEU:C	2:B:663:ALA:H	2.18	0.45
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.41	0.45
2:B:388:CYS:O	2:B:390:LEU:N	2.49	0.45
4:D:220:LEU:HD13	4:D:221:TYR:C	2.37	0.45
5:E:117:THR:C	5:E:119:SER:N	2.70	0.45
7:G:29:LYS:O	7:G:30:LEU:C	2.55	0.45
1:A:447:GLN:CD	13:T:20:BRU:H4'	2.36	0.45
11:K:12:LEU:HD21	11:K:18:LYS:N	2.32	0.45
11:K:16:GLU:OE1	11:K:37:LYS:HE2	2.16	0.45
1:A:1154:TYR:CD2	1:A:1156:PRO:HD3	2.52	0.45
1:A:122:MET:HG3	1:A:126:LEU:HD12	1.98	0.45
3:C:193:TYR:C	3:C:193:TYR:CD1	2.90	0.45
2:B:172:ILE:CD1	2:B:172:ILE:N	2.76	0.45
1:A:225:ASN:ND2	1:A:227:VAL:N	2.58	0.45
1:A:1255:GLU:OE1	1:A:1258:HIS:HB3	2.17	0.45
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.99	0.45
5:E:153:HIS:O	5:E:154:ILE:CG1	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:HIS:C	5:E:154:ILE:HG13	2.37	0.45
3:C:179:GLU:HG2	3:C:180:TYR:H	1.81	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.82	0.45
10:J:53:HIS:CD2	10:J:53:HIS:C	2.89	0.45
1:A:1453:TYR:N	1:A:1453:TYR:CD2	2.82	0.45
1:A:1332:PHE:O	1:A:1336:MET:HB2	2.16	0.45
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.99	0.45
4:D:23:ASN:N	4:D:23:ASN:HD22	2.15	0.45
1:A:829:VAL:C	1:A:831:THR:N	2.70	0.45
8:H:59:ILE:CG2	8:H:60:ALA:H	1.95	0.45
2:B:1175:LEU:HD23	2:B:1175:LEU:H	1.81	0.45
3:C:133:ILE:HD13	3:C:236:GLY:O	2.17	0.45
3:C:73:GLN:HA	3:C:73:GLN:OE1	2.15	0.45
3:C:148:ARG:N	3:C:151:GLN:HG3	2.31	0.45
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.30	0.45
5:E:17:ARG:O	5:E:20:LYS:HB2	2.17	0.45
5:E:56:LYS:HB2	5:E:57:MET:HE3	1.97	0.45
2:B:757:PRO:O	2:B:758:PHE:HB2	2.17	0.45
3:C:213:PRO:HG2	3:C:214:ASN:H	1.80	0.45
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.84	0.45
1:A:1191:TRP:HH2	9:I:25:LEU:HD13	1.81	0.45
1:A:765:VAL:HG23	1:A:802:ASN:O	2.16	0.45
1:A:929:LEU:HD13	1:A:929:LEU:O	2.16	0.45
2:B:809:MET:HE1	2:B:814:PHE:CD2	2.52	0.45
8:H:42:ILE:O	8:H:44:VAL:HG23	2.16	0.45
1:A:218:ASP:HA	1:A:221:SER:OG	2.16	0.45
5:E:56:LYS:HB2	5:E:57:MET:CE	2.47	0.45
1:A:705:LYS:HD2	1:A:708:MET:HE2	1.97	0.45
1:A:830:LYS:HE2	1:A:1081:LEU:CB	2.46	0.45
1:A:207:ILE:HA	1:A:210:ILE:CD1	2.46	0.45
2:B:1224:PHE:HZ	5:E:174:GLN:NE2	2.15	0.45
1:A:639:PRO:HG2	1:A:640:GLN:N	2.32	0.45
1:A:431:LYS:HB2	1:A:431:LYS:HE3	1.75	0.45
1:A:443:LEU:HA	1:A:443:LEU:HD23	1.78	0.45
1:A:567:LYS:HD3	8:H:95:TYR:CB	2.47	0.45
7:G:1:MET:HE2	7:G:3:PHE:CE1	2.52	0.45
1:A:1265:ASN:C	1:A:1267:MET:H	2.20	0.45
1:A:755:PHE:O	1:A:757:ASN:N	2.50	0.45
5:E:159:ASP:CG	5:E:162:ARG:HH22	2.20	0.45
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.46	0.45
5:E:94:LYS:O	5:E:98:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:O	1:A:291:GLU:HB2	2.17	0.45
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.80	0.45
5:E:92:THR:O	5:E:95:THR:HB	2.17	0.45
1:A:174:ILE:HG22	1:A:175:ARG:N	2.32	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.17	0.45
14:N:4:DA:H2"	14:N:5:DG:C8	2.52	0.45
2:B:508:LEU:HD12	2:B:508:LEU:H	1.80	0.45
2:B:170:LEU:HA	2:B:171:PRO:HD2	1.89	0.45
3:C:11:ARG:NE	3:C:21:ILE:HD11	2.28	0.45
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.98	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
2:B:446:LEU:O	2:B:447:ALA:HB3	2.17	0.45
11:K:18:LYS:HZ2	11:K:38:GLU:CG	2.30	0.45
2:B:865:LYS:C	2:B:866:TYR:HD1	2.20	0.45
1:A:310:GLY:C	1:A:312:PRO:HD2	2.38	0.45
1:A:418:SER:C	1:A:420:ARG:N	2.70	0.45
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.80	0.45
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.80	0.45
11:K:31:VAL:HG12	11:K:32:VAL:N	2.32	0.45
1:A:1230:GLU:O	1:A:1232:ASN:N	2.50	0.45
2:B:282:ILE:HG13	2:B:283:VAL:N	2.32	0.45
2:B:563:MET:CE	2:B:580:VAL:HB	2.47	0.45
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.81	0.45
1:A:57:ARG:O	1:A:68:GLN:HG2	2.17	0.45
1:A:488:ASN:N	1:A:488:ASN:OD1	2.50	0.45
2:B:1181:GLU:HG2	2:B:1188:LYS:HD3	1.99	0.45
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.81	0.45
5:E:17:ARG:O	5:E:21:GLU:HG3	2.17	0.45
8:H:82:PRO:C	8:H:84:ALA:H	2.17	0.45
2:B:209:GLU:CD	2:B:485:ARG:HE	2.18	0.45
2:B:515:HIS:O	2:B:518:HIS:HB2	2.17	0.45
1:A:559:VAL:O	1:A:560:ILE:C	2.55	0.45
3:C:260:LEU:O	3:C:264:GLN:HG3	2.17	0.45
1:A:115:LEU:O	1:A:122:MET:HG2	2.17	0.45
1:A:737:LEU:HB2	1:A:744:LYS:HD2	1.99	0.45
5:E:82:PHE:N	5:E:82:PHE:CD1	2.84	0.45
2:B:254:LEU:CD2	2:B:381:MET:HE3	2.46	0.44
2:B:891:ASP:C	2:B:893:LEU:N	2.70	0.44
1:A:61:ILE:HG22	1:A:62:ASP:N	2.32	0.44
7:G:74:TYR:CD2	7:G:74:TYR:N	2.85	0.44
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:O	1:A:428:TYR:C	2.54	0.44
6:F:77:ASP:C	6:F:79:ARG:H	2.21	0.44
1:A:1006:ILE:CD1	5:E:164:LEU:HA	2.48	0.44
2:B:755:ILE:CG2	2:B:755:ILE:O	2.65	0.44
1:A:471:ASN:OD1	1:A:472:LEU:N	2.49	0.44
3:C:84:ARG:HG3	3:C:85:ASP:N	2.33	0.44
5:E:102:GLU:O	5:E:104:ASN:N	2.50	0.44
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.52	0.44
3:C:45:ALA:HB3	3:C:170:TRP:NE1	2.32	0.44
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.16	0.44
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.77	0.44
2:B:510:LYS:HG3	2:B:511:PRO:CG	2.44	0.44
2:B:589:VAL:CG1	2:B:590:HIS:N	2.80	0.44
9:I:5:ARG:HD2	9:I:36:GLU:OE2	2.18	0.44
9:I:87:GLN:NE2	9:I:97:MET:HG2	2.32	0.44
3:C:66:ARG:O	3:C:69:LEU:N	2.51	0.44
3:C:147:LEU:HD12	3:C:151:GLN:O	2.17	0.44
12:L:55:ILE:HG12	12:L:56:LEU:N	2.31	0.44
2:B:215:GLN:OE1	2:B:479:VAL:HG22	2.17	0.44
11:K:89:ASN:O	11:K:92:ASN:N	2.51	0.44
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.52	0.44
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.44
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.99	0.44
1:A:1164:PRO:O	1:A:1167:GLU:HG2	2.18	0.44
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.37	0.44
2:B:892:LYS:O	2:B:899:ILE:HG12	2.17	0.44
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.47	0.44
2:B:1174:LYS:O	2:B:1176:ASN:N	2.50	0.44
2:B:703:ILE:HA	2:B:740:HIS:O	2.17	0.44
1:A:1158:PRO:C	1:A:1159:ARG:HG2	2.37	0.44
1:A:255:SER:OG	2:B:918:ILE:CG2	2.65	0.44
2:B:243:ALA:HA	2:B:250:PHE:O	2.18	0.44
13:T:22:DG:N9	13:T:23:DT:H72	2.31	0.44
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.99	0.44
1:A:1332:PHE:CE1	1:A:1381:LEU:HD13	2.51	0.44
1:A:1001:ARG:HD2	6:F:81:THR:O	2.17	0.44
3:C:260:LEU:HD21	3:C:264:GLN:NE2	2.32	0.44
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.33	0.44
8:H:135:LEU:HB3	8:H:137:GLN:H	1.83	0.44
8:H:5:LEU:HD13	8:H:135:LEU:H	1.82	0.44
8:H:27:GLU:CG	8:H:39:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HD2	9:I:97:MET:HG3	1.99	0.44
3:C:148:ARG:CG	3:C:149:LYS:H	2.30	0.44
1:A:466:SER:HB2	2:B:1099:VAL:CG1	2.43	0.44
7:G:51:TYR:HD2	7:G:51:TYR:O	1.99	0.44
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.53	0.44
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.99	0.44
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.47	0.44
1:A:22:PHE:HB2	2:B:1211:ASN:HD21	1.81	0.44
7:G:128:PRO:O	7:G:138:THR:HG23	2.18	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.98	0.44
2:B:225:VAL:HA	2:B:237:VAL:O	2.16	0.44
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.83	0.44
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.53	0.44
5:E:102:GLU:C	5:E:104:ASN:H	2.21	0.44
5:E:52:ARG:HA	5:E:53:PRO:HD2	1.63	0.44
1:A:32:VAL:HG21	1:A:80:HIS:HB3	2.00	0.44
1:A:1444:MET:CG	7:G:58:ARG:HB3	2.48	0.44
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.16	0.44
2:B:110:HIS:CB	12:L:54:ARG:NH2	2.75	0.44
2:B:101:MET:HG2	2:B:110:HIS:O	2.18	0.44
2:B:884:ARG:O	2:B:936:ASP:CB	2.54	0.44
2:B:889:THR:HG22	2:B:891:ASP:N	2.32	0.44
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	2.00	0.44
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.82	0.44
5:E:78:LEU:HD11	5:E:109:ILE:CG1	2.42	0.44
3:C:88:CYS:O	3:C:90:ASP:N	2.51	0.44
2:B:557:PHE:HD2	2:B:557:PHE:C	2.21	0.44
9:I:64:SER:O	9:I:66:PRO:HD3	2.17	0.44
1:A:845:LEU:O	1:A:846:GLU:C	2.55	0.44
1:A:418:SER:O	1:A:420:ARG:N	2.50	0.44
1:A:347:PHE:H	2:B:1107:ALA:HA	1.83	0.44
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.53	0.44
2:B:289:LEU:HD21	2:B:356:LEU:HD22	1.99	0.44
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.44
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.33	0.44
3:C:238:ILE:HA	3:C:239:PRO:HD3	1.83	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.33	0.44
1:A:589:GLN:HA	1:A:605:MET:O	2.18	0.44
8:H:12:VAL:HG13	8:H:26:ILE:HG12	2.00	0.44
1:A:1120:LEU:CD1	1:A:1120:LEU:N	2.80	0.44
1:A:560:ILE:HD11	8:H:78:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HG3	7:G:59:GLY:O	2.18	0.44
3:C:219:PHE:CD2	8:H:45:GLU:HG2	2.53	0.44
2:B:104:GLU:OE2	12:L:54:ARG:NE	2.48	0.44
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.45	0.44
3:C:236:GLY:O	3:C:238:ILE:N	2.50	0.44
1:A:827:THR:HG22	1:A:828:ALA:N	2.33	0.44
1:A:225:ASN:HD22	1:A:227:VAL:N	2.16	0.44
1:A:1143:LEU:HB2	1:A:1271:ILE:CG2	2.47	0.44
2:B:365:THR:HG21	2:B:370:PHE:HD1	1.83	0.44
1:A:374:LEU:O	1:A:436:ILE:HG12	2.18	0.44
1:A:1059:HIS:O	1:A:1060:PRO:C	2.53	0.44
1:A:476:SER:O	1:A:479:ASN:N	2.50	0.44
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.99	0.44
11:K:70:ARG:NH1	11:K:70:ARG:HG2	2.32	0.44
1:A:379:VAL:HG22	1:A:431:LYS:HG3	1.99	0.44
1:A:1176:LEU:HD13	1:A:1176:LEU:O	2.18	0.44
2:B:294:ASP:C	2:B:296:GLU:N	2.70	0.44
12:L:55:ILE:HG12	12:L:56:LEU:H	1.82	0.44
9:I:75:CYS:HB2	9:I:76:PRO:CD	2.48	0.44
1:A:90:VAL:HG13	1:A:297:GLN:HB2	2.00	0.44
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.99	0.44
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.53	0.44
5:E:140:LEU:CD1	5:E:140:LEU:N	2.80	0.44
7:G:138:THR:O	7:G:139:ILE:C	2.55	0.44
1:A:1215:ARG:CG	1:A:1215:ARG:HH11	2.30	0.44
1:A:335:ARG:CZ	2:B:1202:LEU:HD13	2.48	0.44
1:A:1203:ASN:O	1:A:1206:ASP:N	2.50	0.44
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.53	0.44
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.82	0.44
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.00	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.30	0.44
1:A:618:GLU:OE1	1:A:620:LYS:HG3	2.18	0.44
5:E:213:ILE:HG12	5:E:214:CYS:N	2.33	0.44
4:D:180:LEU:HA	4:D:180:LEU:HD23	1.79	0.44
2:B:360:PHE:CE1	2:B:361:LEU:HD13	2.53	0.44
2:B:569:TYR:O	2:B:570:VAL:HG13	2.17	0.44
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.56	0.44
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.53	0.44
1:A:65:LEU:O	1:A:66:LYS:C	2.56	0.44
1:A:64:ASN:O	1:A:66:LYS:N	2.51	0.44
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:HB	5:E:120:ALA:N	2.32	0.44
2:B:362:PRO:C	2:B:363:HIS:O	2.55	0.44
8:H:61:SER:HB3	8:H:139:ASN:HB3	1.99	0.44
11:K:39:ASP:HB2	11:K:40:HIS:H	1.68	0.44
1:A:1203:ASN:O	1:A:1204:ASP:C	2.57	0.44
1:A:281:HIS:C	1:A:282:ASN:HD22	2.22	0.44
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.18	0.44
6:F:82:THR:HA	6:F:83:PRO:HD3	1.83	0.44
1:A:843:LYS:NZ	1:A:1401:SER:OG	2.49	0.44
2:B:638:PHE:HD2	2:B:690:VAL:HG23	1.83	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.43
3:C:238:ILE:CD1	3:C:246:ARG:HD2	2.47	0.43
12:L:39:SER:O	12:L:40:LEU:HD23	2.19	0.43
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.48	0.43
2:B:649:LYS:O	2:B:650:GLU:HB2	2.18	0.43
7:G:11:ILE:HD13	7:G:29:LYS:HB3	2.00	0.43
2:B:549:THR:HB	2:B:628:THR:OG1	2.18	0.43
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.48	0.43
2:B:363:HIS:O	2:B:364:ILE:CB	2.65	0.43
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.99	0.43
6:F:128:LYS:HD2	6:F:149:GLU:HA	2.00	0.43
8:H:143:LEU:C	8:H:144:ILE:HG13	2.37	0.43
9:I:59:VAL:C	9:I:61:ASP:H	2.22	0.43
2:B:547:VAL:H	2:B:612:GLU:CD	2.20	0.43
13:T:22:DG:C8	13:T:23:DT:H72	2.53	0.43
2:B:792:MET:CE	13:T:24:DC:OP1	2.66	0.43
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.17	0.43
5:E:124:VAL:O	5:E:126:SER:N	2.48	0.43
1:A:1450:LEU:HD13	6:F:131:PRO:HG3	2.00	0.43
11:K:70:ARG:CG	11:K:70:ARG:HH11	2.29	0.43
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.99	0.43
10:J:22:LEU:HD12	10:J:22:LEU:HA	1.77	0.43
8:H:135:LEU:HD13	8:H:137:GLN:CB	2.36	0.43
2:B:577:ALA:CA	2:B:589:VAL:HG11	2.48	0.43
8:H:40:LEU:CD2	8:H:142:LEU:HD21	2.48	0.43
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.96	0.43
2:B:918:ILE:CG2	2:B:935:ARG:NH2	2.81	0.43
3:C:259:LEU:CD1	11:K:88:LYS:HG2	2.48	0.43
1:A:326:ARG:NH1	1:A:330:LYS:HE3	2.32	0.43
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.53	0.43
1:A:282:ASN:O	1:A:284:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:ASP:O	3:C:227:THR:CB	2.67	0.43
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.48	0.43
2:B:378:LEU:HD12	2:B:378:LEU:O	2.18	0.43
2:B:192:LEU:O	2:B:193:LYS:HB2	2.18	0.43
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.33	0.43
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.37	0.43
1:A:975:HIS:CD2	1:A:975:HIS:N	2.85	0.43
1:A:1187:GLN:CG	1:A:1188:GLN:N	2.82	0.43
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.18	0.43
1:A:113:LEU:HG	1:A:218:ASP:CG	2.38	0.43
10:J:27:GLU:C	10:J:29:GLU:N	2.66	0.43
2:B:174:LEU:HD21	2:B:204:ILE:HD11	2.01	0.43
2:B:984:HIS:CD2	2:B:1025:HIS:CA	2.99	0.43
6:F:81:THR:HB	6:F:82:THR:H	1.62	0.43
2:B:225:VAL:HG12	2:B:238:ALA:CA	2.48	0.43
1:A:1389:PHE:CG	1:A:1390:ASN:N	2.87	0.43
2:B:504:ARG:HG3	2:B:505:ASP:N	2.21	0.43
2:B:360:PHE:CE2	2:B:361:LEU:HD22	2.54	0.43
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.53	0.43
1:A:741:ASN:HD22	1:A:741:ASN:C	2.20	0.43
3:C:44:LEU:HD22	3:C:129:ILE:HG23	2.00	0.43
10:J:50:ILE:HD13	10:J:50:ILE:HA	1.88	0.43
2:B:313:MET:HE2	2:B:390:LEU:HD21	2.00	0.43
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.18	0.43
2:B:566:LEU:O	2:B:567:GLU:C	2.56	0.43
1:A:549:MET:CE	1:A:577:ILE:HD11	2.49	0.43
8:H:89:LEU:C	8:H:91:ASP:N	2.66	0.43
1:A:326:ARG:NH1	1:A:330:LYS:HZ1	2.13	0.43
2:B:43:LEU:HD23	2:B:43:LEU:HA	1.83	0.43
2:B:616:ILE:HD12	2:B:616:ILE:H	1.81	0.43
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.80	0.43
8:H:50:ALA:O	8:H:53:ASP:OD1	2.35	0.43
5:E:163:GLU:O	5:E:166:LYS:N	2.50	0.43
1:A:485:ASP:OD1	15:P:10:G:H4'	2.18	0.43
1:A:116:ASP:HB2	1:A:118:HIS:H	1.83	0.43
1:A:184:SER:OG	1:A:184:SER:O	2.36	0.43
2:B:297:ILE:C	2:B:299:GLU:N	2.70	0.43
3:C:11:ARG:HE	3:C:21:ILE:CD1	2.27	0.43
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.49	0.43
2:B:830:TYR:O	2:B:832:GLY:N	2.52	0.43
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ALA:CA	8:H:87:ARG:HD2	2.48	0.43
8:H:87:ARG:O	8:H:89:LEU:HG	2.19	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.43
7:G:146:LYS:HD3	7:G:148:GLU:OE2	2.17	0.43
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.48	0.43
3:C:252:GLN:HG3	11:K:95:ILE:HG23	2.00	0.43
7:G:64:THR:HG22	7:G:65:ASP:N	2.34	0.43
10:J:1:MET:H3	10:J:56:LEU:H	1.64	0.43
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.19	0.43
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.17	0.43
5:E:212:ARG:CG	5:E:212:ARG:NH1	2.77	0.43
1:A:742:ASN:HA	1:A:745:GLN:HB2	2.00	0.43
12:L:53:HIS:C	12:L:55:ILE:HD13	2.38	0.43
2:B:313:MET:CE	2:B:390:LEU:HD21	2.49	0.43
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.53	0.43
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.53	0.43
2:B:975:GLN:HG2	2:B:976:ILE:N	2.33	0.43
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.49	0.43
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.02	0.43
1:A:930:ASP:O	1:A:931:GLU:C	2.57	0.43
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.47	0.43
2:B:885:MET:C	2:B:886:LYS:HG2	2.39	0.43
2:B:889:THR:O	2:B:910:VAL:HG23	2.19	0.43
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.34	0.43
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.83	0.43
1:A:574:GLY:O	1:A:575:LYS:C	2.56	0.43
1:A:143:LYS:HG3	1:A:144:THR:N	2.34	0.43
1:A:1142:THR:HG22	1:A:1271:ILE:O	2.19	0.43
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	2.00	0.43
11:K:89:ASN:C	11:K:91:CYS:N	2.72	0.43
2:B:432:MET:C	2:B:434:ARG:H	2.22	0.43
1:A:974:ASP:C	1:A:976:THR:N	2.69	0.43
11:K:17:SER:O	11:K:18:LYS:C	2.57	0.43
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	2.00	0.43
1:A:1280:GLU:O	1:A:1281:ARG:O	2.36	0.43
1:A:608:ILE:CD1	1:A:613:ILE:HD12	2.48	0.43
2:B:840:ILE:HG21	2:B:994:TYR:HD1	1.84	0.43
2:B:258:LEU:CG	2:B:258:LEU:O	2.65	0.43
1:A:1053:PHE:O	1:A:1056:SER:N	2.48	0.43
2:B:383:ASN:C	2:B:387:LEU:HD13	2.39	0.43
1:A:568:PRO:CG	8:H:46:LEU:HD22	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:VAL:HA	1:A:1113:THR:OG1	2.18	0.43
3:C:69:LEU:O	10:J:6:ARG:HD2	2.17	0.43
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.49	0.43
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.48	0.43
2:B:703:ILE:HG22	2:B:704:ALA:N	2.34	0.43
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.49	0.43
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.34	0.43
3:C:124:LEU:O	3:C:126:GLY:N	2.51	0.43
11:K:94:ILE:O	11:K:98:LEU:HG	2.19	0.43
2:B:1095:LEU:C	2:B:1096:ARG:O	2.55	0.43
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.99	0.43
5:E:42:PHE:HZ	5:E:58:MET:CE	2.32	0.43
11:K:35:PHE:N	11:K:35:PHE:CD1	2.86	0.43
1:A:469:ARG:NH2	2:B:991:GLY:O	2.50	0.43
5:E:164:LEU:HD21	5:E:211:TYR:CG	2.54	0.43
7:G:145:VAL:CG1	7:G:146:LYS:N	2.82	0.43
5:E:100:ILE:HG12	5:E:105:PHE:CD1	2.53	0.43
1:A:478:TYR:O	1:A:479:ASN:HB3	2.18	0.43
2:B:1022:THR:HG23	2:B:1022:THR:O	2.19	0.43
2:B:247:GLY:HA2	2:B:418:LYS:NZ	2.34	0.43
1:A:387:ARG:O	1:A:390:GLN:HB3	2.19	0.43
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.82	0.43
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.01	0.43
8:H:94:ASP:N	8:H:94:ASP:OD1	2.51	0.43
2:B:763:GLN:O	2:B:764:SER:C	2.57	0.43
3:C:144:ILE:O	3:C:145:CYS:CB	2.67	0.43
2:B:172:ILE:CG2	2:B:173:MET:N	2.82	0.43
2:B:313:MET:HE2	2:B:390:LEU:HD11	2.01	0.43
1:A:427:GLN:O	1:A:430:TRP:HB2	2.18	0.43
2:B:1187:ASN:HB3	2:B:1188:LYS:H	1.52	0.43
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.00	0.43
2:B:250:PHE:HE1	2:B:359:GLU:OE1	2.02	0.43
8:H:82:PRO:C	8:H:84:ALA:N	2.71	0.43
1:A:701:LEU:N	1:A:701:LEU:HD23	2.34	0.43
1:A:1079:MET:HE1	1:A:1359:ASP:HB2	2.00	0.43
3:C:204:SER:C	3:C:206:ASN:N	2.72	0.43
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.34	0.43
8:H:95:TYR:CE2	8:H:97:MET:CG	3.02	0.43
5:E:26:ARG:NH2	5:E:133:GLU:OE2	2.52	0.43
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.34	0.43
10:J:64:ASN:CB	10:J:65:PRO:CD	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:NH1	1:A:488:ASN:HD21	1.98	0.43
7:G:119:LEU:HD13	7:G:132:SER:HB2	2.00	0.43
1:A:1279:ILE:CD1	1:A:1312:ASN:HB3	2.49	0.43
2:B:244:LEU:O	2:B:246:LYS:N	2.52	0.43
2:B:436:VAL:C	2:B:437:GLU:HG3	2.39	0.43
4:D:170:THR:CB	4:D:172:LEU:HG	2.48	0.43
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.49	0.43
1:A:842:VAL:O	1:A:843:LYS:C	2.57	0.43
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.82	0.43
1:A:100:LYS:HB3	1:A:100:LYS:HE3	1.86	0.43
1:A:648:ASN:O	1:A:649:ILE:C	2.56	0.43
1:A:877:HIS:C	1:A:878:ILE:HG13	2.38	0.42
9:I:69:PRO:HB2	9:I:85:PHE:CZ	2.53	0.42
1:A:710:LEU:HD22	9:I:96:SER:CB	2.49	0.42
2:B:186:GLU:O	2:B:189:LEU:N	2.52	0.42
2:B:787:VAL:O	2:B:787:VAL:HG12	2.19	0.42
7:G:53:ASN:N	7:G:53:ASN:ND2	2.61	0.42
2:B:54:PHE:HA	2:B:58:THR:HB	2.01	0.42
2:B:778:MET:HE1	2:B:853:SER:HB3	2.01	0.42
1:A:1313:LEU:HD12	1:A:1313:LEU:HA	1.86	0.42
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.32	0.42
2:B:990:ILE:HG22	2:B:992:ILE:H	1.83	0.42
1:A:207:ILE:HA	1:A:210:ILE:HD12	2.01	0.42
2:B:1157:ALA:H	2:B:1197:PRO:HA	1.84	0.42
3:C:37:MET:HE3	3:C:176:ILE:HD13	2.01	0.42
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.42
2:B:1053:GLU:O	2:B:1057:LYS:HG3	2.20	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.42
2:B:1071:VAL:HG22	2:B:1084:GLN:HG3	2.01	0.42
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.18	0.42
2:B:25:ILE:HD11	2:B:653:VAL:C	2.39	0.42
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.54	0.42
2:B:604:ARG:O	2:B:607:GLY:N	2.52	0.42
3:C:238:ILE:HD11	3:C:246:ARG:NE	2.32	0.42
2:B:918:ILE:HG21	2:B:935:ARG:CZ	2.48	0.42
1:A:755:PHE:O	1:A:756:ILE:C	2.56	0.42
1:A:577:ILE:HA	1:A:580:VAL:HG23	2.01	0.42
2:B:429:PHE:HA	2:B:432:MET:HE2	2.00	0.42
2:B:52:ASN:O	2:B:53:GLN:C	2.57	0.42
2:B:255:GLN:CB	2:B:272:THR:HB	2.48	0.42
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:O	1:A:202:LEU:HG	2.19	0.42
4:D:166:LEU:HD23	4:D:214:LEU:CD2	2.49	0.42
2:B:295:GLY:CA	9:I:6:PHE:CE2	3.02	0.42
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.55	0.42
2:B:882:THR:HG22	2:B:883:LEU:H	1.80	0.42
2:B:659:ALA:HA	2:B:662:MET:CE	2.48	0.42
8:H:96:VAL:HA	8:H:142:LEU:O	2.19	0.42
1:A:55:ASP:CG	1:A:55:ASP:O	2.56	0.42
3:C:166:GLU:CG	11:K:10:PHE:CZ	2.92	0.42
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.84	0.42
1:A:167:CYS:O	1:A:168:GLY:C	2.58	0.42
9:I:103:CYS:SG	9:I:106:CYS:SG	3.18	0.42
4:D:117:GLU:O	4:D:118:THR:HB	2.19	0.42
5:E:90:VAL:HA	5:E:120:ALA:CB	2.48	0.42
7:G:30:LEU:HD22	7:G:72:VAL:HG11	2.00	0.42
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.54	0.42
8:H:116:TYR:CE2	8:H:140:ALA:CB	3.02	0.42
2:B:707:PRO:CG	2:B:708:GLU:N	2.81	0.42
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.85	0.42
4:D:68:ARG:HB3	4:D:72:ARG:HH21	1.85	0.42
1:A:1353:TYR:HD1	1:A:1368:MET:HE3	1.84	0.42
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.84	0.42
3:C:215:GLU:O	3:C:216:GLY:C	2.57	0.42
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.19	0.42
2:B:957:ASN:O	2:B:960:GLY:N	2.51	0.42
2:B:1072:MET:HE2	2:B:1087:PHE:CD1	2.37	0.42
1:A:709:THR:HG22	1:A:710:LEU:N	2.34	0.42
3:C:238:ILE:HG12	3:C:239:PRO:HD2	2.02	0.42
7:G:137:ILE:HG23	7:G:143:ILE:HD11	2.00	0.42
2:B:333:PHE:C	2:B:334:ILE:HG12	2.39	0.42
1:A:984:LYS:O	1:A:988:LEU:HB2	2.19	0.42
7:G:1:MET:HG3	7:G:85:GLU:OE1	2.20	0.42
3:C:250:THR:O	3:C:253:LYS:N	2.52	0.42
8:H:82:PRO:O	8:H:83:GLN:HB2	2.19	0.42
2:B:53:GLN:HE21	2:B:57:TYR:HB2	1.83	0.42
2:B:1027:ILE:O	2:B:1028:GLU:C	2.57	0.42
2:B:44:VAL:O	2:B:45:SER:C	2.58	0.42
2:B:1033:LYS:CE	2:B:1070:GLU:OE1	2.67	0.42
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.34	0.42
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.33	0.42
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:C	5:E:99:HIS:ND1	2.72	0.42
4:D:32:GLU:HG2	7:G:42:PHE:HE2	1.84	0.42
1:A:318:SER:HB2	13:T:28:DA:N3	2.34	0.42
11:K:102:LYS:HB2	11:K:102:LYS:HE3	1.90	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.52	0.42
4:D:53:SER:O	4:D:56:ARG:HB3	2.20	0.42
5:E:74:ASP:O	5:E:76:GLY:N	2.53	0.42
1:A:730:GLY:O	1:A:733:ALA:N	2.51	0.42
1:A:770:VAL:C	1:A:772:GLY:N	2.72	0.42
1:A:117:GLU:H	1:A:117:GLU:CD	2.22	0.42
1:A:821:ARG:HG3	1:A:821:ARG:O	2.20	0.42
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.36	0.42
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.35	0.42
12:L:54:ARG:HG3	12:L:54:ARG:NH1	2.34	0.42
2:B:885:MET:O	2:B:886:LYS:HG2	2.20	0.42
8:H:40:LEU:HD13	8:H:123:MET:CE	2.50	0.42
3:C:39:ALA:C	3:C:164:ALA:HB3	2.40	0.42
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.20	0.42
1:A:1170:ILE:CD1	1:A:1170:ILE:H	2.18	0.42
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.48	0.42
2:B:640:VAL:CG1	2:B:649:LYS:HG2	2.49	0.42
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.19	0.42
10:J:8:PHE:H	10:J:49:MET:CE	2.30	0.42
12:L:27:LEU:HD13	12:L:37:LYS:CE	2.49	0.42
2:B:225:VAL:HG12	2:B:238:ALA:CB	2.49	0.42
1:A:652:VAL:HG12	1:A:653:VAL:N	2.35	0.42
2:B:371:GLU:N	2:B:371:GLU:OE1	2.51	0.42
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.86	0.42
1:A:932:GLU:HG2	1:A:933:TYR:N	2.34	0.42
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.54	0.42
7:G:73:LYS:HD2	7:G:74:TYR:O	2.20	0.42
2:B:128:LEU:HD11	2:B:170:LEU:H	1.83	0.42
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.58	0.42
2:B:1004:GLU:OE2	2:B:1064:TYR:CE2	2.73	0.42
11:K:37:LYS:O	11:K:38:GLU:CG	2.63	0.42
6:F:101:ILE:HD13	6:F:120:ILE:HG22	2.01	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.54	0.42
2:B:840:ILE:HG21	2:B:994:TYR:CD1	2.55	0.42
9:I:25:LEU:HG	9:I:38:ALA:HB2	2.02	0.42
6:F:84:TYR:CE2	6:F:152:ILE:HG21	2.54	0.42
1:A:770:VAL:C	1:A:772:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HA	1:A:123:ARG:HH21	1.84	0.42
1:A:88:LYS:HB3	1:A:293:GLU:OE2	2.20	0.42
2:B:803:LEU:HD12	2:B:1032:SER:HB3	2.01	0.42
2:B:295:GLY:HA3	9:I:6:PHE:CE2	2.55	0.42
2:B:882:THR:O	2:B:883:LEU:HB2	2.19	0.42
1:A:567:LYS:HE2	8:H:95:TYR:CE2	2.55	0.42
1:A:70:CYS:HA	2:B:1174:LYS:HG2	2.01	0.42
1:A:73:GLY:O	1:A:75:ASN:N	2.53	0.42
5:E:177:ARG:C	5:E:212:ARG:HD3	2.40	0.42
1:A:1313:LEU:O	1:A:1314:SER:C	2.58	0.42
3:C:124:LEU:C	3:C:126:GLY:N	2.73	0.42
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.55	0.42
11:K:18:LYS:HZ3	11:K:38:GLU:HG2	1.82	0.42
3:C:35:ARG:HD3	11:K:41:THR:OG1	2.18	0.42
1:A:1127:ASP:O	1:A:1128:GLN:C	2.57	0.42
2:B:516:ASN:ND2	2:B:516:ASN:H	2.17	0.42
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.02	0.42
4:D:122:GLU:HA	4:D:125:SER:OG	2.19	0.42
7:G:1:MET:HE1	7:G:2:PHE:CA	2.50	0.42
2:B:807:ARG:O	2:B:810:GLU:HB3	2.19	0.42
1:A:1277:GLU:C	1:A:1279:ILE:N	2.73	0.42
2:B:1183:LYS:HG3	2:B:1183:LYS:H	1.69	0.42
1:A:591:PHE:CD2	1:A:595:THR:HB	2.52	0.42
6:F:77:ASP:O	6:F:78:GLN:CB	2.57	0.42
1:A:1215:ARG:O	1:A:1219:THR:N	2.52	0.42
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.82	0.42
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.19	0.42
2:B:465:ASN:HD22	2:B:465:ASN:N	2.17	0.42
4:D:176:GLU:O	4:D:178:ALA:N	2.53	0.42
1:A:171:GLN:HA	1:A:172:PRO:HD2	1.89	0.42
2:B:51:PHE:O	2:B:54:PHE:HB3	2.20	0.42
3:C:3:GLU:CG	3:C:4:GLU:HG3	2.47	0.42
1:A:886:ILE:HG12	1:A:943:LEU:HD12	2.02	0.42
9:I:44:TYR:CD1	9:I:45:ARG:N	2.88	0.42
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.43	0.42
2:B:408:LEU:N	2:B:408:LEU:CD1	2.83	0.42
1:A:1433:MET:HE1	7:G:63:PRO:HB3	2.00	0.42
1:A:699:ALA:CB	1:A:701:LEU:HG	2.49	0.42
5:E:7:ARG:O	5:E:10:SER:HB3	2.19	0.42
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.50	0.42
1:A:1353:TYR:HD1	1:A:1368:MET:CE	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:PHE:CD1	1:A:1332:PHE:C	2.93	0.42
2:B:1020:ARG:O	2:B:1021:MET:C	2.57	0.42
1:A:586:ILE:HD12	1:A:633:VAL:HG22	2.01	0.42
3:C:12:GLU:O	3:C:13:ALA:HB2	2.18	0.42
2:B:40:GLU:OE1	2:B:682:SER:HB2	2.20	0.42
1:A:666:ILE:O	1:A:668:ASP:N	2.53	0.42
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.85	0.42
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.50	0.42
2:B:641:GLU:C	2:B:643:ASP:H	2.22	0.42
1:A:255:SER:OG	2:B:918:ILE:HD13	2.19	0.42
2:B:1182:CYS:HB3	2:B:1187:ASN:HB2	2.00	0.42
1:A:595:THR:C	1:A:596:THR:HG23	2.40	0.42
5:E:69:ILE:HG13	5:E:69:ILE:H	1.50	0.42
5:E:35:VAL:C	5:E:37:LEU:H	2.23	0.42
11:K:54:ARG:C	11:K:56:VAL:H	2.21	0.42
2:B:423:LYS:C	2:B:423:LYS:HD3	2.40	0.42
1:A:514:PRO:O	1:A:515:GLN:C	2.58	0.42
1:A:795:GLU:HG2	2:B:731:VAL:CG2	2.50	0.42
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.85	0.42
3:C:33:LEU:HD12	3:C:37:MET:HE2	2.01	0.42
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.20	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA2	2.01	0.42
1:A:106:VAL:HG13	1:A:112:LYS:N	2.34	0.42
1:A:164:ARG:HG3	1:A:165:GLY:O	2.19	0.42
3:C:15:LYS:HG2	3:C:16:ASP:OD1	2.20	0.42
2:B:1058:LEU:HA	2:B:1058:LEU:HD23	1.88	0.42
8:H:3:ASN:HB3	8:H:4:THR:H	1.70	0.41
2:B:763:GLN:HG2	2:B:765:PRO:CG	2.49	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.38	0.41
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.85	0.41
3:C:113:VAL:HG23	3:C:147:LEU:HD21	2.02	0.41
4:D:122:GLU:O	4:D:124:GLU:N	2.53	0.41
1:A:679:ILE:HG12	1:A:732:LEU:CD1	2.42	0.41
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.41
8:H:92:ASP:C	8:H:93:TYR:CD1	2.94	0.41
1:A:79:GLY:CA	1:A:243:PRO:HG3	2.43	0.41
1:A:130:ASP:O	1:A:132:LYS:N	2.53	0.41
8:H:139:ASN:O	8:H:140:ALA:CB	2.58	0.41
1:A:1072:ILE:HD11	1:A:1368:MET:HA	2.01	0.41
1:A:416:ARG:HE	1:A:417:TYR:HE1	1.68	0.41
1:A:353:ILE:HD13	1:A:487:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD13	3:C:37:MET:HG3	2.01	0.41
4:D:64:VAL:HG12	4:D:65:GLU:N	2.34	0.41
5:E:144:ILE:HG13	5:E:145:THR:N	2.34	0.41
9:I:35:VAL:O	9:I:36:GLU:HB3	2.20	0.41
8:H:40:LEU:HD21	8:H:142:LEU:HD21	2.01	0.41
10:J:21:TYR:HA	10:J:39:LEU:HD11	2.02	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.19	0.41
2:B:172:ILE:H	2:B:172:ILE:HD12	1.81	0.41
9:I:84:VAL:O	9:I:84:VAL:HG13	2.20	0.41
2:B:640:VAL:O	2:B:641:GLU:O	2.38	0.41
3:C:124:LEU:HD12	3:C:124:LEU:H	1.85	0.41
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.55	0.41
7:G:126:ASN:HA	7:G:127:PRO:C	2.40	0.41
8:H:91:ASP:C	8:H:93:TYR:N	2.73	0.41
1:A:42:ASP:C	1:A:44:THR:N	2.73	0.41
2:B:249:ARG:NH1	2:B:418:LYS:HD2	2.35	0.41
3:C:249:ASP:HB2	11:K:102:LYS:HZ3	1.85	0.41
3:C:94:LYS:HE3	3:C:94:LYS:HB2	1.88	0.41
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.38	0.41
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.02	0.41
2:B:313:MET:SD	2:B:390:LEU:HD21	2.60	0.41
7:G:119:LEU:HD21	7:G:137:ILE:HD12	2.02	0.41
2:B:334:ILE:C	2:B:336:ARG:H	2.23	0.41
2:B:365:THR:HG1	2:B:367:LEU:HG	1.85	0.41
11:K:49:GLU:O	11:K:50:LEU:C	2.59	0.41
5:E:136:ASN:O	5:E:140:LEU:HD13	2.20	0.41
5:E:112:TYR:O	5:E:137:GLU:HG3	2.20	0.41
1:A:524:VAL:HG12	1:A:525:GLN:N	2.26	0.41
2:B:975:GLN:HE21	2:B:975:GLN:HB3	1.48	0.41
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.19	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.24	0.41
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.41
3:C:109:SER:O	3:C:110:THR:C	2.59	0.41
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.50	0.41
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.83	0.41
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.20	0.41
2:B:361:LEU:CD2	2:B:377:PHE:HD2	2.33	0.41
2:B:377:PHE:O	2:B:378:LEU:C	2.58	0.41
8:H:36:CYS:HB2	8:H:129:TYR:OH	2.20	0.41
5:E:177:ARG:HH11	5:E:215:MET:CE	2.33	0.41
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:LYS:O	12:L:29:TYR:HD2	2.03	0.41
4:D:118:THR:CB	4:D:121:LYS:HD2	2.50	0.41
2:B:605:ARG:NH1	2:B:639:ILE:HD13	2.34	0.41
5:E:31:THR:O	5:E:35:VAL:HG23	2.20	0.41
2:B:70:ILE:O	2:B:70:ILE:HG22	2.20	0.41
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.60	0.41
2:B:419:THR:O	2:B:423:LYS:HB2	2.20	0.41
2:B:905:VAL:HG23	2:B:941:LEU:HD22	2.02	0.41
1:A:1011:GLN:HE22	1:A:1015:VAL:CG2	2.33	0.41
1:A:1409:LEU:HD13	2:B:1207:LEU:CD1	2.47	0.41
13:T:25:DA:H1'	13:T:26:DT:C5'	2.50	0.41
1:A:414:ASP:O	1:A:416:ARG:N	2.53	0.41
4:D:32:GLU:O	4:D:33:PHE:CG	2.73	0.41
4:D:63:LEU:O	4:D:129:LEU:HD11	2.20	0.41
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.55	0.41
1:A:924:LYS:HB3	1:A:924:LYS:HE2	1.82	0.41
14:N:5:DG:H2"	14:N:6:DT:OP2	2.20	0.41
8:H:95:TYR:HE2	8:H:97:MET:CG	2.34	0.41
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.45	0.41
5:E:22:MET:CE	5:E:26:ARG:NE	2.68	0.41
6:F:103:MET:CE	7:G:66:GLY:N	2.72	0.41
4:D:48:ILE:HG21	7:G:4:ILE:HB	2.03	0.41
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.56	0.41
5:E:67:GLU:O	5:E:69:ILE:N	2.53	0.41
1:A:1168:GLU:O	1:A:1171:GLN:HG3	2.21	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.22	0.41
1:A:1139:GLU:OE2	1:A:1205:LYS:HE2	2.21	0.41
2:B:1224:PHE:CZ	5:E:171:LYS:HG2	2.56	0.41
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.50	0.41
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.33	0.41
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.20	0.41
8:H:20:TYR:HB3	8:H:23:VAL:O	2.20	0.41
5:E:198:ILE:N	5:E:198:ILE:HD12	2.35	0.41
3:C:76:ASP:O	3:C:79:GLN:HG2	2.20	0.41
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.34	0.41
1:A:143:LYS:HG3	1:A:144:THR:H	1.84	0.41
1:A:255:SER:O	1:A:256:GLN:HG3	2.21	0.41
2:B:412:LEU:CB	2:B:466:TRP:HE1	2.31	0.41
1:A:757:ASN:O	1:A:758:ILE:C	2.57	0.41
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.55	0.41
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.09	0.41
2:B:866:TYR:CD2	2:B:870:ILE:HB	2.55	0.41
6:F:70:LYS:H	6:F:72:LYS:CD	2.33	0.41
9:I:15:TYR:H	9:I:15:TYR:HD1	1.67	0.41
1:A:540:PHE:CE2	1:A:565:ILE:HD12	2.56	0.41
2:B:259:TYR:N	2:B:259:TYR:CD1	2.89	0.41
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.85	0.41
7:G:115:MET:C	7:G:164:LYS:HG3	2.41	0.41
1:A:320:ARG:CB	1:A:320:ARG:NH1	2.83	0.41
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.50	0.41
1:A:21:LEU:HD11	1:A:1414:ALA:HA	2.02	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
2:B:1169:MET:HE3	2:B:1201:LYS:HG2	2.02	0.41
1:A:49:LYS:NZ	1:A:60:SER:HA	2.36	0.41
1:A:69:THR:C	1:A:71:GLN:N	2.74	0.41
12:L:57:LEU:N	12:L:57:LEU:HD23	2.35	0.41
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.55	0.41
9:I:77:LYS:HZ1	9:I:77:LYS:HB3	1.82	0.41
1:A:1315:GLU:C	1:A:1317:MET:N	2.74	0.41
1:A:1157:ASP:C	1:A:1159:ARG:H	2.24	0.41
2:B:70:ILE:HD12	2:B:429:PHE:CZ	2.56	0.41
1:A:447:GLN:HA	1:A:448:PRO:C	2.41	0.41
1:A:746:MET:HE3	2:B:1018:PRO:HG2	2.02	0.41
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.82	0.41
1:A:795:GLU:HG2	2:B:731:VAL:HG22	2.03	0.41
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.84	0.41
3:C:89:GLU:O	3:C:90:ASP:CB	2.66	0.41
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.50	0.41
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.68	0.41
4:D:146:GLN:O	4:D:147:TYR:C	2.59	0.41
7:G:50:ASP:CG	7:G:50:ASP:O	2.58	0.41
1:A:1062:GLU:O	1:A:1064:VAL:N	2.54	0.41
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.99	0.41
2:B:34:ILE:HG12	2:B:542:MET:HE2	2.01	0.41
3:C:100:THR:HG22	3:C:101:LEU:N	2.35	0.41
2:B:955:THR:HG23	12:L:54:ARG:O	2.21	0.41
2:B:1175:LEU:CD2	2:B:1175:LEU:H	2.34	0.41
2:B:852:ARG:HH22	12:L:70:ARG:C	2.24	0.41
1:A:694:THR:O	1:A:698:GLN:HG3	2.20	0.41
5:E:186:LEU:O	5:E:187:TYR:C	2.58	0.41
2:B:167:ILE:O	2:B:453:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:CYS:HB2	9:I:76:PRO:HD2	2.03	0.41
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.51	0.41
4:D:220:LEU:CG	4:D:221:TYR:N	2.83	0.41
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.90	0.41
12:L:61:THR:HG21	12:L:63:ARG:CG	2.49	0.41
3:C:35:ARG:NH1	11:K:41:THR:H	2.18	0.41
4:D:195:ILE:O	4:D:195:ILE:HG22	2.20	0.41
2:B:770:GLN:CD	2:B:983:ARG:HA	2.41	0.41
5:E:101:GLN:HB2	5:E:101:GLN:HE21	1.59	0.41
11:K:107:THR:O	11:K:111:LEU:HG	2.21	0.41
1:A:1446:ASP:HB2	6:F:133:VAL:HG23	2.03	0.41
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.21	0.41
1:A:792:TYR:CD1	1:A:792:TYR:N	2.89	0.41
2:B:345:LYS:C	2:B:347:LYS:HG2	2.41	0.41
13:T:15:DA:H1'	13:T:16:DC:H5'	2.02	0.41
2:B:296:GLU:HA	2:B:299:GLU:HG3	2.03	0.41
2:B:881:ASN:HB2	2:B:933:SER:N	2.36	0.41
2:B:872:GLU:OE2	2:B:914:LYS:HE2	2.21	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.20	0.41
1:A:1111:MET:HE2	1:A:1114:PRO:HB3	2.03	0.41
2:B:114:PRO:O	2:B:117:ALA:N	2.53	0.41
12:L:56:LEU:C	12:L:57:LEU:HD23	2.41	0.41
2:B:125:SER:HA	2:B:172:ILE:HD12	2.03	0.41
2:B:51:PHE:HB2	2:B:173:MET:CE	2.51	0.41
5:E:116:ILE:HG22	5:E:117:THR:N	2.36	0.41
1:A:982:THR:HG22	1:A:983:ILE:N	2.36	0.41
4:D:54:GLU:O	4:D:58:VAL:HG23	2.21	0.41
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.21	0.41
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.02	0.41
1:A:1030:ARG:HG3	1:A:1034:GLU:CG	2.51	0.41
3:C:141:GLY:O	3:C:142:VAL:O	2.38	0.41
3:C:123:ASN:OD1	3:C:125:MET:N	2.52	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.21	0.41
11:K:85:ASP:O	11:K:88:LYS:N	2.54	0.41
1:A:541:ILE:HD13	1:A:549:MET:HE3	2.03	0.41
5:E:78:LEU:HG	5:E:79:TRP:N	2.36	0.41
5:E:190:LEU:HD21	5:E:196:VAL:CG2	2.51	0.41
1:A:1002:GLY:O	1:A:1008:GLN:NE2	2.45	0.41
3:C:179:GLU:CG	3:C:180:TYR:N	2.82	0.41
5:E:124:VAL:C	5:E:126:SER:N	2.74	0.41
7:G:9:LEU:CG	7:G:10:ASN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:O	1:A:470:LEU:HD12	2.20	0.41
1:A:526:ASP:O	1:A:527:THR:C	2.58	0.41
7:G:91:VAL:CG1	7:G:92:VAL:N	2.84	0.41
1:A:451:HIS:HB3	1:A:453:MET:N	2.36	0.41
11:K:51:LEU:HA	11:K:51:LEU:HD12	1.83	0.41
8:H:56:THR:HB	8:H:145:ARG:HG2	2.02	0.41
3:C:77:ILE:HD13	3:C:77:ILE:HA	1.74	0.41
4:D:120:GLU:HG2	4:D:120:GLU:O	2.20	0.41
6:F:96:THR:O	6:F:100:GLN:HG3	2.21	0.41
2:B:265:SER:O	2:B:266:ALA:HB3	2.21	0.41
2:B:652:LYS:CB	2:B:689:LEU:HD23	2.46	0.41
1:A:60:SER:O	1:A:61:ILE:HG13	2.21	0.41
10:J:36:LEU:O	10:J:39:LEU:N	2.54	0.41
12:L:41:SER:O	12:L:44:ASP:OD1	2.39	0.41
2:B:313:MET:CE	2:B:386:LEU:HB3	2.51	0.41
1:A:1239:ARG:HH11	1:A:1239:ARG:CB	2.34	0.41
7:G:113:HIS:C	7:G:114:LEU:HD12	2.41	0.41
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.21	0.41
9:I:58:VAL:HG12	9:I:58:VAL:O	2.22	0.41
11:K:18:LYS:O	11:K:35:PHE:HA	2.21	0.41
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.51	0.41
2:B:966:VAL:CG1	2:B:967:ARG:N	2.84	0.41
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.84	0.41
1:A:248:PRO:O	1:A:260:ASP:HB2	2.21	0.41
2:B:728:ARG:O	2:B:729:ILE:CG1	2.69	0.41
4:D:129:LEU:HD12	4:D:129:LEU:O	2.21	0.41
2:B:723:VAL:HG12	2:B:724:ASP:N	2.36	0.41
1:A:1422:ARG:HH21	2:B:1220:ARG:NH1	2.19	0.41
2:B:360:PHE:CD1	2:B:361:LEU:HD13	2.56	0.40
8:H:135:LEU:HD11	8:H:137:GLN:NE2	2.36	0.40
2:B:680:THR:OG1	2:B:681:TRP:N	2.54	0.40
2:B:883:LEU:O	2:B:885:MET:N	2.53	0.40
2:B:167:ILE:C	2:B:450:ALA:HB1	2.40	0.40
9:I:77:LYS:H	9:I:77:LYS:HD2	1.85	0.40
2:B:1103:ILE:O	2:B:1103:ILE:HG23	2.21	0.40
1:A:407:ARG:O	1:A:408:ASP:C	2.60	0.40
1:A:756:ILE:O	1:A:759:ALA:HB3	2.21	0.40
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.03	0.40
2:B:486:TYR:N	2:B:486:TYR:HD2	2.18	0.40
1:A:809:THR:O	1:A:811:GLN:N	2.55	0.40
3:C:208:GLU:C	3:C:210:GLU:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ASP:OD1	11:K:82:ASP:C	2.58	0.40
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.68	0.40
2:B:399:ASP:O	2:B:515:HIS:CD2	2.74	0.40
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.55	0.40
1:A:2:VAL:HG23	2:B:1157:ALA:C	2.41	0.40
3:C:161:LYS:O	3:C:170:TRP:NE1	2.54	0.40
2:B:784:ASN:O	2:B:785:TYR:C	2.59	0.40
2:B:27:ALA:O	2:B:30:SER:OG	2.34	0.40
7:G:12:THR:O	7:G:12:THR:HG22	2.20	0.40
2:B:508:LEU:HD12	2:B:508:LEU:N	2.36	0.40
2:B:297:ILE:C	2:B:299:GLU:H	2.24	0.40
2:B:296:GLU:HA	2:B:299:GLU:CG	2.51	0.40
3:C:236:GLY:O	3:C:237:SER:C	2.60	0.40
1:A:853:ASP:OD1	1:A:855:THR:CB	2.69	0.40
2:B:579:ARG:NH1	2:B:579:ARG:CG	2.83	0.40
2:B:579:ARG:CB	2:B:586:TRP:NE1	2.74	0.40
2:B:830:TYR:C	2:B:832:GLY:H	2.23	0.40
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.52	0.40
11:K:56:VAL:HG12	11:K:56:VAL:O	2.20	0.40
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.21	0.40
8:H:12:VAL:HG11	8:H:26:ILE:CD1	2.48	0.40
2:B:857:ARG:O	2:B:967:ARG:HA	2.21	0.40
1:A:1091:SER:HB3	1:A:1307:GLU:OE1	2.21	0.40
6:F:84:TYR:CD1	6:F:84:TYR:N	2.88	0.40
2:B:1197:PRO:O	2:B:1200:ALA:N	2.45	0.40
3:C:175:ALA:O	3:C:176:ILE:CG1	2.70	0.40
2:B:1112:GLN:HG3	15:P:2:A:OP1	2.21	0.40
6:F:114:GLU:OE2	6:F:114:GLU:HA	2.20	0.40
4:D:37:GLN:OE1	7:G:5:LYS:NZ	2.53	0.40
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.37	0.40
2:B:542:MET:CG	2:B:747:MET:HE3	2.51	0.40
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.51	0.40
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.39	0.40
2:B:654:ARG:C	2:B:656:GLY:H	2.25	0.40
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.56	0.40
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.84	0.40
10:J:14:VAL:HG12	10:J:50:ILE:HD11	2.03	0.40
12:L:30:ILE:CG2	12:L:31:CYS:N	2.84	0.40
12:L:38:LEU:HD11	12:L:48:CYS:SG	2.61	0.40
2:B:127:GLY:C	2:B:128:LEU:HD12	2.42	0.40
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.51	0.40
2:B:1096:ARG:HH11	2:B:1096:ARG:CG	2.35	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HG22	2.02	0.40
5:E:154:ILE:H	5:E:196:VAL:HG13	1.85	0.40
8:H:12:VAL:O	8:H:52:GLN:N	2.54	0.40
5:E:156:LEU:HB3	5:E:160:GLU:HB2	2.03	0.40
4:D:172:LEU:HD13	4:D:198:LEU:HD21	2.02	0.40
1:A:655:PHE:O	1:A:658:LEU:HB3	2.20	0.40
1:A:818:MET:N	2:B:514:LEU:HD23	2.36	0.40
1:A:317:LYS:O	1:A:318:SER:CB	2.68	0.40
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.41	0.40
10:J:1:MET:CE	10:J:60:PHE:HE2	2.34	0.40
9:I:5:ARG:HG2	9:I:6:PHE:H	1.84	0.40
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.86	0.40
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.56	0.40
1:A:34:LYS:CB	1:A:36:ARG:NH1	2.84	0.40
3:C:242:GLN:OE1	3:C:245:VAL:CG2	2.69	0.40
10:J:13:VAL:HG12	10:J:15:GLY:H	1.85	0.40
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.52	0.40
7:G:119:LEU:HA	7:G:131:GLN:O	2.21	0.40
2:B:284:ILE:HD13	2:B:324:ILE:HD12	2.03	0.40
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.86	0.40
2:B:565:PRO:O	2:B:566:LEU:C	2.60	0.40
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.56	0.40
6:F:147:SER:C	6:F:149:GLU:H	2.25	0.40
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.02	0.40
1:A:313:GLN:O	1:A:314:ALA:C	2.59	0.40
1:A:555:ASP:O	1:A:556:TRP:O	2.38	0.40
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.36	0.40
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.57	0.40
8:H:10:PHE:CD1	8:H:10:PHE:N	2.89	0.40
2:B:1084:GLN:OE1	3:C:189:THR:HG23	2.21	0.40
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.57	0.40
1:A:54:ASN:CB	1:A:247:ARG:HH12	2.34	0.40
9:I:5:ARG:HD3	9:I:36:GLU:OE1	2.22	0.40
2:B:889:THR:HG22	2:B:890:TYR:N	2.35	0.40
3:C:166:GLU:O	11:K:6:ARG:NH1	2.54	0.40
3:C:235:VAL:HG13	10:J:13:VAL:HG23	2.03	0.40
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	2.03	0.40
2:B:334:ILE:HG22	2:B:334:ILE:O	2.21	0.40
7:G:30:LEU:HD23	7:G:54:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:SER:O	1:A:574:GLY:C	2.60	0.40
1:A:408:ASP:O	1:A:410:GLY:N	2.55	0.40
1:A:541:ILE:HD13	1:A:549:MET:CE	2.52	0.40
11:K:78:THR:O	11:K:79:GLU:O	2.39	0.40
5:E:58:MET:O	5:E:59:SER:C	2.59	0.40
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.57	0.40
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.57	0.40
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.20	0.40
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.85	0.40
1:A:112:LYS:HZ1	1:A:165:GLY:H	1.68	0.40
5:E:129:PRO:O	5:E:130:ALA:C	2.59	0.40
1:A:1005:GLU:O	1:A:1009:ASN:ND2	2.55	0.40
2:B:760:ASP:OD1	2:B:760:ASP:N	2.55	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	1409/1733 (81%)	1031 (73%)	264 (19%)	114 (8%)	1 11
2	B	1087/1224 (89%)	798 (73%)	191 (18%)	98 (9%)	1 9
3	C	264/347 (76%)	192 (73%)	49 (19%)	23 (9%)	1 10
4	D	174/221 (79%)	121 (70%)	35 (20%)	18 (10%)	1 7
5	E	211/215 (98%)	155 (74%)	41 (19%)	15 (7%)	1 15
6	F	85/155 (55%)	72 (85%)	10 (12%)	3 (4%)	4 35
7	G	169/171 (99%)	143 (85%)	20 (12%)	6 (4%)	4 34
8	H	129/146 (88%)	83 (64%)	26 (20%)	20 (16%)	0 2
9	I	117/122 (96%)	78 (67%)	27 (23%)	12 (10%)	1 7
10	J	63/70 (90%)	39 (62%)	15 (24%)	9 (14%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	112/120 (93%)	91 (81%)	15 (13%)	6 (5%)	2 22
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0 0
All	All	3864/4594 (84%)	2821 (73%)	707 (18%)	336 (9%)	1 10

All (336) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	59	GLY
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	93	VAL
1	A	130	ASP
1	A	167	CYS
1	A	168	GLY
1	A	223	GLY
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	335	ARG
1	A	399	HIS
1	A	400	PRO
1	A	525	GLN
1	A	543	LEU
1	A	556	TRP
1	A	567	LYS
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	628	GLY
1	A	1124	HIS
1	A	1127	ASP
1	A	1255	GLU
1	A	1281	ARG
2	B	21	GLU
2	B	22	SER
2	B	68	THR
2	B	108	VAL

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Mol	Chain	Res	Type
2	B	115	GLN
2	B	184	ALA
2	B	186	GLU
2	B	229	ALA
2	B	259	TYR
2	B	333	PHE
2	B	367	LEU
2	B	505	ASP
2	B	506	GLY
2	B	567	GLU
2	B	591	ARG
2	B	641	GLU
2	B	643	ASP
2	B	709	ASP
2	B	711	GLU
2	B	728	ARG
2	B	792	MET
2	B	867	GLY
2	B	869	SER
2	B	907	GLY
2	B	992	ILE
2	B	1046	PRO
2	B	1069	PHE
2	B	1100	ASP
2	B	1156	ASP
2	B	1176	ASN
3	C	110	THR
3	C	142	VAL
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
4	D	8	PHE
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	52	LEU
4	D	131	GLU
4	D	199	ASN
4	D	218	GLU
5	E	59	SER

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Mol	Chain	Res	Type
6	F	81	THR
6	F	112	GLU
7	G	139	ILE
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
8	H	135	LEU
8	H	140	ALA
9	I	50	THR
9	I	57	GLY
9	I	60	GLN
9	I	79	HIS
10	J	2	ILE
10	J	6	ARG
10	J	28	ASP
10	J	64	ASN
11	K	79	GLU
12	L	26	THR
12	L	35	SER
12	L	50	ASP
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	4	GLN
1	A	42	ASP
1	A	48	ALA
1	A	54	ASN
1	A	65	LEU
1	A	66	LYS
1	A	76	GLU
1	A	128	ILE
1	A	131	SER
1	A	169	ASN
1	A	253	ASN
1	A	276	LEU
1	A	287	HIS
1	A	331	GLY

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Mol	Chain	Res	Type
1	A	410	GLY
1	A	415	LEU
1	A	426	LEU
1	A	546	VAL
1	A	673	GLY
1	A	692	ASP
1	A	886	ILE
1	A	975	HIS
1	A	1036	ARG
1	A	1212	VAL
1	A	1221	LYS
1	A	1231	ASP
1	A	1403	GLU
1	A	1438	THR
2	B	45	SER
2	B	66	ASP
2	B	124	TYR
2	B	245	GLU
2	B	249	ARG
2	B	295	GLY
2	B	334	ILE
2	B	365	THR
2	B	419	THR
2	B	449	ASN
2	B	466	TRP
2	B	512	ARG
2	B	605	ARG
2	B	629	ASP
2	B	655	LYS
2	B	731	VAL
2	B	803	LEU
2	B	879	ARG
2	B	1155	SER
2	B	1175	LEU
2	B	1186	ASP
2	B	1222	ARG
3	C	12	GLU
3	C	90	ASP
3	C	126	GLY
3	C	214	ASN
3	C	215	GLU
3	C	223	ALA

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Mol	Chain	Res	Type
4	D	12	ARG
4	D	30	GLY
4	D	119	ARG
4	D	168	LYS
5	E	45	LYS
5	E	68	SER
5	E	87	SER
6	F	114	GLU
7	G	154	VAL
8	H	84	ALA
8	H	90	ALA
9	I	3	THR
9	I	9	ASP
9	I	51	ASN
9	I	78	CYS
9	I	106	CYS
10	J	17	LYS
10	J	42	LYS
12	L	43	THR
12	L	54	ARG
12	L	56	LEU
1	A	58	LEU
1	A	113	LEU
1	A	219	PHE
1	A	332	LYS
1	A	700	ASN
1	A	755	PHE
1	A	756	ILE
1	A	885	THR
1	A	958	VAL
1	A	968	GLN
1	A	986	ILE
1	A	1014	ALA
1	A	1114	PRO
1	A	1115	SER
1	A	1309	ASP
1	A	1314	SER
1	A	1386	ARG
1	A	1405	THR
1	A	1437	GLY
2	B	24	PRO
2	B	65	GLU

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Mol	Chain	Res	Type
2	B	206	ASN
2	B	258	LEU
2	B	264	SER
2	B	294	ASP
2	B	511	PRO
2	B	531	GLN
2	B	648	HIS
2	B	688	GLY
2	B	881	ASN
2	B	937	ALA
2	B	958	GLN
2	B	1017	ILE
2	B	1096	ARG
2	B	1157	ALA
2	B	1178	ASN
3	C	11	ARG
3	C	125	MET
3	C	141	GLY
3	C	213	PRO
4	D	20	GLU
5	E	4	GLU
5	E	103	LYS
5	E	115	ASN
8	H	59	ILE
8	H	77	ARG
8	H	134	ASN
8	H	139	ASN
9	I	47	GLU
9	I	54	GLU
10	J	24	LEU
12	L	39	SER
12	L	45	ALA
12	L	53	HIS
1	A	5	GLN
1	A	44	THR
1	A	149	GLU
1	A	154	SER
1	A	317	LYS
1	A	419	LYS
1	A	424	ILE
1	A	1062	GLU
1	A	1109	LYS

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Mol	Chain	Res	Type
1	A	1123	GLY
1	A	1223	ASP
1	A	1242	VAL
1	A	1266	THR
1	A	1308	THR
1	A	1398	MET
1	A	1454	MET
2	B	67	SER
2	B	277	LYS
2	B	391	ASP
2	B	436	VAL
2	B	560	GLU
2	B	658	ILE
2	B	708	GLU
2	B	906	SER
2	B	1182	CYS
2	B	1188	LYS
3	C	10	ILE
3	C	233	GLU
3	C	240	VAL
4	D	118	THR
4	D	138	ASN
4	D	166	LEU
5	E	36	GLU
5	E	65	THR
5	E	73	PRO
5	E	192	ARG
7	G	2	PHE
7	G	50	ASP
7	G	52	ASP
7	G	156	SER
8	H	78	SER
8	H	92	ASP
10	J	8	PHE
11	K	90	ALA
1	A	35	ILE
1	A	138	ILE
1	A	220	THR
1	A	284	ALA
1	A	322	VAL
1	A	380	VAL
1	A	526	ASP

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Mol	Chain	Res	Type
1	A	536	LEU
1	A	591	PHE
1	A	718	VAL
1	A	932	GLU
1	A	1093	LYS
2	B	114	PRO
2	B	257	LYS
2	B	571	PRO
2	B	734	HIS
2	B	744	HIS
2	B	810	GLU
2	B	1108	ARG
2	B	1171	VAL
2	B	1181	GLU
3	C	78	GLU
5	E	75	MET
5	E	86	PRO
11	K	64	GLU
11	K	103	THR
11	K	111	LEU
1	A	829	VAL
1	A	871	ASP
1	A	1049	ILE
1	A	1378	GLN
2	B	1061	GLU
3	C	18	VAL
3	C	153	LEU
8	H	107	VAL
9	I	62	ILE
11	K	41	THR
1	A	916	GLY
2	B	729	ILE
2	B	758	PHE
2	B	901	PRO
2	B	1018	PRO
5	E	90	VAL
8	H	44	VAL
1	A	283	GLY
1	A	336	ILE
2	B	575	PRO
4	D	18	VAL
5	E	38	PRO

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Mol	Chain	Res	Type
10	J	14	VAL
2	B	260	GLY
2	B	530	GLY
2	B	1214	PRO
3	C	25	VAL
1	A	51	GLY
1	A	574	GLY
2	B	369	GLY

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	1242/1520 (82%)	1106 (89%)	136 (11%)	8 34
2	B	958/1061 (90%)	859 (90%)	99 (10%)	9 37
3	C	234/299 (78%)	209 (89%)	25 (11%)	8 35
4	D	141/200 (70%)	124 (88%)	17 (12%)	6 28
5	E	195/197 (99%)	175 (90%)	20 (10%)	9 37
6	F	77/137 (56%)	70 (91%)	7 (9%)	12 44
7	G	152/152 (100%)	140 (92%)	12 (8%)	15 52
8	H	117/128 (91%)	108 (92%)	9 (8%)	16 53
9	I	113/116 (97%)	95 (84%)	18 (16%)	3 17
10	J	60/65 (92%)	52 (87%)	8 (13%)	5 24
11	K	99/102 (97%)	94 (95%)	5 (5%)	29 69
12	L	40/57 (70%)	34 (85%)	6 (15%)	3 20
All	All	3428/4034 (85%)	3066 (89%)	362 (11%)	8 36

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	22	PHE

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Mol	Chain	Res	Type
1	A	34	LYS
1	A	37	PHE
1	A	54	ASN
1	A	57	ARG
1	A	68	GLN
1	A	93	VAL
1	A	110	CYS
1	A	116	ASP
1	A	144	THR
1	A	150	THR
1	A	157	ASP
1	A	170	THR
1	A	187	LYS
1	A	200	ARG
1	A	202	LEU
1	A	208	LEU
1	A	221	SER
1	A	225	ASN
1	A	244	PRO
1	A	245	PRO
1	A	261	ASP
1	A	265	LYS
1	A	289	ILE
1	A	297	GLN
1	A	302	THR
1	A	312	PRO
1	A	322	VAL
1	A	333	GLU
1	A	337	ARG
1	A	344	ARG
1	A	369	SER
1	A	385	ILE
1	A	393	ARG
1	A	394	ASN
1	A	408	ASP
1	A	412	ARG
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	461	LYS

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Mol	Chain	Res	Type
1	A	474	VAL
1	A	476	SER
1	A	481	ASP
1	A	488	ASN
1	A	493	GLN
1	A	501	LEU
1	A	504	LEU
1	A	505	CYS
1	A	524	VAL
1	A	545	GLN
1	A	547	LEU
1	A	557	ASP
1	A	560	ILE
1	A	571	LEU
1	A	590	ARG
1	A	593	GLU
1	A	618	GLU
1	A	629	LEU
1	A	635	ARG
1	A	640	GLN
1	A	660	ASN
1	A	664	THR
1	A	666	ILE
1	A	682	THR
1	A	685	GLU
1	A	701	LEU
1	A	710	LEU
1	A	711	ARG
1	A	716	ASP
1	A	735	VAL
1	A	741	ASN
1	A	768	GLN
1	A	786	HIS
1	A	795	GLU
1	A	806	ARG
1	A	816	HIS
1	A	821	ARG
1	A	827	THR
1	A	839	ARG
1	A	858	ASN
1	A	873	MET
1	A	880	LYS

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Mol	Chain	Res	Type
1	A	904	THR
1	A	929	LEU
1	A	941	LYS
1	A	948	VAL
1	A	961	ARG
1	A	976	THR
1	A	983	ILE
1	A	1006	ILE
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1060	PRO
1	A	1067	LEU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1124	HIS
1	A	1129	GLU
1	A	1146	VAL
1	A	1176	LEU
1	A	1193	LEU
1	A	1215	ARG
1	A	1222	ASN
1	A	1223	ASP
1	A	1255	GLU
1	A	1259	MET
1	A	1264	GLU
1	A	1274	ARG
1	A	1276	VAL
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1315	GLU
1	A	1333	ILE
1	A	1336	MET
1	A	1345	ARG
1	A	1364	ASN
1	A	1368	MET
1	A	1376	THR
1	A	1393	ASN
1	A	1400	CYS

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Mol	Chain	Res	Type
1	A	1406	VAL
1	A	1417	GLU
1	A	1418	LEU
1	A	1422	ARG
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1445	ILE
2	B	22	SER
2	B	30	SER
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	106	ASP
2	B	118	ARG
2	B	119	LEU
2	B	167	ILE
2	B	175	ARG
2	B	199	MET
2	B	217	ARG
2	B	250	PHE
2	B	253	THR
2	B	261	ARG
2	B	268	THR
2	B	299	GLU
2	B	303	TYR
2	B	328	GLU
2	B	329	THR
2	B	336	ARG
2	B	364	ILE
2	B	370	PHE
2	B	371	GLU
2	B	376	PHE
2	B	401	PHE
2	B	403	LYS
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	466	TRP
2	B	484	ASN
2	B	485	ARG

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Mol	Chain	Res	Type
2	B	490	SER
2	B	496	ARG
2	B	502	ILE
2	B	505	ASP
2	B	508	LEU
2	B	510	LYS
2	B	533	CYS
2	B	552	MET
2	B	557	PHE
2	B	563	MET
2	B	570	VAL
2	B	572	HIS
2	B	574	SER
2	B	582	VAL
2	B	603	LEU
2	B	616	ILE
2	B	619	ILE
2	B	628	THR
2	B	643	ASP
2	B	690	VAL
2	B	705	MET
2	B	786	ASN
2	B	790	ASP
2	B	796	LEU
2	B	797	TYR
2	B	811	TYR
2	B	815	ARG
2	B	816	GLU
2	B	830	TYR
2	B	831	SER
2	B	839	MET
2	B	858	SER
2	B	860	MET
2	B	868	MET
2	B	878	GLN
2	B	882	THR
2	B	895	ASP
2	B	953	LEU
2	B	956	THR
2	B	970	THR
2	B	997	GLU
2	B	999	MET

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Mol	Chain	Res	Type
2	B	1001	PHE
2	B	1006	ILE
2	B	1020	ARG
2	B	1073	TYR
2	B	1076	HIS
2	B	1082	MET
2	B	1087	PHE
2	B	1096	ARG
2	B	1112	GLN
2	B	1113	VAL
2	B	1147	LEU
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1183	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1202	LEU
2	B	1218	THR
2	B	1224	PHE
3	C	3	GLU
3	C	8	VAL
3	C	26	ASP
3	C	33	LEU
3	C	55	THR
3	C	62	PHE
3	C	66	ARG
3	C	69	LEU
3	C	73	GLN
3	C	77	ILE
3	C	89	GLU
3	C	91	HIS
3	C	99	LEU
3	C	108	GLU
3	C	145	CYS
3	C	147	LEU
3	C	151	GLN
3	C	166	GLU
3	C	202	PRO

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Mol	Chain	Res	Type
3	C	211	ASP
3	C	233	GLU
3	C	238	ILE
3	C	245	VAL
3	C	259	LEU
3	C	262	LEU
4	D	35	LEU
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	63	LEU
4	D	128	VAL
4	D	133	THR
4	D	139	LYS
4	D	159	THR
4	D	170	THR
4	D	182	SER
4	D	187	THR
4	D	208	GLU
4	D	209	ARG
4	D	213	GLU
4	D	219	THR
4	D	220	LEU
5	E	3	GLN
5	E	8	ASN
5	E	26	ARG
5	E	37	LEU
5	E	65	THR
5	E	72	PHE
5	E	82	PHE
5	E	84	ASP
5	E	99	HIS
5	E	101	GLN
5	E	104	ASN
5	E	107	THR
5	E	123	LEU
5	E	132	ILE
5	E	134	THR
5	E	136	ASN
5	E	204	THR
5	E	207	ARG
5	E	212	ARG

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Mol	Chain	Res	Type
5	E	214	CYS
6	F	79	ARG
6	F	90	ARG
6	F	103	MET
6	F	111	LEU
6	F	115	THR
6	F	119	ARG
6	F	123	LYS
7	G	1	MET
7	G	10	ASN
7	G	12	THR
7	G	13	LEU
7	G	17	PHE
7	G	51	TYR
7	G	53	ASN
7	G	64	THR
7	G	74	TYR
7	G	80	LYS
7	G	88	ASP
7	G	152	SER
8	H	35	GLN
8	H	39	THR
8	H	94	ASP
8	H	95	TYR
8	H	102	TYR
8	H	128	ASN
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
9	I	2	THR
9	I	5	ARG
9	I	7	CYS
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	31	THR
9	I	44	TYR
9	I	45	ARG
9	I	59	VAL
9	I	62	ILE
9	I	77	LYS
9	I	85	PHE

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Mol	Chain	Res	Type
9	I	98	VAL
9	I	104	LEU
9	I	106	CYS
9	I	110	PHE
9	I	116	ASN
10	J	4	PRO
10	J	7	CYS
10	J	16	ASP
10	J	23	ASN
10	J	24	LEU
10	J	26	GLN
10	J	28	ASP
10	J	48	ARG
11	K	25	THR
11	K	47	ARG
11	K	51	LEU
11	K	70	ARG
11	K	111	LEU
12	L	27	LEU
12	L	54	ARG
12	L	55	ILE
12	L	64	LEU
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	109	HIS
1	A	169	ASN
1	A	225	ASN
1	A	282	ASN
1	A	297	GLN
1	A	339	ASN
1	A	435	HIS
1	A	445	ASN
1	A	447	GLN
1	A	479	ASN
1	A	488	ASN
1	A	503	GLN
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	611	GLN
1	A	654	ASN
1	A	700	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	975	HIS
1	A	994	GLN
1	A	1009	ASN
1	A	1052	GLN
1	A	1173	HIS
1	A	1187	GLN
1	A	1203	ASN
1	A	1218	GLN
1	A	1432	GLN
2	B	53	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	366	GLN
2	B	383	ASN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	667	GLN
2	B	686	ASN
2	B	744	HIS
2	B	842	ASN
2	B	951	GLN
2	B	957	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1205	GLN
2	B	1211	ASN
3	C	31	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	135	GLN
3	C	231	ASN
3	C	252	GLN
4	D	23	ASN
4	D	39	ASN
4	D	40	HIS
4	D	41	GLN
4	D	74	GLN
4	D	143	ASN
4	D	150	ASN
5	E	54	GLN
5	E	61	GLN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	122	ASN
7	G	126	ASN
8	H	128	ASN
8	H	137	GLN
9	I	12	ASN
9	I	51	ASN
9	I	87	GLN
10	J	53	HIS
11	K	29	ASN

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Mol	Chain	Res	Type
11	K	65	HIS
11	K	104	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/20 (45%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
13	BRU	T	20	13,15	13,21,22	4.58	4 (30%)	16,30,33	4.12	3 (18%)

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
13	BRU	T	20	13,15	-	0/3/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	20	BRU	BR-C5	-15.10	1.50	1.90
13	T	20	BRU	C6-N1	2.41	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	20	BRU	C4-N3	3.15	1.39	1.33
13	T	20	BRU	C4-C5	4.95	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	20	BRU	C5-C4-N3	-8.18	115.27	124.00
13	T	20	BRU	C2'-C1'-N1	-2.84	107.25	114.16
13	T	20	BRU	C4-N3-C2	13.54	126.95	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	20	BRU	8	0

5.5 Carbohydrates (i)

There are no carbohydrates 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1419/1733 (81%)	0.16	37 (2%) 59 54	21, 68, 106, 122	0
2	B	1105/1224 (90%)	0.23	46 (4%) 40 35	28, 78, 111, 122	0
3	C	266/347 (76%)	0.12	2 (0%) 87 83	38, 66, 91, 115	0
4	D	178/221 (80%)	0.13	1 (0%) 90 86	46, 77, 106, 115	0
5	E	213/215 (99%)	0.54	23 (10%) 8 7	47, 91, 115, 121	0
6	F	87/155 (56%)	-0.18	0 100 100	29, 49, 75, 86	0
7	G	171/171 (100%)	0.15	2 (1%) 81 75	45, 67, 96, 108	0
8	H	133/146 (91%)	0.75	16 (12%) 6 6	81, 98, 112, 118	0
9	I	119/122 (97%)	0.56	10 (8%) 14 13	64, 97, 116, 124	0
10	J	65/70 (92%)	-0.01	1 (1%) 76 71	42, 63, 88, 99	0
11	K	114/120 (95%)	0.21	2 (1%) 71 65	33, 70, 88, 101	0
12	L	46/70 (65%)	0.86	6 (13%) 5 4	53, 105, 121, 123	0
13	T	18/41 (43%)	1.74	7 (38%) 0 1	79, 107, 129, 134	1 (5%)
14	N	7/41 (17%)	2.49	7 (100%) 0 0	113, 116, 124, 126	1 (14%)
15	P	10/20 (50%)	1.09	2 (20%) 1 2	80, 99, 124, 127	0
All	All	3951/4696 (84%)	0.24	162 (4%) 41 36	21, 74, 111, 134	2 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	T	28	DA	5.8
2	B	883	LEU	5.3
12	L	26	THR	5.1
1	A	161	LEU	5.1
1	A	1455	PRO	4.8
9	I	116	ASN	4.7
1	A	158	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
13	T	11	DA	4.3
1	A	155	GLU	4.3
1	A	159	THR	4.3
9	I	119	THR	4.2
8	H	108	SER	4.1
5	E	117	THR	4.0
2	B	433	GLN	4.0
1	A	255	SER	3.9
2	B	918	ILE	3.9
2	B	505	ASP	3.9
8	H	107	VAL	3.9
2	B	882	THR	3.8
2	B	346	GLU	3.8
13	T	13	DT	3.7
13	T	12	DC	3.7
5	E	118	PRO	3.6
15	P	1	U	3.6
1	A	253	ASN	3.6
5	E	123	LEU	3.5
9	I	118	ARG	3.5
12	L	25	ALA	3.5
1	A	44	THR	3.4
2	B	432	MET	3.4
2	B	867	GLY	3.4
2	B	431	TYR	3.4
1	A	154	SER	3.3
5	E	93	MET	3.2
2	B	868	MET	3.2
5	E	89	GLY	3.2
2	B	250	PHE	3.2
2	B	349	ILE	3.2
2	B	435	THR	3.1
5	E	126	SER	3.1
8	H	139	ASN	3.1
9	I	76	PRO	3.1
2	B	422	LYS	3.1
14	N	2	DA	3.0
3	C	4	GLU	3.0
5	E	121	MET	3.0
1	A	197	PRO	2.9
2	B	881	ASN	2.9
3	C	3	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
8	H	2	SER	2.9
1	A	251	SER	2.9
14	N	1	DG	2.9
5	E	47	CYS	2.9
1	A	160	GLN	2.9
9	I	120	GLN	2.8
1	A	157	ASP	2.8
8	H	109	LYS	2.8
1	A	1256	GLU	2.8
12	L	50	ASP	2.8
5	E	122	LYS	2.8
14	N	3	DA	2.8
13	T	10	DT	2.8
8	H	86	ASP	2.8
1	A	1125	ALA	2.8
2	B	429	PHE	2.7
8	H	132	LEU	2.7
2	B	436	VAL	2.7
5	E	97	VAL	2.7
2	B	866	TYR	2.6
1	A	1257	ASP	2.6
1	A	257	ARG	2.6
8	H	111	LEU	2.6
2	B	919	SER	2.6
7	G	125	SER	2.6
15	P	3	A	2.6
1	A	1236	LEU	2.6
2	B	132	VAL	2.6
2	B	715	ALA	2.6
13	T	14	DT	2.5
2	B	725	PRO	2.5
1	A	156	ASP	2.5
1	A	1169	ILE	2.5
9	I	83	ASN	2.5
5	E	110	PHE	2.5
5	E	120	ALA	2.5
5	E	88	VAL	2.5
2	B	467	GLY	2.4
2	B	428	ILE	2.4
7	G	122	ASN	2.4
2	B	434	ARG	2.4
5	E	116	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
9	I	110	PHE	2.4
5	E	105	PHE	2.4
1	A	45	GLN	2.4
2	B	679	TYR	2.4
2	B	870	ILE	2.4
2	B	865	LYS	2.4
14	N	4	DA	2.4
2	B	229	ALA	2.4
9	I	117	LYS	2.4
2	B	252	SER	2.4
8	H	83	GLN	2.3
2	B	167	ILE	2.3
1	A	69	THR	2.3
1	A	1091	SER	2.3
1	A	1188	GLN	2.3
8	H	131	ASN	2.3
5	E	51	GLY	2.3
8	H	36	CYS	2.3
1	A	56	PRO	2.3
5	E	100	ILE	2.3
8	H	129	TYR	2.3
12	L	27	LEU	2.3
8	H	127	GLY	2.3
11	K	77	THR	2.3
2	B	709	ASP	2.3
2	B	426	LYS	2.3
8	H	133	ASN	2.2
2	B	69	LEU	2.2
14	N	5	DG	2.2
1	A	163	SER	2.2
9	I	77	LYS	2.2
1	A	153	PRO	2.2
2	B	102	VAL	2.2
12	L	51	CYS	2.2
11	K	113	THR	2.2
2	B	430	ARG	2.2
2	B	935	ARG	2.2
13	T	15	DA	2.2
1	A	150	THR	2.2
1	A	1258	HIS	2.2
1	A	708	MET	2.2
1	A	3	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	130	VAL	2.2
1	A	1175	SER	2.2
2	B	643	ASP	2.2
1	A	254	GLU	2.1
9	I	115	LYS	2.1
1	A	250	ILE	2.1
2	B	916	THR	2.1
1	A	256	GLN	2.1
5	E	86	PRO	2.1
12	L	53	HIS	2.1
2	B	111	ALA	2.1
5	E	119	SER	2.1
14	N	6	DT	2.1
2	B	91	SER	2.1
5	E	50	MET	2.1
1	A	162	VAL	2.1
8	H	146	ARG	2.1
5	E	127	ILE	2.1
2	B	665	GLU	2.1
8	H	112	ILE	2.0
2	B	871	THR	2.0
5	E	96	PHE	2.0
4	D	76	LYS	2.0
10	J	27	GLU	2.0
14	N	7	DA	2.0
2	B	437	GLU	2.0
1	A	258	GLY	2.0
2	B	103	ASN	2.0
5	E	41	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	BRU	T	20	20/21	0.80	0.26	-	75,80,83,84	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	ZN	J	1066	1/1	1.00	0.22	0.08	64,64,64,64	0
17	MG	A	2458	1/1	0.62	0.18	-1.54	100,100,100,100	0
16	ZN	A	2457	1/1	0.99	0.16	-1.57	53,53,53,53	0
16	ZN	C	1269	1/1	0.99	0.11	-2.19	65,65,65,65	0
16	ZN	I	1122	1/1	0.95	0.09	-2.31	134,134,134,134	0
16	ZN	I	1121	1/1	0.98	0.10	-2.33	75,75,75,75	0
16	ZN	A	2456	1/1	0.97	0.09	-2.56	85,85,85,85	0
16	ZN	L	1071	1/1	0.95	0.06	-2.98	119,119,119,119	0
16	ZN	B	2225	1/1	0.99	0.23	-	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.