



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:00 am BST

PDB ID : 2VUM
Title : Alpha-amanitin inhibited complete RNA polymerase II elongation complex
Authors : Brueckner, F.; Cramer, P.
Deposited on : 2008-05-27
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

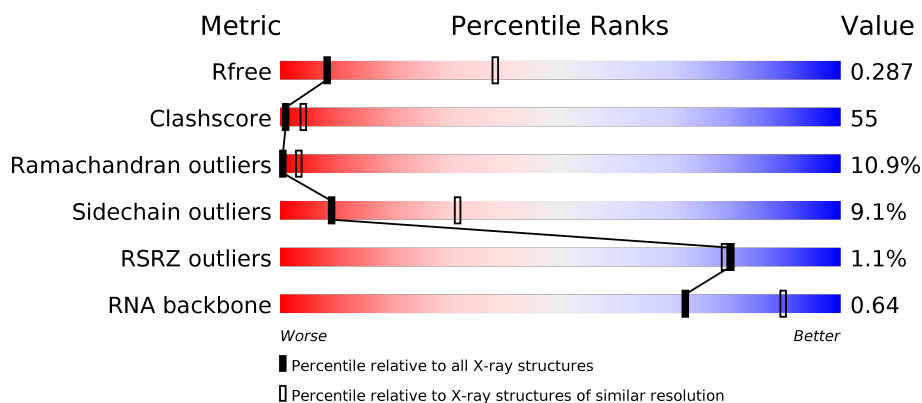
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	8	
14	N	14	
15	P	11	
16	T	26	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32083 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	1418	Total	C	N	O	S	0	0	0
			11158	7032	1949	2115	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- 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			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	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	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	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	84	Total	C	N	O	S	0	0	0
			679	434	115	127	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 protein called AMATOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	13	Total	C	N	O	P	0	0	0
			262	127	47	76	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- Molecule 16 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	25	Total	Br	C	N	O	P	0	0
			509	1	243	92	149	24		

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

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

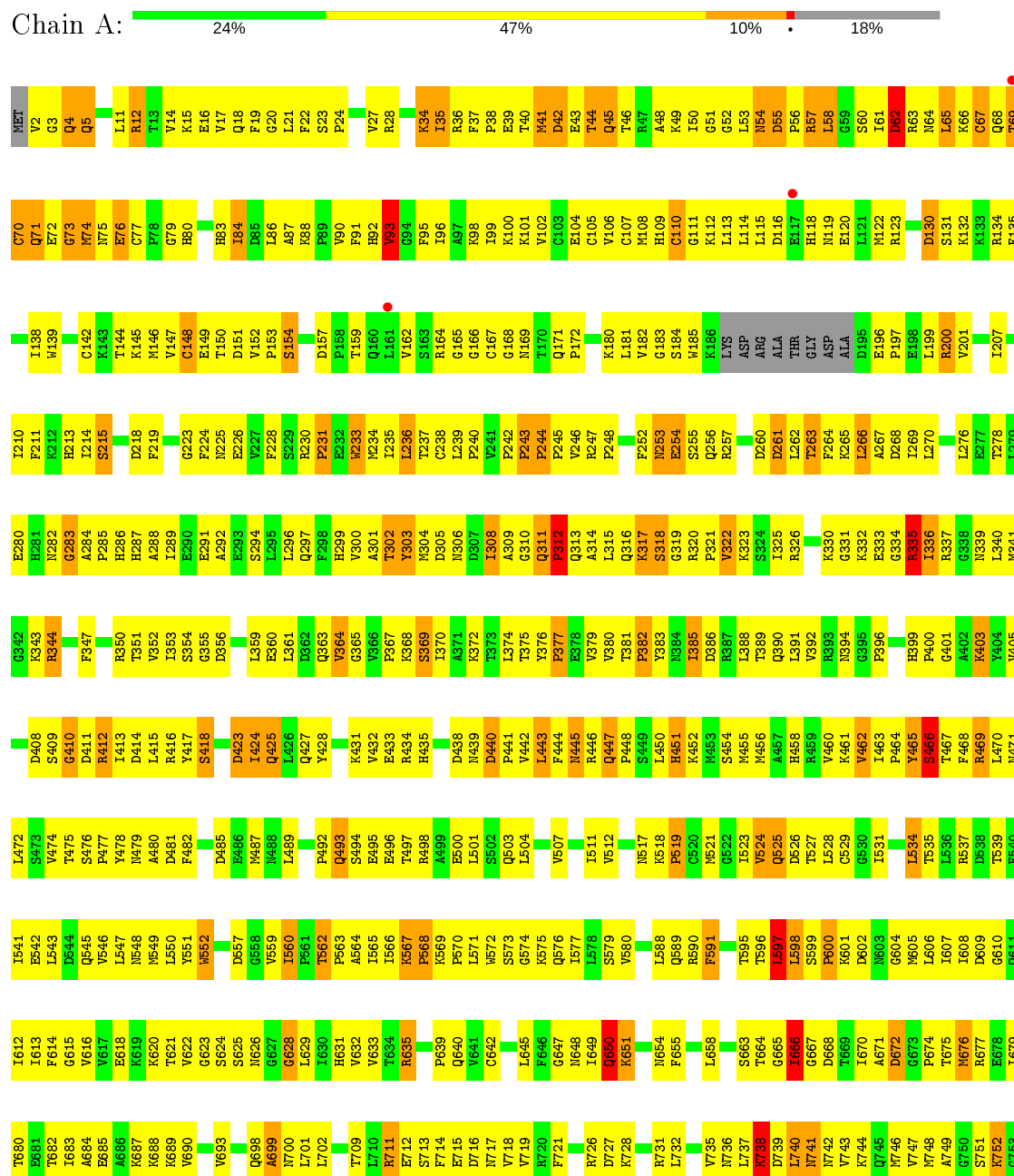
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

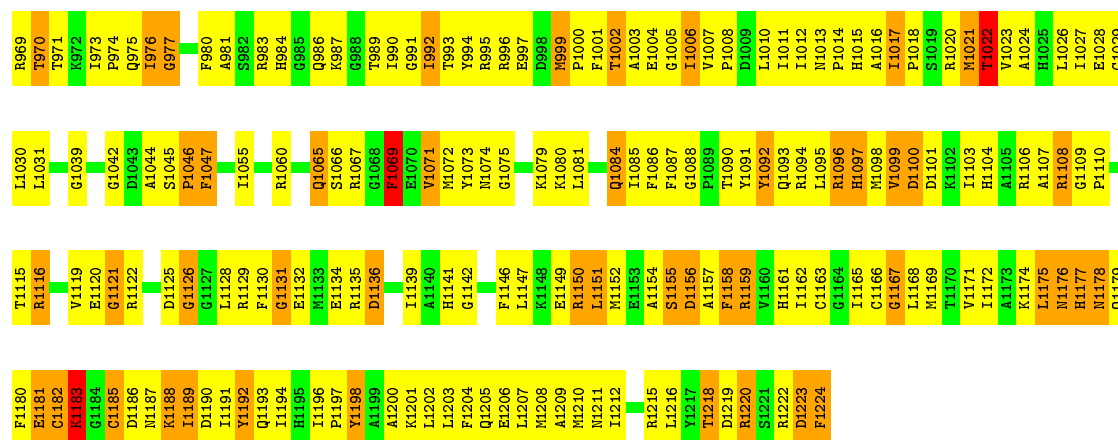
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



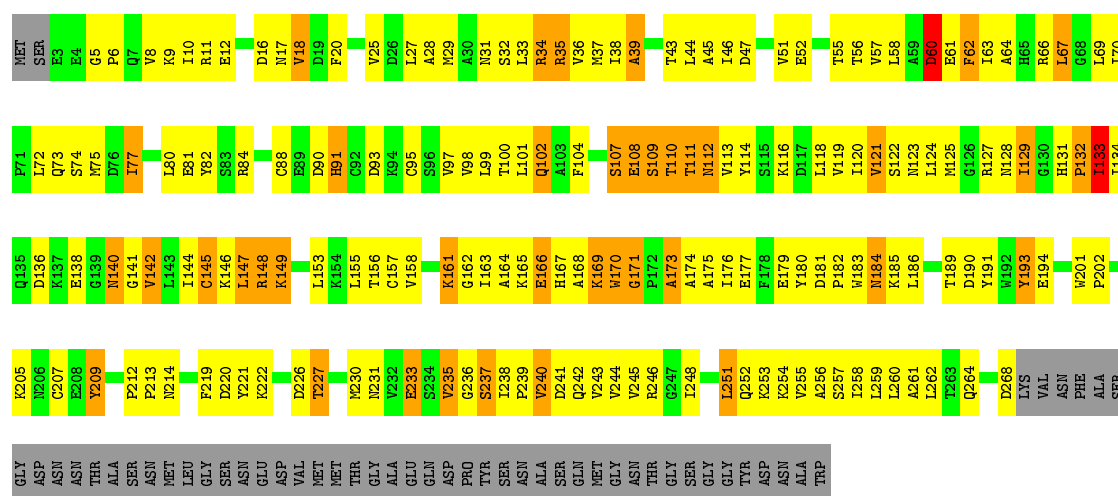
- Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





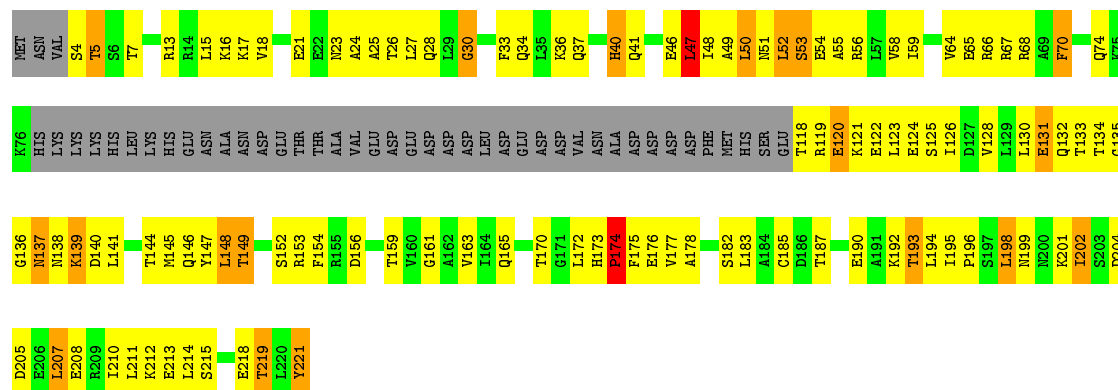
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 28% 43% 12% 16%

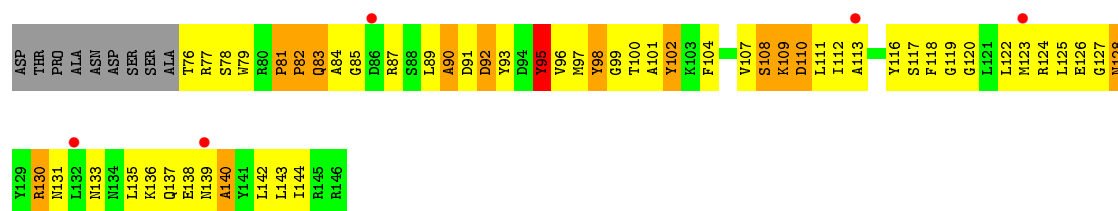


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

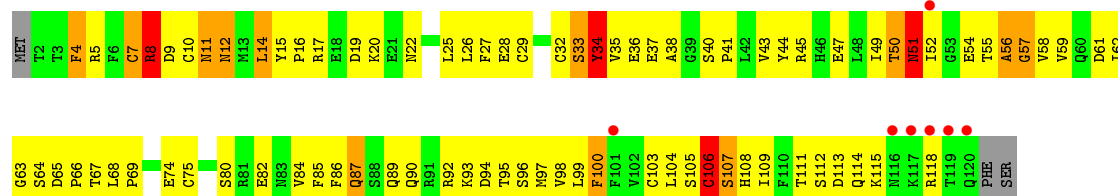
Chain D: 29% 42% 9% 20%



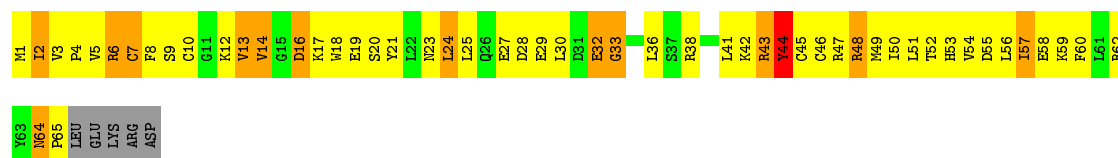
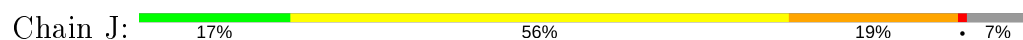
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1



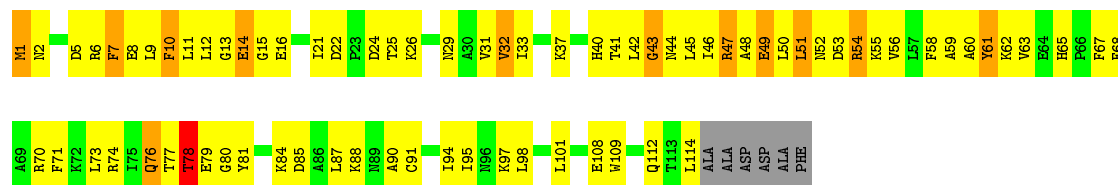
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



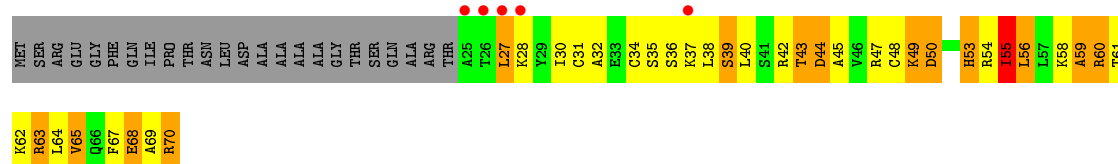
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

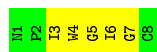


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

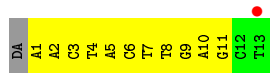


• Molecule 13: AMATOXIN

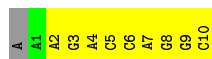




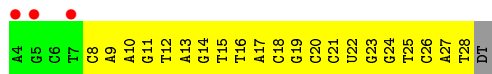
- Molecule 14: 5'-D(*AP*AP*AP*CP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'



- Molecule 15: 5'-R(*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'



- Molecule 16: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *GP*TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.62Å 394.23Å 283.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (49.75-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.288 0.251 , 0.287	Depositor DCC
R_{free} test set	7809 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.077 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.085 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32083	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/11359	0.73	1/15364 (0.0%)
2	B	0.43	0/8963	0.73	0/12086
3	C	0.44	0/2133	0.71	1/2891 (0.0%)
4	D	0.40	0/1365	0.65	0/1837
5	E	0.40	0/1788	0.63	0/2406
6	F	0.49	0/691	0.75	0/933
7	G	0.45	0/1368	0.71	0/1844
8	H	0.41	0/1086	0.66	0/1470
9	I	0.39	0/989	0.67	0/1331
10	J	0.46	0/541	0.76	0/727
11	K	0.48	0/937	0.71	0/1265
12	L	0.44	0/365	0.77	0/485
13	M	1.80	1/22 (4.5%)	1.60	0/26
14	N	0.59	0/293	0.84	0/450
15	P	0.45	0/240	0.77	0/373
16	T	0.55	0/547	0.95	0/840
All	All	0.44	1/32687 (0.0%)	0.72	2/44328 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	7	GLY	N-CA	5.81	1.54	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	5.43	125.66	111.00
1	A	266	LEU	N-CA-C	-5.29	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11222	1335	0
2	B	8792	0	8823	1107	0
3	C	2095	0	2051	245	0
4	D	1356	0	1319	127	0
5	E	1752	0	1776	162	0
6	F	679	0	701	86	0
7	G	1340	0	1357	170	0
8	H	1068	0	1040	160	0
9	I	971	0	931	108	0
10	J	532	0	543	128	0
11	K	919	0	929	103	0
12	L	363	0	388	54	0
13	M	64	0	50	4	0
14	N	262	0	149	20	0
15	P	214	0	111	7	0
16	T	509	0	281	41	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32083	0	31671	3527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (3527) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:THR:HG22	1:A:1331:SER:H	1.05	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.14	1.10
6:F:109:VAL:HG12	6:F:110:ASP:H	1.15	1.09
1:A:40:THR:HB	1:A:41:MET:HE2	1.15	1.09
3:C:43:THR:HG22	3:C:44:LEU:H	1.08	1.08
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.35	1.07
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.70	1.06
1:A:53:LEU:HD23	1:A:54:ASN:N	1.68	1.06
2:B:589:VAL:HG12	2:B:590:HIS:H	1.17	1.06
14:N:2:DA:H2''	14:N:3:DC:H5''	1.28	1.06
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.34	1.04
9:I:34:TYR:HD2	9:I:35:VAL:N	1.56	1.04
1:A:738:LYS:HB2	1:A:740:LEU:HD23	1.40	1.03
1:A:53:LEU:HD23	1:A:54:ASN:H	1.15	1.03
1:A:41:MET:HB3	1:A:49:LYS:HA	1.36	1.03
1:A:332:LYS:H	1:A:337:ARG:HB3	1.23	1.02
1:A:552:TRP:HE1	11:K:62:LYS:HB2	1.24	1.02
1:A:50:ILE:HG22	1:A:52:GLY:H	1.21	1.02
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.25	1.02
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.40	1.01
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.43	1.00
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.21	0.99
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.41	0.99
14:N:2:DA:C2'	14:N:3:DC:H5''	1.93	0.99
9:I:111:THR:HG22	9:I:112:SER:H	1.26	0.99
7:G:138:THR:HG22	7:G:139:ILE:H	1.28	0.99
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	1.78	0.98
1:A:1276:VAL:HB	1:A:1279:ILE:HD12	1.46	0.98
8:H:112:ILE:HB	8:H:130:ARG:HH12	1.28	0.98
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	0.98	0.98
8:H:59:ILE:HG22	8:H:60:ALA:H	1.28	0.97
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.45	0.97
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.44	0.97
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.43	0.97
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.79	0.96
1:A:903:ASN:HD22	1:A:904:THR:N	1.64	0.95
1:A:55:ASP:C	1:A:57:ARG:H	1.68	0.95
3:C:66:ARG:NH2	10:J:5:VAL:HG23	1.82	0.95
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.49	0.95
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.48	0.95
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.66	0.94
6:F:82:THR:HG22	6:F:84:TYR:H	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:HG22	7:G:139:ILE:N	1.78	0.94
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.48	0.94
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.31	0.94
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.46	0.94
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.50	0.93
1:A:265:LYS:HD2	1:A:265:LYS:H	1.34	0.93
5:E:84:ASP:O	5:E:86:PRO:HD3	1.68	0.93
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.50	0.93
10:J:1:MET:HB2	10:J:56:LEU:HD12	1.50	0.92
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.49	0.92
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.34	0.92
8:H:135:LEU:HD13	8:H:137:GLN:NE2	1.83	0.92
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.98	0.91
2:B:359:GLU:O	2:B:362:PRO:HD3	1.69	0.91
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.34	0.91
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.33	0.91
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.50	0.91
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.53	0.90
14:N:1:DA:H2"	14:N:2:DA:OP2	1.68	0.90
2:B:168:GLY:H	2:B:450:ALA:HB1	1.36	0.90
2:B:642:ASP:HA	2:B:649:LYS:HA	1.54	0.90
1:A:709:THR:HB	1:A:712:GLU:HG3	1.52	0.90
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	2.02	0.90
2:B:278:GLN:HG2	2:B:279:ASP:H	1.37	0.89
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.87	0.89
1:A:1329:THR:HG22	1:A:1331:SER:N	1.86	0.89
2:B:580:VAL:HG13	2:B:624:LEU:HB3	1.55	0.89
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.53	0.89
1:A:265:LYS:HD2	1:A:265:LYS:N	1.88	0.88
2:B:806:THR:HG22	2:B:808:ALA:H	1.38	0.88
1:A:984:LYS:HB3	1:A:988:LEU:HD12	1.53	0.88
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.53	0.88
10:J:1:MET:N	10:J:56:LEU:H	1.72	0.88
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.39	0.88
1:A:984:LYS:O	1:A:988:LEU:HB2	1.74	0.88
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.56	0.88
7:G:138:THR:CG2	7:G:139:ILE:H	1.87	0.88
2:B:1181:GLU:HA	2:B:1187:ASN:O	1.75	0.87
2:B:169:ARG:HB3	2:B:169:ARG:HH11	1.36	0.87
5:E:153:HIS:O	5:E:154:ILE:HG13	1.73	0.87
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:O	5:E:23:VAL:HG23	1.74	0.87
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.04	0.87
2:B:589:VAL:HG12	2:B:590:HIS:N	1.89	0.87
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.56	0.87
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.55	0.86
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.56	0.86
2:B:996:ARG:NH2	3:C:175:ALA:H	1.72	0.86
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.57	0.86
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.55	0.86
2:B:526:GLU:OE2	2:B:752:ALA:HB2	1.74	0.86
2:B:821:GLN:HE22	2:B:851:PHE:H	1.21	0.86
1:A:69:THR:C	1:A:71:GLN:H	1.78	0.86
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.89	0.86
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	1.74	0.86
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.54	0.86
3:C:31:ASN:O	3:C:34:ARG:HB3	1.75	0.86
1:A:738:LYS:H	1:A:738:LYS:HD2	1.39	0.86
1:A:901:LEU:H	1:A:926:GLN:HE21	1.22	0.86
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.58	0.86
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.58	0.85
1:A:446:ARG:HB2	1:A:487:MET:SD	2.15	0.85
2:B:516:ASN:N	2:B:516:ASN:HD22	1.70	0.85
3:C:10:ILE:HD11	11:K:108:GLU:HB3	1.58	0.85
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.58	0.85
2:B:1207:LEU:HB3	2:B:1212:ILE:HG22	1.57	0.85
14:N:2:DA:H2''	14:N:3:DC:C5'	2.05	0.85
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.39	0.85
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.56	0.85
3:C:43:THR:HG22	3:C:44:LEU:N	1.90	0.85
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.59	0.84
2:B:766:ARG:HH22	2:B:1020:ARG:NH1	1.75	0.84
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.12	0.84
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.59	0.84
2:B:755:ILE:HA	2:B:809:MET:HE2	1.58	0.84
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.42	0.84
1:A:1351:GLU:O	1:A:1355:VAL:HG23	1.78	0.84
1:A:928:LEU:HD23	1:A:931:GLU:OE1	1.76	0.84
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.43	0.84
1:A:492:PRO:HB3	1:A:501:LEU:HD12	1.59	0.84
1:A:763:ALA:O	1:A:803:SER:HB3	1.78	0.84
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.12	0.84
7:G:1:MET:HE3	7:G:80:LYS:O	1.78	0.84
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.07	0.84
2:B:801:LYS:O	10:J:52:THR:HG23	1.78	0.84
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.42	0.84
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.76	0.84
7:G:80:LYS:HG2	7:G:80:LYS:O	1.76	0.84
9:I:95:THR:HG22	9:I:96:SER:H	1.43	0.83
2:B:295:GLY:H	2:B:298:LEU:HD23	1.43	0.83
15:P:5:C:H2'	15:P:6:C:H6	1.42	0.83
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.11	0.83
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.58	0.83
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.59	0.83
8:H:98:TYR:HD1	8:H:99:GLY:N	1.76	0.83
1:A:1385:THR:HG23	1:A:1387:HIS:H	1.42	0.83
8:H:93:TYR:HB3	8:H:144:ILE:O	1.77	0.83
2:B:549:THR:HG22	2:B:550:ASP:H	1.43	0.83
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.61	0.83
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.61	0.82
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.41	0.82
3:C:175:ALA:CB	10:J:43:ARG:HH22	1.91	0.82
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.61	0.82
4:D:40:HIS:HB2	7:G:73:LYS:NZ	1.94	0.82
2:B:574:SER:HA	2:B:591:ARG:HH22	1.44	0.82
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.61	0.82
4:D:144:THR:O	4:D:148:LEU:HB2	1.80	0.82
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.61	0.82
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.61	0.82
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.15	0.82
3:C:257:SER:HA	3:C:260:LEU:HB3	1.60	0.82
3:C:98:VAL:O	3:C:99:LEU:HD23	1.79	0.82
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.61	0.82
1:A:1370:LEU:O	1:A:1374:VAL:HG23	1.80	0.82
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.60	0.82
1:A:1121:GLU:HG3	1:A:1322:ILE:O	1.80	0.82
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.62	0.81
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.61	0.81
1:A:51:GLY:O	1:A:56:PRO:HB3	1.78	0.81
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.60	0.81
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.61	0.81
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.11	0.81
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.80	0.81
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.62	0.81
9:I:14:LEU:HD12	9:I:27:PHE:HB3	1.63	0.81
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.62	0.81
1:A:50:ILE:HG22	1:A:52:GLY:N	1.94	0.81
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.62	0.81
6:F:109:VAL:HG12	6:F:110:ASP:N	1.96	0.81
1:A:41:MET:O	1:A:50:ILE:HG13	1.79	0.81
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.79	0.81
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.62	0.81
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.63	0.81
1:A:567:LYS:HB3	8:H:96:VAL:H	1.46	0.81
10:J:43:ARG:H	10:J:43:ARG:HD3	1.45	0.81
2:B:996:ARG:HH22	3:C:175:ALA:H	1.29	0.80
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.63	0.80
1:A:709:THR:HG22	1:A:711:ARG:H	1.46	0.80
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.63	0.80
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.81	0.80
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	1.64	0.80
12:L:49:LYS:O	12:L:50:ASP:HB2	1.81	0.80
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.64	0.80
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.63	0.80
2:B:1169:MET:HE2	2:B:1204:PHE:HB2	1.64	0.80
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.64	0.80
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.63	0.80
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.64	0.80
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.64	0.80
2:B:215:GLN:NE2	2:B:499:ASN:HB3	1.96	0.80
3:C:244:VAL:O	3:C:248:ILE:HG13	1.81	0.80
7:G:138:THR:CG2	7:G:139:ILE:N	2.45	0.80
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.47	0.80
1:A:528:LEU:O	1:A:531:ILE:HG22	1.82	0.79
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.63	0.79
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.64	0.79
1:A:567:LYS:CB	8:H:95:TYR:HA	2.13	0.79
2:B:1129:ARG:HG2	2:B:1131:GLY:H	1.47	0.79
6:F:111:LEU:HD12	6:F:111:LEU:H	1.48	0.79
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.64	0.79
1:A:61:ILE:HG22	1:A:62:ASP:H	1.47	0.79
1:A:866:PHE:C	1:A:867:ILE:HD12	2.03	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:942:ARG:HB2	2:B:945:GLU:HG3	1.62	0.79
2:B:333:PHE:O	2:B:334:ILE:HG13	1.82	0.79
2:B:364:ILE:O	2:B:365:THR:HB	1.83	0.79
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.13	0.79
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.64	0.79
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.27	0.79
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.13	0.79
7:G:111:THR:HB	7:G:114:LEU:HD13	1.65	0.79
9:I:34:TYR:CD2	9:I:35:VAL:N	2.47	0.79
2:B:65:GLU:HG3	2:B:66:ASP:H	1.46	0.78
1:A:537:ARG:HH22	8:H:122:LEU:HD12	1.48	0.78
2:B:942:ARG:HH22	16:T:24:DG:P	2.06	0.78
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.49	0.78
1:A:567:LYS:HB3	8:H:96:VAL:N	1.97	0.78
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.65	0.78
1:A:86:LEU:HD21	1:A:239:LEU:HB2	1.64	0.78
1:A:412:ARG:HH22	2:B:1108:ARG:HH22	1.32	0.78
2:B:852:ARG:HH22	12:L:70:ARG:C	1.86	0.78
2:B:800:GLN:HG2	10:J:52:THR:HG22	1.64	0.78
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.66	0.78
2:B:1207:LEU:HB3	2:B:1212:ILE:CG2	2.13	0.78
1:A:1134:ILE:HG22	1:A:1138:ILE:HD11	1.66	0.78
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.65	0.78
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.84	0.78
1:A:1441:PHE:HE2	6:F:89:GLU:HG2	1.48	0.78
1:A:605:MET:HE3	1:A:606:LEU:H	1.49	0.78
1:A:853:ASP:O	1:A:854:ASN:HB2	1.84	0.78
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.66	0.77
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.14	0.77
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.99	0.77
2:B:498:THR:HG22	2:B:537:LYS:H	1.49	0.77
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.98	0.77
10:J:1:MET:H1	10:J:57:ILE:H	1.32	0.77
3:C:133:ILE:HD12	3:C:237:SER:N	1.99	0.77
5:E:26:ARG:HH22	5:E:133:GLU:CD	1.87	0.77
1:A:41:MET:HB3	1:A:49:LYS:CA	2.12	0.77
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.49	0.77
9:I:50:THR:HG22	9:I:51:ASN:H	1.50	0.77
11:K:47:ARG:HD3	11:K:59:ALA:O	1.85	0.77
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.66	0.77
2:B:542:MET:HG2	2:B:747:MET:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:HE1	6:F:92:ARG:HD3	1.48	0.77
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.66	0.77
5:E:29:PHE:O	5:E:30:ILE:HG13	1.84	0.77
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.49	0.77
8:H:14:GLU:O	8:H:26:ILE:HG23	1.83	0.77
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.66	0.77
1:A:58:LEU:HD22	1:A:80:HIS:O	1.85	0.77
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.66	0.77
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	1.64	0.77
9:I:15:TYR:O	9:I:28:GLU:HG2	1.84	0.77
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.67	0.77
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.66	0.77
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.19	0.77
3:C:32:SER:O	3:C:36:VAL:HG23	1.84	0.77
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.15	0.77
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.66	0.77
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.25	0.76
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.67	0.76
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.14	0.76
1:A:332:LYS:O	1:A:333:GLU:HB2	1.83	0.76
2:B:797:TYR:C	2:B:798:TYR:HD2	1.87	0.76
3:C:236:GLY:O	3:C:238:ILE:N	2.19	0.76
1:A:1158:PRO:O	1:A:1159:ARG:HG3	1.85	0.76
1:A:308:ILE:HG22	1:A:309:ALA:H	1.50	0.76
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.67	0.76
1:A:709:THR:HG21	9:I:93:LYS:O	1.85	0.76
7:G:153:GLN:CG	7:G:154:VAL:H	1.98	0.76
8:H:100:THR:HG23	8:H:138:GLU:HA	1.68	0.76
1:A:482:PHE:O	2:B:989:THR:HG23	1.86	0.76
3:C:107:SER:O	3:C:109:SER:N	2.19	0.76
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.66	0.76
8:H:59:ILE:HG22	8:H:60:ALA:N	2.01	0.76
15:P:5:C:H2'	15:P:6:C:C6	2.20	0.76
1:A:494:SER:O	1:A:498:ARG:HG3	1.86	0.76
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.48	0.76
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.00	0.76
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.21	0.76
1:A:596:THR:O	1:A:598:LEU:N	2.17	0.76
1:A:765:VAL:HG23	1:A:802:ASN:O	1.84	0.76
2:B:295:GLY:N	2:B:298:LEU:HD23	1.99	0.76
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.51	0.76
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.68	0.76
5:E:117:THR:HG22	5:E:119:SER:H	1.51	0.76
1:A:40:THR:HB	1:A:41:MET:CE	2.08	0.76
1:A:41:MET:HA	1:A:50:ILE:H	1.50	0.76
1:A:443:LEU:HD23	1:A:501:LEU:HD21	1.68	0.75
1:A:53:LEU:CD2	1:A:54:ASN:H	1.97	0.75
2:B:542:MET:HE2	2:B:743:ILE:HG21	1.69	0.75
10:J:48:ARG:HE	10:J:49:MET:HE2	1.49	0.75
2:B:1016:ALA:O	2:B:1020:ARG:HG3	1.87	0.75
5:E:202:SER:OG	5:E:204:THR:HG22	1.87	0.75
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.69	0.75
3:C:165:LYS:O	11:K:6:ARG:NH1	2.19	0.75
2:B:363:HIS:O	2:B:364:ILE:HB	1.86	0.75
8:H:63:LEU:C	8:H:90:ALA:HB3	2.05	0.75
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.21	0.75
1:A:56:PRO:O	1:A:57:ARG:HG3	1.86	0.75
2:B:744:HIS:HD2	2:B:746:SER:OG	1.69	0.75
4:D:52:LEU:O	4:D:54:GLU:N	2.20	0.75
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.52	0.75
2:B:46:GLN:HG3	2:B:47:GLN:H	1.50	0.75
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.52	0.75
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.52	0.75
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.34	0.75
1:A:252:PHE:O	1:A:253:ASN:HB2	1.86	0.74
2:B:260:GLY:O	2:B:267:ARG:HD3	1.87	0.74
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.22	0.74
1:A:35:ILE:O	1:A:35:ILE:HG22	1.86	0.74
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.85	0.74
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.69	0.74
2:B:464:GLY:O	2:B:477:ALA:HA	1.87	0.74
1:A:302:THR:HG22	1:A:303:TYR:N	2.01	0.74
3:C:44:LEU:HD13	3:C:129:ILE:HD11	1.68	0.74
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.23	0.74
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.67	0.74
11:K:56:VAL:HA	11:K:77:THR:HG22	1.69	0.74
1:A:4:GLN:O	1:A:5:GLN:HB2	1.86	0.74
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.70	0.74
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.51	0.74
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.67	0.74
7:G:143:ILE:HG22	7:G:145:VAL:HG23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ILE:HG23	9:I:49:ILE:HB	1.70	0.74
1:A:855:THR:HG21	1:A:857:ARG:HE	1.53	0.74
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.02	0.74
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.70	0.74
1:A:858:ASN:ND2	1:A:860:LEU:H	1.84	0.74
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.69	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.02	0.74
1:A:236:LEU:N	1:A:236:LEU:HD23	2.02	0.74
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.69	0.74
1:A:535:THR:HG21	1:A:616:VAL:HA	1.70	0.74
2:B:510:LYS:HG2	2:B:511:PRO:CD	2.17	0.74
2:B:782:LEU:HD12	2:B:788:ARG:NH1	2.03	0.74
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.53	0.74
1:A:666:ILE:HD12	1:A:667:GLY:H	1.53	0.74
1:A:858:ASN:C	1:A:858:ASN:HD22	1.91	0.74
2:B:1172:ILE:O	2:B:1172:ILE:HG22	1.88	0.74
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.88	0.73
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.51	0.73
2:B:48:LEU:HD23	2:B:173:MET:SD	2.28	0.73
2:B:992:ILE:HG12	2:B:993:THR:H	1.53	0.73
1:A:321:PRO:O	1:A:322:VAL:HB	1.88	0.73
1:A:353:ILE:CG2	1:A:487:MET:HG3	2.17	0.73
2:B:1202:LEU:HD23	2:B:1206:GLU:HG3	1.70	0.73
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.53	0.73
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.70	0.73
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.88	0.73
2:B:491:THR:O	2:B:495:LEU:HD12	1.86	0.73
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.71	0.73
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.88	0.73
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.89	0.73
2:B:559:SER:HA	2:B:563:MET:HB3	1.71	0.73
10:J:43:ARG:N	10:J:43:ARG:HD3	2.02	0.73
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.17	0.73
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	1.71	0.73
1:A:317:LYS:O	1:A:318:SER:HB3	1.88	0.73
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.24	0.73
2:B:882:THR:HG22	2:B:884:ARG:H	1.54	0.73
1:A:885:THR:O	1:A:940:ARG:HD2	1.88	0.73
2:B:563:MET:CE	2:B:580:VAL:HB	2.19	0.73
2:B:889:THR:HG22	2:B:891:ASP:H	1.53	0.73
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.04	0.73
1:A:12:ARG:HE	2:B:1192:TYR:HE2	1.36	0.73
2:B:298:LEU:N	2:B:298:LEU:HD22	2.04	0.73
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.71	0.73
7:G:80:LYS:HE2	7:G:80:LYS:N	2.04	0.73
8:H:89:LEU:C	8:H:91:ASP:H	1.91	0.73
1:A:55:ASP:CG	1:A:55:ASP:O	2.20	0.72
1:A:671:ALA:HB3	1:A:676:MET:HG2	1.70	0.72
2:B:170:LEU:HD12	2:B:171:PRO:CD	2.19	0.72
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.71	0.72
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.24	0.72
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.71	0.72
6:F:109:VAL:HG13	6:F:127:GLU:OE1	1.88	0.72
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.88	0.72
1:A:443:LEU:HD23	1:A:501:LEU:CD2	2.18	0.72
2:B:882:THR:O	2:B:883:LEU:HB2	1.87	0.72
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.89	0.72
7:G:1:MET:HE2	7:G:3:PHE:HE1	1.54	0.72
7:G:21:ARG:NH1	7:G:23:LYS:HB3	2.02	0.72
9:I:51:ASN:HD21	9:I:118:ARG:NH2	1.86	0.72
1:A:605:MET:HE3	1:A:606:LEU:N	2.03	0.72
3:C:147:LEU:HD23	3:C:147:LEU:N	2.04	0.72
6:F:97:ARG:O	6:F:101:ILE:HG13	1.89	0.72
8:H:142:LEU:C	8:H:143:LEU:HD12	2.10	0.72
1:A:973:ILE:HG21	1:A:1036:ARG:O	1.89	0.72
5:E:61:GLN:HG2	5:E:62:ALA:H	1.54	0.72
7:G:14:HIS:CD2	7:G:16:SER:HB3	2.24	0.72
1:A:91:PHE:H	1:A:297:GLN:HE22	1.36	0.72
1:A:639:PRO:HG2	1:A:640:GLN:H	1.55	0.72
7:G:91:VAL:HB	7:G:139:ILE:O	1.89	0.72
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.70	0.72
2:B:378:LEU:O	2:B:382:ILE:HG13	1.89	0.72
7:G:163:ILE:HG22	7:G:168:LEU:HB3	1.71	0.72
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.72	0.72
1:A:335:ARG:NH1	2:B:1202:LEU:HD22	2.05	0.72
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.05	0.72
1:A:511:ILE:HA	1:A:521:MET:HE3	1.71	0.72
2:B:558:LEU:C	2:B:560:GLU:H	1.93	0.72
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.69	0.72
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.70	0.72
1:A:16:GLU:HG2	1:A:1418:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:PHE:HE1	1:A:785:PRO:CD	2.00	0.72
1:A:901:LEU:H	1:A:926:GLN:NE2	1.87	0.72
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.70	0.71
1:A:1364:ASN:HD22	1:A:1365:TYR:N	1.87	0.71
1:A:84:ILE:CD1	1:A:270:LEU:HD13	2.20	0.71
2:B:126:SER:OG	2:B:172:ILE:HD11	1.90	0.71
7:G:127:PRO:HG2	7:G:138:THR:CG2	2.20	0.71
1:A:737:LEU:HD13	1:A:741:ASN:OD1	1.88	0.71
11:K:53:ASP:C	11:K:55:LYS:H	1.92	0.71
11:K:90:ALA:O	11:K:94:ILE:HG13	1.90	0.71
16:T:20:DC:H2''	16:T:21:DC:H5'	1.72	0.71
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.72	0.71
2:B:563:MET:HE3	2:B:580:VAL:HB	1.70	0.71
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.53	0.71
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.73	0.71
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.72	0.71
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.72	0.71
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.56	0.71
1:A:1068:ALA:HA	1:A:1367:HIS:ND1	2.06	0.71
1:A:591:PHE:HA	1:A:595:THR:HG21	1.72	0.71
2:B:296:GLU:O	2:B:299:GLU:HB2	1.91	0.71
2:B:332:ASP:O	2:B:334:ILE:N	2.23	0.71
5:E:48:ASP:CG	5:E:49:SER:H	1.92	0.71
1:A:182:VAL:HG13	1:A:200:ARG:O	1.90	0.71
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.04	0.71
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.72	0.71
2:B:992:ILE:HG12	2:B:993:THR:N	2.06	0.71
4:D:122:GLU:HA	4:D:125:SER:OG	1.91	0.71
8:H:130:ARG:H	8:H:130:ARG:HD2	1.56	0.71
9:I:106:CYS:SG	9:I:107:SER:N	2.64	0.71
1:A:564:ALA:HB2	1:A:576:GLN:OE1	1.91	0.71
10:J:1:MET:N	10:J:56:LEU:N	2.38	0.71
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.73	0.71
8:H:41:ASP:O	8:H:42:ILE:HG13	1.91	0.70
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.20	0.70
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.72	0.70
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.21	0.70
3:C:35:ARG:HD3	11:K:41:THR:OG1	1.91	0.70
2:B:576:ASP:HB3	2:B:622:LYS:NZ	2.07	0.70
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.57	0.70
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.06	0.70
1:A:923:LEU:O	1:A:927:VAL:HG23	1.91	0.70
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.27	0.70
1:A:67:CYS:O	1:A:70:CYS:SG	2.50	0.70
11:K:65:HIS:CD2	11:K:67:PHE:H	2.09	0.70
1:A:134:ARG:O	1:A:138:ILE:HG13	1.90	0.70
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.27	0.70
2:B:957:ASN:ND2	2:B:961:LEU:HD12	2.06	0.70
1:A:283:GLY:O	1:A:285:PRO:HD3	1.92	0.70
1:A:335:ARG:HH11	2:B:1202:LEU:HD22	1.57	0.70
2:B:411:PRO:O	2:B:414:ALA:HB3	1.91	0.70
2:B:90:ILE:HD12	2:B:432:MET:SD	2.32	0.70
1:A:552:TRP:NE1	11:K:62:LYS:HB2	2.03	0.70
1:A:225:ASN:HD22	1:A:228:PHE:H	1.37	0.70
1:A:463:ILE:HD12	1:A:464:PRO:O	1.91	0.70
1:A:55:ASP:C	1:A:57:ARG:N	2.40	0.70
2:B:916:THR:HB	2:B:935:ARG:HG3	1.74	0.70
9:I:105:SER:O	9:I:106:CYS:HB3	1.92	0.70
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.22	0.70
2:B:383:ASN:O	2:B:387:LEU:HD13	1.91	0.69
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.22	0.69
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.73	0.69
2:B:582:VAL:HG23	2:B:626:ILE:HD12	1.72	0.69
3:C:112:ASN:N	3:C:112:ASN:HD22	1.90	0.69
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.07	0.69
1:A:385:ILE:HG22	1:A:386:ASP:N	2.07	0.69
1:A:55:ASP:N	1:A:56:PRO:HD3	2.07	0.69
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.57	0.69
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.19	0.69
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.74	0.69
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	1.90	0.69
4:D:65:GLU:HA	4:D:68:ARG:HD2	1.73	0.69
7:G:145:VAL:HG12	7:G:146:LYS:N	2.07	0.69
1:A:715:GLU:O	1:A:719:VAL:HG23	1.93	0.69
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.75	0.69
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.72	0.69
3:C:251:LEU:O	3:C:255:VAL:HG23	1.92	0.69
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.74	0.69
4:D:40:HIS:HB2	7:G:73:LYS:CE	2.23	0.69
1:A:282:ASN:O	1:A:284:ALA:N	2.26	0.69
1:A:858:ASN:HD22	1:A:860:LEU:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.57	0.69
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.07	0.69
6:F:90:ARG:HG2	6:F:91:ALA:N	2.05	0.69
6:F:89:GLU:O	6:F:93:ILE:HG13	1.92	0.69
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.08	0.69
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.72	0.69
1:A:857:ARG:HD3	1:A:861:GLY:O	1.91	0.69
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.06	0.69
2:B:112:LEU:HD12	2:B:113:TYR:H	1.57	0.69
2:B:123:THR:HG21	2:B:458:LYS:HE2	1.74	0.69
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.12	0.69
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.92	0.69
1:A:1385:THR:CG2	1:A:1387:HIS:H	2.05	0.69
1:A:569:LYS:O	1:A:571:LEU:HD12	1.91	0.69
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.58	0.69
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.28	0.69
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.12	0.69
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.73	0.69
8:H:89:LEU:O	8:H:91:ASP:N	2.22	0.69
13:M:3:ILX:OG1	13:M:3:ILX:C	2.40	0.69
14:N:1:DA:H1'	14:N:2:DA:H5'	1.75	0.69
4:D:47:LEU:CD1	4:D:48:ILE:H	2.06	0.69
2:B:661:LEU:C	2:B:663:ALA:H	1.95	0.69
2:B:890:TYR:O	2:B:893:LEU:HB2	1.93	0.69
4:D:34:GLN:O	4:D:47:LEU:HD23	1.93	0.69
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.28	0.69
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.75	0.69
3:C:254:LYS:O	3:C:258:ILE:HD13	1.91	0.69
11:K:87:LEU:O	11:K:91:CYS:HB2	1.93	0.69
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.28	0.68
16:T:8:DC:H2"	16:T:9:DA:OP2	1.90	0.68
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.75	0.68
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.08	0.68
7:G:13:LEU:HD12	7:G:26:LEU:HD21	1.73	0.68
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.33	0.68
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.27	0.68
2:B:516:ASN:H	2:B:516:ASN:HD22	1.38	0.68
2:B:616:ILE:HD12	2:B:616:ILE:N	2.08	0.68
3:C:73:GLN:HE21	3:C:74:SER:H	1.41	0.68
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.75	0.68
1:A:1082:ASN:HB3	1:A:1084:PHE:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.93	0.68
2:B:575:PRO:HG2	2:B:576:ASP:H	1.59	0.68
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.59	0.68
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.92	0.68
11:K:109:TRP:O	11:K:112:GLN:HG2	1.93	0.68
14:N:1:DA:H1'	14:N:2:DA:C5'	2.24	0.68
1:A:440:ASP:O	1:A:460:VAL:HG23	1.94	0.68
1:A:597:LEU:N	1:A:597:LEU:HD12	2.08	0.68
2:B:1069:PHE:HA	2:B:1085:ILE:O	1.93	0.68
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.94	0.68
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.23	0.68
2:B:763:GLN:HG2	2:B:765:PRO:HG2	1.74	0.68
7:G:21:ARG:HH11	7:G:23:LYS:HB3	1.58	0.68
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.76	0.68
1:A:63:ARG:HA	1:A:74:MET:CE	2.24	0.68
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.29	0.68
2:B:912:ILE:O	2:B:938:SER:HB3	1.94	0.68
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.24	0.68
9:I:34:TYR:HD2	9:I:35:VAL:H	1.40	0.68
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.23	0.68
1:A:837:ILE:HG12	1:A:840:ARG:NH1	2.08	0.68
1:A:837:ILE:HG12	1:A:840:ARG:HH11	1.59	0.68
1:A:982:THR:O	1:A:985:ASP:HB2	1.94	0.68
2:B:589:VAL:CG1	2:B:590:HIS:H	1.98	0.68
12:L:28:LYS:HB2	12:L:39:SER:HA	1.75	0.68
1:A:1420:ASP:OD1	1:A:1422:ARG:HD2	1.94	0.68
4:D:201:LYS:O	4:D:202:ILE:HB	1.93	0.68
3:C:175:ALA:HB1	10:J:43:ARG:HH12	1.59	0.68
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.23	0.68
2:B:596:LEU:O	2:B:600:LEU:HG	1.94	0.68
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.75	0.68
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.59	0.67
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.67
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.91	0.67
4:D:215:SER:HA	4:D:218:GLU:HB2	1.77	0.67
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.78	0.67
1:A:1333:ILE:HD13	1:A:1381:LEU:HD12	1.76	0.67
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.94	0.67
1:A:903:ASN:HD22	1:A:903:ASN:C	1.93	0.67
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.75	0.67
2:B:698:GLU:O	2:B:701:ILE:HG12	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:HE3	5:E:26:ARG:HE	1.60	0.67
6:F:118:LEU:O	6:F:122:MET:HG3	1.95	0.67
10:J:43:ARG:CD	10:J:43:ARG:H	2.07	0.67
2:B:798:TYR:HD1	10:J:4:PRO:HG3	1.60	0.67
1:A:741:ASN:HD22	1:A:742:ASN:N	1.92	0.67
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.75	0.67
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.76	0.67
1:A:913:LEU:HG	1:A:915:SER:H	1.59	0.67
2:B:737:THR:CG2	9:I:66:PRO:HA	2.25	0.67
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.60	0.67
1:A:560:ILE:HG13	8:H:79:TRP:H	1.60	0.67
2:B:484:ASN:O	2:B:485:ARG:HD2	1.95	0.67
9:I:56:ALA:HB3	9:I:89:GLN:HG3	1.76	0.67
1:A:1407:GLU:H	1:A:1407:GLU:CD	1.98	0.67
1:A:475:THR:HG23	1:A:476:SER:N	2.09	0.67
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.30	0.67
1:A:786:HIS:CD2	2:B:703:ILE:HB	2.30	0.67
6:F:109:VAL:CG1	6:F:110:ASP:H	1.99	0.67
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.59	0.67
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.30	0.67
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.75	0.67
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.75	0.67
10:J:52:THR:HG22	10:J:52:THR:O	1.93	0.67
11:K:7:PHE:O	11:K:11:LEU:HD23	1.94	0.67
1:A:1004:ASN:O	1:A:1008:GLN:HG2	1.95	0.66
1:A:597:LEU:O	1:A:598:LEU:HB2	1.93	0.66
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.76	0.66
2:B:33:VAL:O	2:B:36:ALA:HB3	1.95	0.66
4:D:130:LEU:O	4:D:132:GLN:N	2.27	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.77	0.66
8:H:112:ILE:HB	8:H:130:ARG:NH1	2.08	0.66
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.10	0.66
1:A:1152:ILE:HG23	1:A:1193:LEU:HD13	1.78	0.66
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.10	0.66
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.07	0.66
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.93	0.66
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.94	0.66
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.94	0.66
3:C:17:ASN:N	3:C:240:VAL:HG11	2.11	0.66
1:A:367:PRO:HG2	1:A:370:ILE:HG13	1.75	0.66
1:A:557:ASP:OD2	1:A:559:VAL:HB	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.77	0.66
4:D:47:LEU:HD13	4:D:48:ILE:H	1.61	0.66
11:K:55:LYS:HB3	11:K:81:TYR:HE1	1.59	0.66
1:A:1198:ASP:O	1:A:1202:MET:HG2	1.96	0.66
1:A:405:VAL:HG22	1:A:432:VAL:HG22	1.76	0.66
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.31	0.66
12:L:30:ILE:O	12:L:56:LEU:HA	1.94	0.66
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.77	0.66
1:A:466:SER:HB2	2:B:1099:VAL:HG11	1.78	0.66
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.76	0.66
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.66
7:G:4:ILE:HD13	7:G:49:LEU:HD11	1.77	0.66
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.59	0.66
1:A:1005:GLU:HG3	1:A:1009:ASN:ND2	2.11	0.66
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	1.96	0.66
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.77	0.66
1:A:42:ASP:HA	1:A:46:THR:O	1.96	0.66
1:A:463:ILE:HD13	1:A:469:ARG:HD2	1.77	0.66
2:B:737:THR:HG21	9:I:66:PRO:HA	1.77	0.66
2:B:542:MET:SD	2:B:747:MET:HE2	2.35	0.66
1:A:628:GLY:O	1:A:632:VAL:HG23	1.96	0.66
1:A:932:GLU:OE1	1:A:987:VAL:HG22	1.95	0.66
2:B:637:LEU:HD22	2:B:741:CYS:O	1.95	0.66
2:B:873:THR:O	2:B:914:LYS:HA	1.96	0.66
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.77	0.66
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.96	0.66
1:A:738:LYS:H	1:A:738:LYS:CD	2.06	0.66
2:B:1176:ASN:C	2:B:1178:ASN:H	1.98	0.66
4:D:55:ALA:HB3	4:D:148:LEU:HD11	1.78	0.66
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.96	0.66
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.77	0.66
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.95	0.66
4:D:53:SER:H	4:D:148:LEU:CD2	2.09	0.66
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.25	0.66
1:A:821:ARG:O	1:A:825:ILE:HG13	1.95	0.65
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.26	0.65
2:B:850:LEU:HD12	2:B:851:PHE:N	2.11	0.65
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.26	0.65
2:B:60:GLN:OE1	2:B:95:ILE:HG22	1.96	0.65
1:A:1325:THR:O	5:E:148:GLU:HB2	1.96	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.97	0.65
2:B:884:ARG:HB2	2:B:935:ARG:HA	1.78	0.65
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.96	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.97	0.65
2:B:1151:LEU:H	2:B:1151:LEU:HD13	1.61	0.65
12:L:40:LEU:HD22	12:L:44:ASP:HB3	1.77	0.65
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.62	0.65
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.11	0.65
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.77	0.65
2:B:847:ASP:C	2:B:849:GLY:H	2.00	0.65
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.61	0.65
10:J:36:LEU:CB	10:J:47:ARG:HH12	2.10	0.65
10:J:9:SER:CB	10:J:45:CYS:HB2	2.26	0.65
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.78	0.65
2:B:649:LYS:HD3	2:B:736:THR:O	1.96	0.65
3:C:142:VAL:HG12	3:C:142:VAL:O	1.94	0.65
3:C:235:VAL:HG12	10:J:13:VAL:CG2	2.27	0.65
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.95	0.65
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.62	0.65
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.60	0.65
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.32	0.65
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.61	0.65
2:B:278:GLN:HG2	2:B:279:ASP:N	2.10	0.65
2:B:582:VAL:HA	2:B:626:ILE:HB	1.76	0.65
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.78	0.65
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.32	0.65
5:E:61:GLN:HG2	5:E:62:ALA:N	2.12	0.65
4:D:40:HIS:HB2	7:G:73:LYS:HZ1	1.62	0.65
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.79	0.65
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.77	0.65
1:A:567:LYS:CB	1:A:568:PRO:CD	2.74	0.65
7:G:153:GLN:HG2	7:G:154:VAL:H	1.61	0.65
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.36	0.65
1:A:69:THR:C	1:A:71:GLN:N	2.50	0.65
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.76	0.65
4:D:185:CYS:HB3	4:D:211:LEU:HD22	1.78	0.65
5:E:157:SER:C	5:E:159:ASP:H	1.99	0.65
8:H:101:ALA:HA	8:H:116:TYR:HA	1.78	0.65
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.27	0.65
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.30	0.65
1:A:855:THR:HG21	1:A:857:ARG:NE	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.79	0.65
3:C:241:ASP:O	3:C:245:VAL:HG23	1.97	0.65
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.32	0.65
7:G:1:MET:SD	7:G:79:PHE:CD1	2.90	0.65
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.79	0.65
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.44	0.64
1:A:84:ILE:HD11	1:A:270:LEU:CD1	2.25	0.64
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.78	0.64
2:B:1157:ALA:O	2:B:1158:PHE:HB2	1.97	0.64
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.79	0.64
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.79	0.64
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.31	0.64
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.79	0.64
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.78	0.64
8:H:15:VAL:HG22	8:H:26:ILE:HD13	1.78	0.64
1:A:1025:ARG:O	1:A:1026:LEU:HD23	1.97	0.64
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.62	0.64
1:A:534:LEU:HA	1:A:539:THR:HG21	1.79	0.64
2:B:983:ARG:HH11	2:B:1091:TYR:CB	2.10	0.64
2:B:234:ILE:HG21	2:B:237:VAL:CG2	2.26	0.64
2:B:298:LEU:H	2:B:298:LEU:CD2	2.11	0.64
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.79	0.64
2:B:294:ASP:O	2:B:296:GLU:N	2.29	0.64
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.78	0.64
8:H:139:ASN:O	8:H:140:ALA:HB2	1.96	0.64
1:A:844:ALA:O	1:A:845:LEU:HD23	1.98	0.64
3:C:119:VAL:HG12	3:C:120:ILE:N	2.12	0.64
3:C:43:THR:CG2	3:C:44:LEU:H	1.90	0.64
1:A:1441:PHE:CE1	6:F:92:ARG:HD3	2.33	0.64
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.79	0.64
2:B:298:LEU:H	2:B:298:LEU:HD22	1.62	0.64
3:C:253:LYS:O	3:C:256:ALA:HB3	1.97	0.64
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.12	0.64
1:A:590:ARG:O	1:A:591:PHE:HB2	1.96	0.64
8:H:143:LEU:O	8:H:144:ILE:HG13	1.98	0.64
9:I:33:SER:O	9:I:35:VAL:HG23	1.98	0.64
1:A:1152:ILE:CG1	9:I:44:TYR:HB3	2.27	0.64
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.80	0.64
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.79	0.64
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.32	0.64
2:B:35:SER:HA	2:B:811:TYR:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.33	0.64
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.80	0.64
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.80	0.64
5:E:91:LYS:C	5:E:93:MET:H	1.99	0.64
4:D:40:HIS:HB2	7:G:73:LYS:HE3	1.79	0.64
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.27	0.64
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.12	0.63
1:A:889:SER:HB3	1:A:1297:GLU:CG	2.28	0.63
2:B:603:LEU:HD12	2:B:609:ILE:HG23	1.78	0.63
6:F:110:ASP:O	6:F:112:GLU:N	2.31	0.63
9:I:62:ILE:HG12	9:I:62:ILE:O	1.98	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.63
1:A:40:THR:CB	1:A:41:MET:HE2	2.10	0.63
4:D:67:ARG:HB2	4:D:133:THR:HG21	1.80	0.63
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.79	0.63
1:A:224:PHE:CG	1:A:231:PRO:HG3	2.33	0.63
2:B:558:LEU:O	2:B:560:GLU:N	2.30	0.63
3:C:184:ASN:HD21	3:C:189:THR:HB	1.63	0.63
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.34	0.63
1:A:590:ARG:HB3	1:A:605:MET:H	1.64	0.63
1:A:738:LYS:HB2	1:A:740:LEU:CD2	2.24	0.63
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.80	0.63
2:B:408:LEU:HD13	2:B:545:ILE:HD12	1.81	0.63
3:C:167:HIS:HD2	3:C:168:ALA:H	1.46	0.63
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.81	0.63
12:L:28:LYS:HG3	12:L:39:SER:OG	1.99	0.63
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.80	0.63
2:B:105:SER:O	2:B:106:ASP:HB2	1.98	0.63
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.80	0.63
1:A:401:GLY:C	1:A:435:HIS:HD2	2.02	0.63
2:B:710:LEU:HD22	2:B:733:HIS:HB3	1.80	0.63
2:B:756:ILE:O	2:B:759:PRO:HD3	1.99	0.63
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.62	0.63
3:C:43:THR:HB	3:C:170:TRP:HD1	1.63	0.63
3:C:73:GLN:NE2	3:C:74:SER:H	1.97	0.63
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.64	0.63
1:A:416:ARG:O	1:A:417:TYR:HD2	1.82	0.63
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.12	0.63
2:B:273:LEU:HB2	2:B:276:ILE:CD1	2.28	0.63
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.63	0.63
2:B:916:THR:HB	2:B:935:ARG:CG	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:LEU:O	2:B:953:LEU:HD23	1.99	0.63
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.81	0.63
10:J:2:ILE:CG2	10:J:3:VAL:N	2.61	0.63
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.80	0.63
1:A:41:MET:CB	1:A:49:LYS:HA	2.22	0.63
1:A:95:PHE:HE2	1:A:1410:PHE:HB3	1.63	0.63
2:B:127:GLY:C	2:B:128:LEU:HD12	2.19	0.63
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.17	0.63
3:C:39:ALA:O	3:C:164:ALA:HB3	1.98	0.63
9:I:14:LEU:HD13	9:I:28:GLU:O	1.99	0.63
16:T:17:DA:H3'	16:T:17:DA:OP1	1.98	0.63
1:A:445:ASN:HB2	1:A:454:SER:O	1.99	0.63
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.80	0.63
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.13	0.63
2:B:50:SER:OG	2:B:411:PRO:HD3	1.99	0.63
4:D:170:THR:CG2	4:D:172:LEU:HG	2.29	0.63
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.81	0.63
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.81	0.63
3:C:175:ALA:HB2	10:J:43:ARG:HH22	1.63	0.63
1:A:1323:ASP:O	1:A:1325:THR:N	2.24	0.62
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.81	0.62
7:G:1:MET:CE	7:G:3:PHE:HE1	2.11	0.62
15:P:6:C:O2'	15:P:7:A:H5'	1.99	0.62
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.33	0.62
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.34	0.62
4:D:134:THR:HG22	4:D:136:GLY:H	1.64	0.62
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.34	0.62
9:I:69:PRO:HB2	9:I:85:PHE:CZ	2.34	0.62
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.33	0.62
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.00	0.62
1:A:787:PHE:CE1	1:A:796:SER:HA	2.34	0.62
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.80	0.62
2:B:1151:LEU:N	2:B:1151:LEU:HD13	2.13	0.62
10:J:2:ILE:HG23	10:J:3:VAL:N	2.14	0.62
1:A:884:ASP:HB2	1:A:1024:SER:OG	1.99	0.62
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.26	0.62
1:A:979:SER:OG	1:A:980:ASP:N	2.32	0.62
2:B:1169:MET:CE	2:B:1204:PHE:HB2	2.29	0.62
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.62
3:C:201:TRP:HE3	3:C:202:PRO:HD2	1.63	0.62
4:D:37:GLN:HB2	7:G:5:LYS:HZ1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:PHE:CD2	8:H:45:GLU:HG2	2.34	0.62
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.80	0.62
2:B:365:THR:OG1	2:B:367:LEU:HG	1.99	0.62
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.14	0.62
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.29	0.62
3:C:226:ASP:O	3:C:227:THR:HB	2.00	0.62
7:G:160:ILE:HG22	7:G:161:GLY:N	2.14	0.62
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.34	0.62
11:K:40:HIS:HD1	11:K:61:TYR:HH	1.46	0.62
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.81	0.62
1:A:826:ASP:O	1:A:830:LYS:HG2	2.00	0.62
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.81	0.62
2:B:298:LEU:HD12	2:B:314:LEU:HD13	1.81	0.62
2:B:487:THR:O	2:B:490:SER:HB3	2.00	0.62
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.29	0.62
3:C:164:ALA:HA	3:C:167:HIS:O	1.99	0.62
4:D:55:ALA:CB	4:D:148:LEU:HD11	2.29	0.62
7:G:51:TYR:O	7:G:54:ILE:HG13	1.99	0.62
1:A:772:GLY:O	13:M:6:ILE:HD13	2.00	0.62
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.30	0.62
2:B:1003:ALA:O	3:C:177:GLU:HG2	2.00	0.62
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.99	0.62
2:B:20:ASP:C	2:B:22:SER:H	2.02	0.62
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.82	0.62
2:B:423:LYS:NZ	2:B:423:LYS:HB2	2.15	0.62
2:B:65:GLU:HG3	2:B:66:ASP:N	2.15	0.62
2:B:996:ARG:HH22	3:C:175:ALA:N	1.97	0.62
5:E:2:ASP:O	5:E:3:GLN:HG2	2.00	0.62
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.99	0.62
1:A:919:ILE:HG21	1:A:983:ILE:HD11	1.80	0.62
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.13	0.62
2:B:842:ASN:ND2	2:B:845:SER:OG	2.33	0.62
5:E:17:ARG:O	5:E:21:GLU:HG3	2.00	0.62
7:G:51:TYR:HD2	7:G:51:TYR:C	2.03	0.62
1:A:1328:TYR:CD1	1:A:1335:ILE:HD11	2.35	0.62
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.81	0.62
1:A:320:ARG:HH22	1:A:323:LYS:HE3	1.64	0.62
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.35	0.62
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.81	0.62
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.00	0.62
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:VAL:HG21	2:B:1090:THR:HB	1.80	0.62
2:B:800:GLN:HG2	10:J:52:THR:CG2	2.30	0.62
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.63	0.62
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.00	0.61
1:A:751:SER:O	1:A:752:LYS:HG2	1.99	0.61
2:B:262:GLU:HG2	2:B:262:GLU:O	2.00	0.61
2:B:57:TYR:N	2:B:57:TYR:HD1	1.98	0.61
2:B:815:ARG:O	10:J:54:VAL:HG21	2.00	0.61
4:D:50:LEU:CD1	4:D:55:ALA:HA	2.29	0.61
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.81	0.61
1:A:351:THR:HG21	2:B:1103:ILE:HD12	1.81	0.61
1:A:960:ILE:O	1:A:963:ILE:HG22	2.00	0.61
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.61
2:B:834:ASN:HA	2:B:838:SER:O	2.00	0.61
6:F:99:LEU:C	6:F:99:LEU:HD12	2.21	0.61
1:A:63:ARG:HA	1:A:74:MET:HE1	1.82	0.61
1:A:965:GLN:HA	1:A:968:GLN:CG	2.30	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.36	0.61
2:B:125:SER:HB2	2:B:170:LEU:C	2.20	0.61
2:B:744:HIS:ND1	2:B:745:PRO:HD2	2.15	0.61
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.35	0.61
2:B:798:TYR:CD2	2:B:798:TYR:N	2.68	0.61
2:B:883:LEU:O	2:B:885:MET:N	2.33	0.61
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.36	0.61
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.01	0.61
1:A:370:ILE:HG22	1:A:374:LEU:HD12	1.80	0.61
2:B:188:ASP:O	2:B:192:LEU:HD12	2.00	0.61
2:B:955:THR:HG22	2:B:956:THR:N	2.14	0.61
4:D:24:ALA:C	4:D:26:THR:H	2.02	0.61
6:F:82:THR:HG22	6:F:84:TYR:N	2.10	0.61
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.30	0.61
11:K:70:ARG:O	11:K:71:PHE:HB3	2.00	0.61
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.82	0.61
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.36	0.61
5:E:121:MET:O	5:E:124:VAL:HG23	1.99	0.61
8:H:58:THR:HG22	8:H:59:ILE:N	2.15	0.61
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.83	0.61
1:A:1364:ASN:HD22	1:A:1365:TYR:H	1.47	0.61
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.00	0.61
3:C:167:HIS:CD2	3:C:168:ALA:H	2.19	0.61
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:ASP:OD1	9:I:22:ASN:HB2	2.00	0.61
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.63	0.61
1:A:1328:TYR:HD1	1:A:1335:ILE:HD11	1.66	0.61
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.61
2:B:798:TYR:HD2	2:B:798:TYR:N	1.98	0.61
3:C:184:ASN:ND2	3:C:189:THR:HB	2.15	0.61
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.36	0.61
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.16	0.61
2:B:1220:ARG:CZ	2:B:1220:ARG:HB3	2.29	0.61
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.34	0.61
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.66	0.61
3:C:259:LEU:HD11	11:K:88:LYS:HA	1.82	0.61
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.40	0.61
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.83	0.61
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.31	0.61
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.35	0.61
4:D:208:GLU:O	4:D:212:LYS:HG3	2.01	0.61
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.66	0.61
10:J:13:VAL:O	10:J:14:VAL:HG22	2.01	0.61
12:L:60:ARG:HG2	12:L:61:THR:H	1.64	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.61
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.27	0.61
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.66	0.61
2:B:345:LYS:O	2:B:347:LYS:HG2	2.01	0.61
2:B:424:LEU:O	2:B:428:ILE:HG13	2.00	0.61
3:C:148:ARG:CG	3:C:149:LYS:H	2.13	0.61
1:A:698:GLN:HA	9:I:97:MET:O	2.01	0.61
10:J:2:ILE:H	10:J:57:ILE:HG22	1.65	0.61
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.13	0.60
1:A:774:ARG:HB2	1:A:797:LYS:HB3	1.83	0.60
2:B:220:GLY:O	2:B:222:ILE:HG13	2.01	0.60
2:B:254:LEU:HD23	2:B:381:MET:CE	2.30	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.81	0.60
9:I:95:THR:HG22	9:I:96:SER:N	2.15	0.60
1:A:34:LYS:N	1:A:34:LYS:HD3	2.15	0.60
1:A:537:ARG:HH22	8:H:122:LEU:CD1	2.14	0.60
1:A:70:CYS:O	1:A:72:GLU:HG2	2.01	0.60
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.82	0.60
1:A:1444:MET:O	6:F:133:VAL:HG23	2.02	0.60
10:J:48:ARG:NE	10:J:49:MET:HE2	2.16	0.60
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HG22	1:A:952:ALA:HB2	1.83	0.60
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.82	0.60
2:B:735:ALA:O	2:B:738:PHE:HE1	1.84	0.60
7:G:51:TYR:C	7:G:51:TYR:CD2	2.75	0.60
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.82	0.60
1:A:1323:ASP:C	1:A:1325:THR:H	2.05	0.60
1:A:577:ILE:O	1:A:580:VAL:HG23	2.00	0.60
1:A:847:ASP:O	1:A:858:ASN:HA	2.00	0.60
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.31	0.60
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.82	0.60
2:B:453:ILE:O	2:B:457:LEU:HG	2.00	0.60
2:B:54:PHE:HA	2:B:58:THR:HB	1.84	0.60
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.82	0.60
7:G:28:THR:O	7:G:32:GLU:HG3	2.00	0.60
3:C:169:LYS:HZ3	12:L:69:ALA:HB3	1.67	0.60
1:A:108:MET:C	1:A:110:CYS:H	2.03	0.60
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.83	0.60
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.01	0.60
1:A:534:LEU:O	1:A:574:GLY:HA3	2.02	0.60
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.31	0.60
2:B:266:ALA:O	2:B:268:THR:HG22	2.02	0.60
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.17	0.60
1:A:262:LEU:C	1:A:264:PHE:H	2.03	0.60
1:A:364:VAL:O	1:A:364:VAL:HG13	2.02	0.60
1:A:416:ARG:HG3	1:A:417:TYR:CD2	2.36	0.60
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.82	0.60
7:G:34:VAL:HG11	7:G:74:TYR:OH	2.01	0.60
7:G:9:LEU:HG	7:G:10:ASN:N	2.16	0.60
10:J:7:CYS:SG	10:J:49:MET:HE3	2.42	0.60
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.00	0.60
1:A:86:LEU:HG	1:A:237:THR:O	2.02	0.60
2:B:274:PRO:O	2:B:275:TYR:HB2	2.02	0.60
3:C:167:HIS:HE1	12:L:70:ARG:HA	1.66	0.60
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.84	0.60
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.15	0.60
1:A:1445:ILE:HG21	7:G:18:PHE:CE2	2.37	0.60
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.01	0.60
9:I:55:THR:O	9:I:58:VAL:HG23	2.02	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.31	0.60
1:A:518:LYS:HE2	1:A:624:SER:O	2.02	0.60
1:A:738:LYS:HD2	1:A:738:LYS:N	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:C	2:B:643:ASP:H	2.05	0.60
2:B:770:GLN:HG2	2:B:983:ARG:O	2.02	0.60
5:E:17:ARG:HG2	5:E:35:VAL:HG13	1.83	0.60
6:F:85:MET:HE3	6:F:153:VAL:HG22	1.84	0.60
1:A:1444:MET:CG	7:G:60:ARG:HA	2.31	0.60
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.83	0.60
12:L:55:ILE:HD13	12:L:55:ILE:H	1.67	0.60
1:A:1373:ASP:O	1:A:1376:THR:HG22	2.02	0.60
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.84	0.60
1:A:409:SER:O	1:A:411:ASP:N	2.35	0.60
1:A:743:VAL:O	1:A:747:VAL:HG23	2.01	0.60
1:A:886:ILE:HG13	1:A:943:LEU:HB2	1.84	0.60
2:B:654:ARG:H	2:B:657:HIS:HD2	1.50	0.60
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.16	0.60
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.32	0.60
8:H:61:SER:O	8:H:62:SER:HB2	2.01	0.60
1:A:830:LYS:O	1:A:834:THR:HB	2.02	0.59
2:B:804:GLY:HA2	2:B:1042:GLY:O	2.02	0.59
1:A:447:GLN:NE2	16:T:20:DC:H4'	2.17	0.59
1:A:69:THR:O	1:A:71:GLN:N	2.35	0.59
2:B:190:TYR:CD2	10:J:62:ARG:HB3	2.37	0.59
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.02	0.59
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.84	0.59
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.35	0.59
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.36	0.59
2:B:942:ARG:NH2	16:T:24:DG:OP1	2.35	0.59
5:E:17:ARG:NH1	5:E:17:ARG:HG3	2.17	0.59
5:E:22:MET:CE	5:E:26:ARG:HH21	2.15	0.59
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.37	0.59
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.37	0.59
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.82	0.59
2:B:473:MET:HE3	2:B:474:SER:HA	1.85	0.59
3:C:251:LEU:HD12	3:C:251:LEU:O	2.02	0.59
5:E:15:ALA:O	5:E:19:VAL:HG23	2.01	0.59
5:E:22:MET:CE	5:E:26:ARG:HE	2.15	0.59
7:G:81:PRO:HG3	7:G:106:MET:SD	2.42	0.59
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.02	0.59
2:B:1166:CYS:O	2:B:1168:LEU:N	2.35	0.59
2:B:614:SER:OG	2:B:627:PHE:HB2	2.02	0.59
3:C:67:LEU:HD23	3:C:67:LEU:N	2.16	0.59
1:A:495:GLU:HB3	6:F:99:LEU:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.33	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
1:A:53:LEU:CD2	1:A:54:ASN:N	2.57	0.59
1:A:680:THR:HG23	2:B:729:ILE:CD1	2.32	0.59
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.50	0.59
2:B:43:LEU:HD13	2:B:492:LEU:HD13	1.84	0.59
8:H:59:ILE:CG2	8:H:60:ALA:H	2.09	0.59
9:I:17:ARG:HD2	9:I:28:GLU:OE1	2.03	0.59
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.18	0.59
1:A:925:LEU:HD13	1:A:983:ILE:HD12	1.85	0.59
2:B:1129:ARG:HG2	2:B:1131:GLY:N	2.17	0.59
2:B:799:PRO:HG2	10:J:56:LEU:HD11	1.84	0.59
3:C:243:VAL:HG12	3:C:243:VAL:O	2.02	0.59
8:H:143:LEU:C	8:H:144:ILE:HG13	2.23	0.59
1:A:55:ASP:N	1:A:56:PRO:CD	2.66	0.59
1:A:576:GLN:O	1:A:579:SER:HB2	2.02	0.59
1:A:790:ASP:OD2	9:I:87:GLN:HG3	2.03	0.59
1:A:965:GLN:O	1:A:968:GLN:HB2	2.02	0.59
2:B:278:GLN:CG	2:B:279:ASP:H	2.12	0.59
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.38	0.59
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.85	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.17	0.59
2:B:168:GLY:N	2:B:450:ALA:HB1	2.15	0.59
2:B:1165:ILE:HD13	4:D:17:LYS:CB	2.33	0.59
11:K:53:ASP:O	11:K:55:LYS:N	2.36	0.59
1:A:1083:THR:HG21	1:A:1095:THR:HA	1.85	0.59
1:A:1400:CYS:SG	1:A:1409:LEU:HD21	2.43	0.59
1:A:492:PRO:CB	1:A:497:THR:HG22	2.32	0.59
1:A:50:ILE:C	1:A:52:GLY:H	2.06	0.59
2:B:376:PHE:HB3	2:B:586:TRP:HZ3	1.67	0.59
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.85	0.59
2:B:955:THR:CG2	2:B:956:THR:N	2.65	0.59
3:C:193:TYR:C	3:C:193:TYR:CD1	2.76	0.59
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.38	0.59
1:A:1368:MET:CE	1:A:1368:MET:H	2.16	0.58
1:A:263:THR:HG22	1:A:263:THR:O	2.01	0.58
1:A:511:ILE:O	1:A:519:PRO:HA	2.03	0.58
2:B:1208:MET:O	2:B:1211:ASN:N	2.31	0.58
2:B:294:ASP:C	2:B:296:GLU:H	2.06	0.58
2:B:167:ILE:CG2	2:B:453:ILE:HD12	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.18	0.58
2:B:656:GLY:O	2:B:660:LYS:HB2	2.03	0.58
2:B:995:ARG:O	2:B:999:MET:HB2	2.03	0.58
6:F:111:LEU:H	6:F:111:LEU:CD1	2.16	0.58
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.38	0.58
9:I:111:THR:HG22	9:I:113:ASP:H	1.67	0.58
12:L:61:THR:HG22	12:L:62:LYS:N	2.18	0.58
1:A:800:VAL:HG13	1:A:812:GLU:OE1	2.03	0.58
1:A:918:GLU:HG3	1:A:918:GLU:O	2.03	0.58
2:B:35:SER:O	2:B:39:ARG:HG3	2.02	0.58
8:H:98:TYR:CD1	8:H:99:GLY:N	2.65	0.58
1:A:1313:LEU:O	1:A:1315:GLU:N	2.36	0.58
1:A:1423:GLY:O	1:A:1426:GLU:HG2	2.03	0.58
1:A:42:ASP:HB3	1:A:45:GLN:H	1.68	0.58
1:A:54:ASN:C	1:A:56:PRO:HD3	2.24	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.32	0.58
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.32	0.58
2:B:300:HIS:O	2:B:303:TYR:HE2	1.86	0.58
2:B:857:ARG:HG2	2:B:859:TYR:CE1	2.38	0.58
2:B:948:ILE:O	2:B:968:VAL:HG13	2.04	0.58
8:H:59:ILE:O	8:H:60:ALA:CB	2.50	0.58
10:J:1:MET:H3	10:J:56:LEU:H	1.50	0.58
12:L:31:CYS:HA	12:L:56:LEU:HD23	1.84	0.58
1:A:316:GLN:HB2	1:A:322:VAL:CG2	2.34	0.58
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.85	0.58
1:A:63:ARG:HG2	1:A:74:MET:HE1	1.85	0.58
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.02	0.58
2:B:1202:LEU:HD23	2:B:1206:GLU:CG	2.32	0.58
2:B:429:PHE:HA	2:B:432:MET:HE3	1.84	0.58
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.33	0.58
6:F:111:LEU:N	6:F:111:LEU:HD12	2.18	0.58
1:A:524:VAL:HG12	1:A:525:GLN:H	1.67	0.58
5:E:176:PRO:O	5:E:212:ARG:HA	2.03	0.58
8:H:18:GLY:O	8:H:19:ARG:HB2	2.02	0.58
16:T:17:DA:C8	16:T:18:DC:H5	2.21	0.58
1:A:903:ASN:ND2	1:A:903:ASN:C	2.57	0.58
2:B:744:HIS:CD2	2:B:746:SER:OG	2.53	0.58
4:D:118:THR:HB	4:D:121:LYS:HD2	1.84	0.58
5:E:85:GLU:HB2	5:E:88:VAL:HG22	1.85	0.58
1:A:567:LYS:CB	8:H:96:VAL:H	2.16	0.58
8:H:9:ILE:HG12	8:H:56:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.03	0.58
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.84	0.58
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.67	0.58
2:B:950:ASP:O	2:B:951:GLN:HB2	2.03	0.58
4:D:204:ASP:O	4:D:208:GLU:HB2	2.03	0.58
4:D:59:ILE:HG21	4:D:145:MET:SD	2.44	0.58
1:A:1265:ASN:O	1:A:1267:MET:N	2.36	0.58
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.67	0.58
1:A:242:PRO:HB3	2:B:1209:ALA:HB2	1.85	0.58
1:A:575:LYS:HE2	1:A:615:GLY:O	2.03	0.58
2:B:249:ARG:CZ	2:B:418:LYS:NZ	2.67	0.58
2:B:641:GLU:O	2:B:643:ASP:N	2.35	0.58
2:B:745:PRO:O	2:B:748:ILE:HG12	2.04	0.58
3:C:148:ARG:HG2	3:C:149:LYS:N	2.19	0.58
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.37	0.58
8:H:12:VAL:HG21	8:H:53:ASP:HB2	1.85	0.58
1:A:105:CYS:O	1:A:114:LEU:HG	2.04	0.58
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.86	0.58
2:B:487:THR:HG22	2:B:488:TYR:N	2.19	0.58
2:B:628:THR:O	2:B:629:ASP:O	2.21	0.58
7:G:1:MET:HE1	7:G:80:LYS:HE3	1.86	0.58
1:A:1322:ILE:HG13	1:A:1324:PRO:HD3	1.86	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
2:B:1169:MET:HE2	2:B:1204:PHE:CB	2.33	0.58
3:C:113:VAL:O	3:C:144:ILE:HB	2.04	0.58
1:A:1318:THR:HB	5:E:141:VAL:HG11	1.85	0.58
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.44	0.58
14:N:4:DT:H2"	14:N:5:DA:OP2	2.04	0.58
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.85	0.57
2:B:129:PHE:HA	2:B:165:VAL:O	2.04	0.57
2:B:298:LEU:CD2	2:B:298:LEU:N	2.67	0.57
2:B:601:ARG:O	2:B:605:ARG:HG3	2.03	0.57
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.39	0.57
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.33	0.57
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.85	0.57
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.34	0.57
1:A:107:CYS:N	1:A:114:LEU:HD21	2.20	0.57
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.05	0.57
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.57
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.86	0.57
2:B:976:ILE:O	2:B:976:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:36:CYS:HA	8:H:126:GLU:O	2.03	0.57
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.69	0.57
1:A:1152:ILE:HG13	9:I:44:TYR:HB3	1.85	0.57
1:A:105:CYS:SG	1:A:139:TRP:HA	2.44	0.57
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.69	0.57
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.68	0.57
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.34	0.57
3:C:111:THR:O	3:C:147:LEU:HD23	2.04	0.57
1:A:568:PRO:CG	8:H:46:LEU:HD22	2.34	0.57
1:A:1022:LEU:CD1	1:A:1026:LEU:HD12	2.33	0.57
1:A:1120:LEU:H	1:A:1120:LEU:HD13	1.68	0.57
1:A:352:VAL:O	1:A:467:THR:HB	2.04	0.57
1:A:855:THR:CG2	1:A:857:ARG:HE	2.17	0.57
2:B:225:VAL:HG12	2:B:238:ALA:HB2	1.86	0.57
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.04	0.57
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.34	0.57
11:K:10:PHE:CD2	11:K:10:PHE:N	2.72	0.57
16:T:25:DT:H2"	16:T:26:DC:O5'	2.04	0.57
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.86	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.39	0.57
11:K:31:VAL:HG12	11:K:32:VAL:N	2.19	0.57
14:N:2:DA:C1'	14:N:3:DC:H5"	2.35	0.57
1:A:1035:TYR:O	1:A:1037:LEU:N	2.38	0.57
1:A:1083:THR:HG23	1:A:1096:SER:H	1.69	0.57
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.85	0.57
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.38	0.57
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.85	0.57
2:B:292:ILE:HD11	2:B:327:ARG:HB2	1.86	0.57
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.19	0.57
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.40	0.57
5:E:105:PHE:O	5:E:106:GLN:CB	2.52	0.57
7:G:153:GLN:CG	7:G:154:VAL:N	2.67	0.57
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.25	0.57
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.86	0.57
2:B:286:PHE:CD1	2:B:297:ILE:HG23	2.39	0.57
2:B:644:GLU:C	2:B:646:LEU:H	2.07	0.57
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.87	0.57
2:B:882:THR:HG21	2:B:935:ARG:HA	1.87	0.57
3:C:100:THR:HB	3:C:119:VAL:HB	1.87	0.57
10:J:1:MET:H1	10:J:56:LEU:N	2.01	0.57
1:A:100:LYS:O	1:A:104:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:ARG:HB2	1:A:1403:GLU:OE1	2.04	0.57
1:A:331:GLY:O	1:A:332:LYS:HB3	2.03	0.57
2:B:99:LYS:HB3	2:B:100:PRO:HD2	1.85	0.57
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.40	0.57
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.63	0.57
2:B:860:MET:CG	2:B:965:LYS:HG2	2.35	0.57
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.35	0.57
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.34	0.57
1:A:41:MET:CE	1:A:41:MET:H	2.17	0.57
2:B:1096:ARG:HD2	2:B:1097:HIS:ND1	2.19	0.57
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.86	0.57
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.86	0.57
3:C:235:VAL:HG12	10:J:13:VAL:HG22	1.86	0.57
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.05	0.57
1:A:224:PHE:CD1	1:A:231:PRO:HG3	2.39	0.57
1:A:315:LEU:CD2	1:A:321:PRO:HA	2.35	0.57
1:A:897:TYR:CE2	1:A:1030:ARG:HD2	2.40	0.57
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.19	0.57
3:C:189:THR:HG22	3:C:190:ASP:N	2.19	0.57
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.19	0.56
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.69	0.56
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.05	0.56
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.35	0.56
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.05	0.56
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.05	0.56
2:B:215:GLN:HE22	2:B:499:ASN:CB	2.15	0.56
2:B:600:LEU:O	2:B:609:ILE:HD11	2.05	0.56
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.05	0.56
2:B:640:VAL:O	2:B:641:GLU:O	2.23	0.56
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.56
2:B:821:GLN:NE2	2:B:851:PHE:H	1.98	0.56
2:B:892:LYS:O	2:B:899:ILE:HG23	2.05	0.56
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.20	0.56
4:D:137:ASN:HD22	4:D:138:ASN:N	2.02	0.56
5:E:175:LEU:HD23	5:E:176:PRO:CD	2.28	0.56
8:H:11:GLN:O	8:H:28:ALA:HB1	2.05	0.56
1:A:1083:THR:O	1:A:1083:THR:HG22	2.05	0.56
1:A:315:LEU:HD23	1:A:321:PRO:HA	1.86	0.56
1:A:73:GLY:O	1:A:75:ASN:N	2.38	0.56
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.33	0.56
2:B:644:GLU:HB2	2:B:648:HIS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:LEU:C	2:B:663:ALA:N	2.59	0.56
2:B:882:THR:HG22	2:B:884:ARG:N	2.19	0.56
8:H:102:TYR:HE2	8:H:117:SER:HB2	1.71	0.56
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.45	0.56
1:A:551:TYR:CE2	11:K:62:LYS:HG2	2.40	0.56
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.87	0.56
1:A:853:ASP:O	1:A:1000:LEU:HD21	2.04	0.56
2:B:1002:THR:HG21	2:B:1006:ILE:HG13	1.87	0.56
2:B:776:GLN:O	2:B:1095:LEU:HA	2.05	0.56
4:D:37:GLN:HB2	7:G:5:LYS:NZ	2.20	0.56
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.40	0.56
10:J:53:HIS:CD2	10:J:54:VAL:N	2.73	0.56
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.87	0.56
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.04	0.56
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.40	0.56
1:A:316:GLN:OE1	1:A:320:ARG:HD3	2.05	0.56
1:A:590:ARG:HB3	1:A:605:MET:N	2.20	0.56
2:B:1004:GLU:HB2	2:B:1006:ILE:CG1	2.35	0.56
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.86	0.56
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.69	0.56
7:G:137:ILE:HD13	7:G:143:ILE:HD11	1.87	0.56
8:H:95:TYR:HE2	8:H:97:MET:CG	2.18	0.56
12:L:38:LEU:O	12:L:39:SER:CB	2.54	0.56
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.87	0.56
1:A:332:LYS:N	1:A:337:ARG:HB3	2.06	0.56
2:B:130:VAL:O	2:B:132:VAL:HG23	2.05	0.56
4:D:120:GLU:HA	4:D:123:LEU:HG	1.86	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56
4:D:66:ARG:C	4:D:68:ARG:H	2.08	0.56
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.87	0.56
9:I:64:SER:O	9:I:66:PRO:HD3	2.04	0.56
12:L:61:THR:HG22	12:L:62:LYS:H	1.71	0.56
16:T:27:DA:C4	16:T:28:DT:H71	2.41	0.56
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.35	0.56
1:A:219:PHE:HE1	1:A:230:ARG:HH21	1.51	0.56
1:A:39:GLU:O	1:A:53:LEU:HB3	2.04	0.56
1:A:895:LYS:HG2	1:A:895:LYS:O	2.06	0.56
2:B:1207:LEU:HD13	2:B:1212:ILE:HG21	1.87	0.56
2:B:400:HIS:O	2:B:402:GLY:N	2.39	0.56
1:A:1276:VAL:HB	1:A:1279:ILE:CD1	2.29	0.56
1:A:405:VAL:HG12	1:A:413:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HG3	1:A:276:LEU:CD2	2.36	0.56
2:B:1029:CYS:SG	2:B:1088:GLY:HA3	2.45	0.56
2:B:526:GLU:HA	2:B:771:SER:HB3	1.88	0.56
5:E:90:VAL:HB	5:E:119:SER:HB2	1.87	0.56
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.87	0.56
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.35	0.56
1:A:1164:PRO:O	1:A:1166:ASP:N	2.39	0.56
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.51	0.56
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.36	0.56
2:B:613:VAL:HG13	2:B:627:PHE:O	2.06	0.56
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.56
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.18	0.56
8:H:127:GLY:O	8:H:128:ASN:HB2	2.05	0.56
1:A:107:CYS:HA	1:A:171:GLN:OE1	2.06	0.56
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.93	0.56
1:A:391:LEU:HA	1:A:394:ASN:HD22	1.71	0.56
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.88	0.56
1:A:564:ALA:HB2	1:A:576:GLN:CD	2.26	0.56
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.36	0.56
2:B:124:TYR:HE2	2:B:179:CYS:HG	1.49	0.56
2:B:114:PRO:HG3	2:B:181:LEU:HD21	1.88	0.56
3:C:132:PRO:O	3:C:134:ILE:HG13	2.05	0.56
4:D:176:GLU:O	4:D:178:ALA:N	2.39	0.56
9:I:111:THR:CG2	9:I:112:SER:H	2.07	0.56
10:J:47:ARG:HG2	10:J:47:ARG:NH1	2.18	0.56
12:L:31:CYS:HA	12:L:56:LEU:CD2	2.35	0.56
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.88	0.56
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.06	0.56
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.36	0.56
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.41	0.56
1:A:842:VAL:C	1:A:844:ALA:H	2.10	0.56
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.69	0.56
2:B:999:MET:CE	2:B:1011:ILE:HD11	2.35	0.56
2:B:811:TYR:N	2:B:811:TYR:CD1	2.73	0.56
2:B:831:SER:HB3	2:B:994:TYR:OH	2.05	0.56
3:C:98:VAL:C	3:C:99:LEU:HD23	2.26	0.56
5:E:42:PHE:HZ	5:E:58:MET:HE1	1.71	0.56
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.29	0.56
8:H:84:ALA:HA	8:H:87:ARG:HD2	1.86	0.56
14:N:7:DT:O2	16:T:11:DG:N2	2.38	0.56
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HG2	1:A:1336:MET:O	2.06	0.56
1:A:590:ARG:HH22	1:A:620:LYS:HB3	1.68	0.56
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.34	0.56
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.71	0.56
11:K:42:LEU:HD23	11:K:42:LEU:O	2.06	0.56
1:A:485:ASP:OD1	15:P:10:C:H4'	2.04	0.56
1:A:858:ASN:ND2	1:A:858:ASN:C	2.60	0.55
2:B:95:ILE:HG13	2:B:129:PHE:O	2.05	0.55
2:B:287:ARG:HA	2:B:291:ILE:O	2.07	0.55
6:F:75:PRO:HG2	6:F:77:ASP:O	2.06	0.55
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.87	0.55
7:G:14:HIS:HD2	7:G:16:SER:HB3	1.71	0.55
9:I:56:ALA:CB	9:I:89:GLN:HG3	2.35	0.55
10:J:48:ARG:HE	10:J:49:MET:CE	2.19	0.55
1:A:1120:LEU:CD1	1:A:1120:LEU:N	2.69	0.55
1:A:443:LEU:CD1	1:A:455:MET:HB3	2.27	0.55
1:A:940:ARG:O	1:A:944:ARG:HG3	2.06	0.55
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.88	0.55
2:B:574:SER:HA	2:B:591:ARG:NH2	2.18	0.55
2:B:25:ILE:CG2	2:B:658:ILE:HD11	2.36	0.55
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.88	0.55
2:B:792:MET:HE1	16:T:24:DG:H5'	1.87	0.55
8:H:143:LEU:N	8:H:143:LEU:HD12	2.20	0.55
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	1.88	0.55
1:A:278:THR:O	1:A:278:THR:HG22	2.06	0.55
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.88	0.55
1:A:49:LYS:NZ	1:A:60:SER:HA	2.22	0.55
1:A:709:THR:HB	1:A:712:GLU:CG	2.31	0.55
1:A:787:PHE:HE1	1:A:796:SER:HA	1.69	0.55
1:A:93:VAL:HG23	1:A:304:MET:CE	2.36	0.55
2:B:945:GLU:O	2:B:946:ASN:HB3	2.04	0.55
3:C:242:GLN:C	3:C:244:VAL:H	2.08	0.55
1:A:1444:MET:HB3	7:G:59:GLY:O	2.07	0.55
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.07	0.55
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.55
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.79	0.55
1:A:2:VAL:HG23	2:B:1157:ALA:HB1	1.87	0.55
1:A:471:ASN:OD1	1:A:472:LEU:N	2.40	0.55
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.88	0.55
3:C:161:LYS:O	3:C:170:TRP:NE1	2.40	0.55
3:C:213:PRO:O	3:C:214:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.36	0.55
12:L:28:LYS:HG3	12:L:39:SER:CB	2.36	0.55
16:T:21:DC:C6	16:T:22:BRU:BR	3.14	0.55
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.06	0.55
1:A:549:MET:SD	1:A:577:ILE:HD12	2.47	0.55
1:A:940:ARG:HH11	1:A:940:ARG:HG2	1.70	0.55
2:B:240:ILE:O	2:B:240:ILE:HG23	2.07	0.55
2:B:556:THR:O	2:B:558:LEU:N	2.39	0.55
2:B:723:VAL:HG12	2:B:724:ASP:N	2.22	0.55
2:B:878:GLN:O	2:B:879:ARG:C	2.45	0.55
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.88	0.55
7:G:49:LEU:N	7:G:49:LEU:HD23	2.21	0.55
9:I:113:ASP:O	9:I:114:GLN:HG3	2.07	0.55
1:A:108:MET:HA	1:A:210:ILE:HD13	1.89	0.55
1:A:130:ASP:O	1:A:132:LYS:N	2.40	0.55
1:A:230:ARG:HG3	1:A:233:TRP:CH2	2.41	0.55
1:A:534:LEU:HG	1:A:574:GLY:HA3	1.89	0.55
1:A:655:PHE:O	1:A:658:LEU:HB3	2.07	0.55
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.89	0.55
9:I:106:CYS:SG	9:I:108:HIS:HB2	2.46	0.55
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.55
1:A:738:LYS:CB	1:A:740:LEU:HD23	2.26	0.55
7:G:145:VAL:CG1	7:G:146:LYS:N	2.69	0.55
8:H:12:VAL:CG2	8:H:53:ASP:HB2	2.37	0.55
1:A:148:CYS:O	1:A:168:GLY:HA2	2.07	0.55
1:A:90:VAL:HG12	1:A:91:PHE:N	2.22	0.55
2:B:1103:ILE:O	2:B:1103:ILE:HG23	2.06	0.55
2:B:465:ASN:HD22	2:B:465:ASN:N	2.03	0.55
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.87	0.55
7:G:1:MET:SD	7:G:1:MET:O	2.64	0.55
8:H:58:THR:HG22	8:H:59:ILE:H	1.72	0.55
2:B:294:ASP:H	9:I:12:ASN:ND2	2.05	0.55
1:A:789:LYS:HG3	9:I:67:THR:O	2.06	0.55
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.05	0.55
1:A:447:GLN:HA	1:A:448:PRO:C	2.27	0.55
1:A:590:ARG:NH1	1:A:590:ARG:HG3	2.21	0.55
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.33	0.55
2:B:345:LYS:C	2:B:347:LYS:H	2.09	0.55
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.88	0.55
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.27	0.55
2:B:975:GLN:O	2:B:977:GLY:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.89	0.55
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.06	0.55
1:A:102:VAL:HG11	1:A:211:PHE:CE2	2.41	0.55
1:A:243:PRO:O	1:A:246:VAL:HB	2.07	0.55
1:A:401:GLY:C	1:A:435:HIS:CD2	2.80	0.55
1:A:933:TYR:O	1:A:937:VAL:HG23	2.06	0.55
2:B:1021:MET:O	2:B:1023:VAL:HG23	2.07	0.55
2:B:1156:ASP:O	2:B:1157:ALA:HB3	2.07	0.55
2:B:1168:LEU:HD13	2:B:1208:MET:CE	2.37	0.55
2:B:345:LYS:O	2:B:347:LYS:N	2.31	0.55
4:D:146:GLN:O	4:D:149:THR:HG22	2.07	0.55
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.88	0.55
10:J:13:VAL:O	10:J:14:VAL:CG2	2.55	0.55
1:A:1121:GLU:HG2	1:A:1122:PRO:CD	2.36	0.54
1:A:475:THR:CG2	1:A:476:SER:N	2.70	0.54
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.72	0.54
1:A:995:GLU:O	1:A:998:LEU:HD21	2.07	0.54
2:B:707:PRO:HG2	2:B:708:GLU:H	1.72	0.54
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.89	0.54
2:B:864:LYS:N	2:B:872:GLU:OE1	2.38	0.54
3:C:112:ASN:N	3:C:112:ASN:ND2	2.55	0.54
3:C:251:LEU:HD11	11:K:45:LEU:CD2	2.38	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.88	0.54
8:H:40:LEU:HD22	8:H:123:MET:CE	2.33	0.54
11:K:29:ASN:O	11:K:76:GLN:HG3	2.07	0.54
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.07	0.54
1:A:1265:ASN:C	1:A:1267:MET:H	2.11	0.54
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.56	0.54
1:A:200:ARG:CB	1:A:200:ARG:HH11	2.19	0.54
1:A:315:LEU:HD22	1:A:319:GLY:O	2.08	0.54
1:A:857:ARG:HA	1:A:864:ILE:HD12	1.89	0.54
2:B:1115:THR:O	2:B:1116:ARG:CB	2.55	0.54
2:B:1151:LEU:N	2:B:1151:LEU:CD1	2.70	0.54
3:C:167:HIS:CD2	3:C:168:ALA:N	2.75	0.54
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.35	0.54
3:C:75:MET:O	3:C:246:ARG:NH2	2.30	0.54
7:G:132:SER:HB3	7:G:135:ASP:H	1.72	0.54
8:H:112:ILE:HG22	8:H:113:ALA:N	2.23	0.54
8:H:82:PRO:C	8:H:84:ALA:H	2.11	0.54
16:T:16:DT:H2"	16:T:17:DA:OP2	2.06	0.54
1:A:12:ARG:HG3	2:B:1192:TYR:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.38	0.54
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.36	0.54
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.42	0.54
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.41	0.54
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.89	0.54
2:B:292:ILE:HD11	2:B:327:ARG:H	1.72	0.54
2:B:312:GLU:O	2:B:315:LYS:HB2	2.06	0.54
2:B:25:ILE:HD11	2:B:653:VAL:C	2.28	0.54
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.42	0.54
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.72	0.54
11:K:91:CYS:O	11:K:94:ILE:HB	2.08	0.54
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.06	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
2:B:105:SER:O	2:B:106:ASP:CB	2.55	0.54
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.89	0.54
2:B:175:ARG:NH1	2:B:175:ARG:HG3	2.22	0.54
2:B:23:ALA:O	2:B:654:ARG:HD2	2.08	0.54
2:B:557:PHE:O	2:B:557:PHE:HD2	1.90	0.54
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.95	0.54
3:C:257:SER:O	3:C:261:ALA:N	2.36	0.54
4:D:153:ARG:C	4:D:154:PHE:CD1	2.81	0.54
4:D:52:LEU:H	4:D:182:SER:HB3	1.73	0.54
7:G:13:LEU:HD22	7:G:14:HIS:O	2.06	0.54
9:I:106:CYS:O	9:I:107:SER:CB	2.54	0.54
1:A:1067:LEU:C	1:A:1067:LEU:HD12	2.28	0.54
1:A:1074:GLU:C	1:A:1076:ALA:H	2.10	0.54
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.89	0.54
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.08	0.54
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.07	0.54
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.89	0.54
4:D:202:ILE:O	4:D:202:ILE:HG23	2.07	0.54
8:H:62:SER:OG	8:H:63:LEU:HG	2.07	0.54
8:H:81:PRO:CB	8:H:82:PRO:CD	2.85	0.54
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.89	0.54
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.08	0.54
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.90	0.54
1:A:841:LEU:O	1:A:845:LEU:HG	2.06	0.54
2:B:465:ASN:N	2:B:465:ASN:ND2	2.55	0.54
2:B:473:MET:CE	2:B:474:SER:HA	2.37	0.54
3:C:108:GLU:O	3:C:109:SER:HB3	2.08	0.54
8:H:61:SER:HB3	8:H:139:ASN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H1	10:J:57:ILE:N	2.04	0.54
10:J:27:GLU:C	10:J:29:GLU:H	2.10	0.54
1:A:311:GLN:O	1:A:312:PRO:C	2.46	0.54
1:A:666:ILE:HD12	1:A:666:ILE:N	2.22	0.54
2:B:1099:VAL:O	2:B:1101:ASP:N	2.41	0.54
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.38	0.54
2:B:637:LEU:HD22	2:B:742:GLU:HA	1.90	0.54
3:C:97:VAL:CG1	3:C:99:LEU:HD21	2.38	0.54
7:G:114:LEU:HB3	7:G:162:SER:HB3	1.90	0.54
9:I:74:GLU:O	9:I:74:GLU:HG3	2.06	0.54
1:A:266:LEU:CD2	1:A:303:TYR:CE1	2.91	0.54
1:A:332:LYS:O	1:A:333:GLU:CB	2.52	0.54
1:A:537:ARG:NH2	8:H:25:ARG:HH21	2.06	0.54
1:A:714:PHE:O	1:A:718:VAL:HG23	2.08	0.54
1:A:343:LYS:HE3	2:B:1151:LEU:CA	2.38	0.54
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.89	0.54
3:C:16:ASP:O	3:C:17:ASN:CG	2.46	0.54
4:D:4:SER:O	4:D:5:THR:CB	2.56	0.54
8:H:111:LEU:HD23	8:H:127:GLY:O	2.07	0.54
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.90	0.54
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.89	0.54
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.22	0.54
1:A:670:ILE:HG23	1:A:805:LEU:CD2	2.36	0.54
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.73	0.54
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.43	0.54
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.90	0.54
1:A:560:ILE:CG1	8:H:78:SER:HB2	2.38	0.54
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.72	0.54
1:A:1230:GLU:O	1:A:1232:ASN:N	2.40	0.54
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.10	0.54
2:B:193:LYS:CD	2:B:787:VAL:HG11	2.38	0.54
2:B:479:VAL:O	2:B:480:SER:HB3	2.08	0.54
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.90	0.54
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.38	0.54
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.72	0.54
5:E:157:SER:C	5:E:159:ASP:N	2.61	0.54
7:G:1:MET:HE1	7:G:80:LYS:H	1.72	0.54
8:H:89:LEU:C	8:H:91:ASP:N	2.58	0.54
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.07	0.53
1:A:1340:GLY:O	1:A:1342:GLU:N	2.41	0.53
1:A:1376:THR:HG23	1:A:1377:THR:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:PRO:O	1:A:1436:ILE:HD12	2.08	0.53
1:A:92:HIS:HB2	1:A:236:LEU:CD2	2.34	0.53
2:B:858:SER:HA	2:B:966:VAL:O	2.08	0.53
3:C:114:TYR:HB3	3:C:140:ASN:O	2.08	0.53
4:D:147:TYR:CD2	4:D:147:TYR:C	2.80	0.53
7:G:153:GLN:HB3	7:G:156:SER:O	2.08	0.53
8:H:26:ILE:HG22	8:H:27:GLU:N	2.23	0.53
12:L:68:GLU:N	12:L:68:GLU:OE1	2.36	0.53
14:N:7:DT:H2"	14:N:8:DT:OP2	2.07	0.53
1:A:1334:ASP:O	1:A:1337:GLU:N	2.40	0.53
1:A:523:ILE:CG2	1:A:527:THR:HB	2.39	0.53
2:B:871:THR:HG22	2:B:872:GLU:N	2.22	0.53
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.89	0.53
5:E:120:ALA:O	5:E:123:LEU:HG	2.07	0.53
10:J:53:HIS:HD2	10:J:54:VAL:N	2.06	0.53
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.70	0.53
1:A:1340:GLY:HA3	5:E:184:VAL:HG23	1.89	0.53
1:A:543:LEU:O	1:A:547:LEU:HG	2.07	0.53
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.43	0.53
2:B:326:ASP:OD2	2:B:328:GLU:HB2	2.09	0.53
2:B:516:ASN:ND2	2:B:516:ASN:N	2.43	0.53
2:B:859:TYR:HD1	2:B:859:TYR:H	1.57	0.53
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.44	0.53
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.43	0.53
4:D:7:THR:CB	7:G:42:PHE:HE2	2.21	0.53
1:A:1164:PRO:C	1:A:1166:ASP:H	2.12	0.53
2:B:423:LYS:HB2	2:B:423:LYS:HZ2	1.72	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CG	2.39	0.53
2:B:848:ARG:HH22	2:B:996:ARG:HD2	1.72	0.53
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.36	0.53
5:E:161:LYS:C	5:E:163:GLU:H	2.09	0.53
8:H:100:THR:OG1	8:H:138:GLU:HG3	2.09	0.53
12:L:58:LYS:O	12:L:59:ALA:O	2.26	0.53
1:A:225:ASN:ND2	1:A:228:PHE:H	2.05	0.53
1:A:545:GLN:HG2	1:A:549:MET:CE	2.39	0.53
2:B:469:GLN:O	2:B:470:LYS:O	2.27	0.53
2:B:542:MET:HG2	2:B:747:MET:CE	2.35	0.53
3:C:82:TYR:CE2	3:C:161:LYS:HB3	2.44	0.53
5:E:105:PHE:O	5:E:106:GLN:HB2	2.09	0.53
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.08	0.53
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.85	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.53
2:B:693:ILE:HD13	2:B:701:ILE:CD1	2.38	0.53
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.49	0.53
4:D:120:GLU:HG3	4:D:123:LEU:HD12	1.89	0.53
7:G:1:MET:O	7:G:3:PHE:CD1	2.62	0.53
11:K:68:PHE:HB3	11:K:70:ARG:NH1	2.23	0.53
1:A:11:LEU:HD12	1:A:12:ARG:N	2.23	0.53
1:A:1265:ASN:C	1:A:1267:MET:N	2.61	0.53
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.38	0.53
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.17	0.53
2:B:199:MET:CE	2:B:492:LEU:HD23	2.39	0.53
2:B:388:CYS:C	2:B:390:LEU:H	2.10	0.53
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.23	0.53
3:C:148:ARG:CG	3:C:149:LYS:N	2.72	0.53
5:E:17:ARG:HG3	5:E:17:ARG:HH11	1.72	0.53
5:E:94:LYS:HG3	5:E:98:ILE:CD1	2.38	0.53
7:G:77:VAL:HG12	7:G:77:VAL:O	2.07	0.53
11:K:12:LEU:HD22	11:K:16:GLU:O	2.09	0.53
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.08	0.53
1:A:839:ARG:NH1	1:A:1402:PHE:HD1	2.07	0.53
1:A:1436:ILE:O	1:A:1437:GLY:C	2.46	0.53
1:A:405:VAL:CG1	1:A:413:ILE:HD12	2.39	0.53
1:A:981:LEU:HD12	1:A:1032:LEU:HD21	1.90	0.53
2:B:1010:LEU:CD2	2:B:1092:TYR:CE1	2.92	0.53
2:B:253:THR:HG22	2:B:254:LEU:N	2.23	0.53
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.90	0.53
2:B:616:ILE:HD13	2:B:625:LYS:HB2	1.91	0.53
5:E:78:LEU:HA	5:E:107:THR:HB	1.90	0.53
5:E:78:LEU:HD23	5:E:78:LEU:C	2.29	0.53
9:I:32:CYS:SG	9:I:33:SER:N	2.81	0.53
12:L:38:LEU:CD1	12:L:49:LYS:HG2	2.38	0.53
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.09	0.53
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.74	0.53
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.44	0.53
1:A:66:LYS:O	1:A:67:CYS:HB2	2.09	0.53
2:B:581:PHE:O	2:B:626:ILE:HB	2.08	0.53
2:B:745:PRO:C	2:B:747:MET:H	2.12	0.53
2:B:770:GLN:CD	2:B:983:ARG:HA	2.28	0.53
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.38	0.53
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:HIS:ND1	11:K:61:TYR:OH	2.38	0.53
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.37	0.53
1:A:2:VAL:CG2	2:B:1157:ALA:HB1	2.38	0.53
1:A:41:MET:HE3	1:A:41:MET:H	1.73	0.53
1:A:41:MET:O	1:A:42:ASP:C	2.47	0.53
1:A:56:PRO:O	1:A:57:ARG:CG	2.54	0.53
1:A:735:VAL:HG12	1:A:735:VAL:O	2.09	0.53
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.21	0.53
2:B:828:ALA:O	2:B:834:ASN:ND2	2.40	0.53
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.09	0.53
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.90	0.53
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.91	0.53
9:I:50:THR:HG22	9:I:51:ASN:N	2.21	0.53
1:A:698:GLN:HE21	9:I:99:LEU:HD21	1.74	0.53
1:A:1022:LEU:HD12	1:A:1026:LEU:HD12	1.90	0.52
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.09	0.52
1:A:1373:ASP:CA	1:A:1376:THR:HG22	2.40	0.52
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.74	0.52
2:B:332:ASP:O	2:B:333:PHE:C	2.48	0.52
2:B:50:SER:O	2:B:410:GLY:HA3	2.09	0.52
2:B:857:ARG:HG3	2:B:858:SER:N	2.25	0.52
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.44	0.52
8:H:128:ASN:CG	8:H:128:ASN:O	2.47	0.52
9:I:58:VAL:HG13	9:I:62:ILE:HG21	1.91	0.52
11:K:65:HIS:HD2	11:K:67:PHE:H	1.54	0.52
1:A:1004:ASN:ND2	5:E:167:ARG:CD	2.67	0.52
1:A:93:VAL:HG21	1:A:301:ALA:HA	1.90	0.52
2:B:166:PHE:C	2:B:167:ILE:HG13	2.28	0.52
2:B:619:ILE:C	2:B:621:GLU:H	2.12	0.52
2:B:955:THR:HG22	2:B:956:THR:O	2.09	0.52
1:A:1059:HIS:HE1	6:F:155:LEU:HD21	1.74	0.52
7:G:101:VAL:HG12	7:G:102:GLN:N	2.22	0.52
7:G:47:CYS:O	7:G:76:ALA:HB1	2.09	0.52
1:A:1006:ILE:HD12	5:E:167:ARG:HG3	1.91	0.52
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.09	0.52
1:A:114:LEU:O	1:A:115:LEU:HG	2.08	0.52
1:A:1332:PHE:HD2	1:A:1332:PHE:N	2.06	0.52
1:A:351:THR:HG21	2:B:1103:ILE:CD1	2.38	0.52
1:A:913:LEU:CD2	1:A:919:ILE:HD12	2.39	0.52
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.89	0.52
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:THR:HG23	2:B:729:ILE:HD11	1.91	0.52
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.08	0.52
2:B:99:LYS:C	2:B:126:SER:HB3	2.30	0.52
5:E:157:SER:OG	5:E:160:GLU:HG3	2.10	0.52
7:G:50:ASP:OD1	7:G:50:ASP:O	2.28	0.52
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.76	0.52
1:A:320:ARG:NH2	1:A:323:LYS:HE3	2.24	0.52
1:A:326:ARG:NH2	1:A:330:LYS:HE3	2.24	0.52
1:A:334:GLY:O	1:A:336:ILE:N	2.42	0.52
1:A:935:GLN:O	1:A:938:LYS:N	2.42	0.52
2:B:189:LEU:O	2:B:192:LEU:N	2.41	0.52
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.91	0.52
4:D:139:LYS:HD3	4:D:140:ASP:N	2.25	0.52
5:E:91:LYS:C	5:E:93:MET:N	2.63	0.52
7:G:113:HIS:C	7:G:114:LEU:HD12	2.30	0.52
7:G:74:TYR:H	7:G:74:TYR:HD2	1.56	0.52
12:L:30:ILE:HG22	12:L:31:CYS:N	2.24	0.52
16:T:26:DC:H2''	16:T:27:DA:H5'	1.91	0.52
2:B:486:TYR:CE1	2:B:1096:ARG:NH2	2.77	0.52
2:B:295:GLY:O	2:B:299:GLU:HG2	2.09	0.52
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.92	0.52
7:G:39:THR:O	7:G:43:GLY:N	2.32	0.52
8:H:48:PRO:O	8:H:49:VAL:HG23	2.09	0.52
3:C:66:ARG:NH2	10:J:3:VAL:O	2.42	0.52
11:K:84:LYS:O	11:K:87:LEU:HB3	2.10	0.52
1:A:1030:ARG:HB3	1:A:1030:ARG:HH11	1.75	0.52
1:A:726:ARG:HD2	13:M:4:TRX:CE3	2.39	0.52
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.92	0.52
2:B:597:MET:HE2	2:B:601:ARG:HG3	1.90	0.52
2:B:705:MET:N	2:B:710:LEU:HD12	2.25	0.52
10:J:20:SER:O	10:J:24:LEU:HG	2.10	0.52
10:J:44:TYR:HD2	10:J:44:TYR:H	1.58	0.52
1:A:1437:GLY:O	1:A:1439:GLY:N	2.43	0.52
1:A:28:ARG:HH21	1:A:238:CYS:HB2	1.75	0.52
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.45	0.52
1:A:986:ILE:HG22	1:A:987:VAL:N	2.24	0.52
2:B:582:VAL:O	2:B:582:VAL:HG12	2.08	0.52
2:B:865:LYS:HG3	2:B:871:THR:OG1	2.10	0.52
2:B:913:GLY:HA2	2:B:938:SER:OG	2.10	0.52
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.43	0.52
5:E:121:MET:C	5:E:123:LEU:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.20	0.52
7:G:88:ASP:OD2	7:G:88:ASP:N	2.42	0.52
9:I:106:CYS:O	9:I:107:SER:HB2	2.08	0.52
9:I:14:LEU:HD22	9:I:28:GLU:O	2.10	0.52
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.50	0.52
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.10	0.52
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.91	0.52
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.57	0.52
1:A:913:LEU:HD11	1:A:981:LEU:O	2.10	0.52
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.92	0.52
2:B:864:LYS:O	2:B:872:GLU:HG3	2.09	0.52
3:C:55:THR:O	3:C:55:THR:HG22	2.10	0.52
10:J:52:THR:O	10:J:52:THR:CG2	2.56	0.52
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.39	0.52
1:A:1082:ASN:HB3	1:A:1084:PHE:CD1	2.41	0.52
1:A:1424:VAL:HG11	2:B:1139:ILE:HG21	1.92	0.52
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.25	0.52
1:A:849:MET:HG3	1:A:849:MET:O	2.09	0.52
2:B:274:PRO:HG3	2:B:359:GLU:HB3	1.91	0.52
2:B:210:LYS:HA	2:B:481:GLN:O	2.09	0.52
2:B:731:VAL:HG12	2:B:732:SER:H	1.74	0.52
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.52
3:C:124:LEU:O	3:C:127:ARG:HG2	2.09	0.52
3:C:251:LEU:HG	11:K:98:LEU:HD11	1.92	0.52
7:G:27:LYS:O	7:G:30:LEU:HB3	2.10	0.52
4:D:23:ASN:O	7:G:83:LYS:HB2	2.10	0.52
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.56	0.52
1:A:711:ARG:O	1:A:714:PHE:HB3	2.09	0.52
1:A:93:VAL:HG23	1:A:304:MET:HE2	1.91	0.52
2:B:167:ILE:HA	2:B:450:ALA:CB	2.40	0.52
2:B:298:LEU:CD1	2:B:314:LEU:HD13	2.40	0.52
2:B:372:SER:O	2:B:375:ALA:HB3	2.10	0.52
4:D:66:ARG:HD2	4:D:133:THR:HB	1.92	0.52
4:D:64:VAL:O	4:D:68:ARG:HG3	2.10	0.52
5:E:96:PHE:CE2	5:E:110:PHE:HB2	2.45	0.52
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.92	0.52
8:H:100:THR:HG22	8:H:101:ALA:N	2.25	0.52
1:A:302:THR:HG22	1:A:303:TYR:H	1.75	0.51
1:A:493:GLN:H	1:A:497:THR:HG21	1.75	0.51
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.91	0.51
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:THR:HG22	1:A:784:LEU:HG	1.92	0.51
2:B:1167:GLY:O	2:B:1168:LEU:HD23	2.09	0.51
2:B:549:THR:HG22	2:B:550:ASP:N	2.19	0.51
2:B:882:THR:OG1	2:B:934:LYS:N	2.42	0.51
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.75	0.51
3:C:73:GLN:HE21	3:C:75:MET:N	2.08	0.51
7:G:111:THR:CB	7:G:114:LEU:HD13	2.39	0.51
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.93	0.51
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.35	0.51
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.91	0.51
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.91	0.51
2:B:97:VAL:HG12	2:B:97:VAL:O	2.08	0.51
4:D:64:VAL:C	4:D:66:ARG:H	2.12	0.51
5:E:93:MET:HE3	5:E:120:ALA:HB1	1.91	0.51
6:F:84:TYR:CE1	6:F:152:ILE:HD12	2.44	0.51
6:F:96:THR:O	6:F:100:GLN:HG3	2.11	0.51
7:G:44:TYR:O	7:G:78:VAL:HG12	2.10	0.51
10:J:27:GLU:O	10:J:29:GLU:N	2.43	0.51
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.45	0.51
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.51
1:A:264:PHE:C	1:A:266:LEU:H	2.13	0.51
1:A:43:GLU:HB2	1:A:46:THR:HB	1.91	0.51
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.75	0.51
1:A:541:ILE:CD1	1:A:577:ILE:HD11	2.38	0.51
1:A:642:CYS:O	1:A:645:LEU:HB3	2.10	0.51
2:B:258:LEU:HG	2:B:258:LEU:O	2.10	0.51
2:B:583:ASN:HD21	2:B:628:THR:HB	1.75	0.51
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.44	0.51
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.10	0.51
3:C:133:ILE:HD12	3:C:237:SER:H	1.71	0.51
3:C:193:TYR:HD1	3:C:193:TYR:C	2.14	0.51
7:G:88:ASP:CB	7:G:144:ARG:HA	2.24	0.51
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.92	0.51
1:A:447:GLN:HE21	16:T:20:DC:H4'	1.74	0.51
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.74	0.51
1:A:1107:VAL:HG13	1:A:1333:ILE:HD11	1.91	0.51
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.45	0.51
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.93	0.51
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.46	0.51
1:A:683:ILE:O	1:A:687:LYS:HG3	2.11	0.51
1:A:91:PHE:HB3	1:A:96:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:THR:HG22	2:B:537:LYS:N	2.20	0.51
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.75	0.51
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.46	0.51
2:B:755:ILE:HG22	2:B:809:MET:CE	2.41	0.51
2:B:997:GLU:HB3	3:C:35:ARG:HB3	1.92	0.51
1:A:370:ILE:HD12	1:A:468:PHE:CE2	2.45	0.51
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.92	0.51
1:A:666:ILE:CD1	1:A:667:GLY:H	2.21	0.51
1:A:886:ILE:CG2	1:A:887:GLY:N	2.73	0.51
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.93	0.51
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.24	0.51
1:A:1409:LEU:CD1	2:B:1207:LEU:HD11	2.41	0.51
2:B:210:LYS:HE2	2:B:462:ALA:O	2.11	0.51
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.26	0.51
3:C:36:VAL:HG21	3:C:251:LEU:CD2	2.39	0.51
3:C:82:TYR:CD2	3:C:161:LYS:HB3	2.46	0.51
8:H:82:PRO:O	8:H:84:ALA:N	2.38	0.51
1:A:215:SER:O	1:A:218:ASP:HB2	2.09	0.51
1:A:425:GLN:N	1:A:425:GLN:OE1	2.44	0.51
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.76	0.51
1:A:605:MET:HG2	1:A:621:THR:CG2	2.40	0.51
1:A:684:ALA:O	1:A:687:LYS:HB2	2.11	0.51
1:A:693:VAL:O	1:A:693:VAL:HG12	2.10	0.51
1:A:866:PHE:O	1:A:867:ILE:HD12	2.09	0.51
2:B:1198:TYR:HE2	2:B:1202:LEU:HD12	1.75	0.51
2:B:1158:PHE:HE2	2:B:1201:LYS:HD2	1.75	0.51
4:D:52:LEU:HD22	4:D:147:TYR:HE2	1.75	0.51
5:E:42:PHE:HZ	5:E:58:MET:CE	2.22	0.51
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.75	0.51
11:K:7:PHE:HA	11:K:10:PHE:HE2	1.76	0.51
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.93	0.51
1:A:49:LYS:NZ	1:A:61:ILE:H	2.09	0.51
1:A:622:VAL:HG13	1:A:622:VAL:O	2.11	0.51
2:B:1005:GLY:O	2:B:1006:ILE:C	2.49	0.51
2:B:1166:CYS:SG	2:B:1185:CYS:SG	3.09	0.51
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.40	0.51
2:B:774:GLY:C	2:B:776:GLN:H	2.14	0.51
4:D:130:LEU:HD21	4:D:141:LEU:HD23	1.92	0.51
6:F:147:SER:OG	6:F:150:GLU:HG3	2.10	0.51
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.92	0.51
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.25	0.51
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.24	0.51
1:A:470:LEU:HD12	1:A:470:LEU:C	2.31	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.64	0.51
2:B:1178:ASN:O	2:B:1179:GLN:C	2.49	0.51
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.93	0.51
2:B:40:GLU:OE1	2:B:681:TRP:HB3	2.11	0.51
2:B:552:MET:C	2:B:554:ILE:H	2.13	0.51
2:B:558:LEU:HD11	2:B:626:ILE:HD11	1.92	0.51
2:B:812:LEU:O	2:B:814:PHE:N	2.44	0.51
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.43	0.51
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.31	0.51
5:E:147:HIS:CD2	5:E:149:LEU:H	2.29	0.51
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.40	0.51
1:A:830:LYS:HD2	1:A:1079:MET:O	2.11	0.51
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.11	0.51
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.44	0.51
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.92	0.51
1:A:444:PHE:CB	1:A:458:HIS:CD2	2.94	0.51
1:A:471:ASN:O	1:A:474:VAL:HG12	2.11	0.51
1:A:647:GLY:O	1:A:651:LYS:HG3	2.11	0.51
1:A:901:LEU:HD11	1:A:983:ILE:CD1	2.40	0.51
2:B:1162:ILE:CD1	2:B:1194:ILE:HD13	2.35	0.51
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.45	0.51
2:B:217:ARG:C	2:B:217:ARG:HD2	2.32	0.51
2:B:209:GLU:OE2	2:B:483:LEU:HD23	2.10	0.51
2:B:522:VAL:HG13	2:B:538:ASN:O	2.10	0.51
2:B:859:TYR:CD1	2:B:859:TYR:N	2.78	0.51
2:B:878:GLN:N	2:B:878:GLN:OE1	2.44	0.51
2:B:954:VAL:HA	2:B:964:VAL:HG22	1.93	0.51
3:C:110:THR:HG22	3:C:112:ASN:HD21	1.75	0.51
9:I:100:PHE:CD1	9:I:100:PHE:N	2.79	0.51
16:T:9:DA:H1'	16:T:10:DA:H5'	1.93	0.51
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.59	0.51
1:A:1410:PHE:C	1:A:1412:ALA:H	2.15	0.51
1:A:147:VAL:O	1:A:149:GLU:N	2.44	0.51
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.15	0.51
1:A:809:THR:O	1:A:810:PRO:C	2.50	0.51
1:A:827:THR:HA	1:A:830:LYS:HE2	1.93	0.51
1:A:976:THR:OG1	1:A:977:LYS:N	2.44	0.51
1:A:15:LYS:HB3	2:B:1220:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:HIS:O	2:B:735:ALA:N	2.44	0.51
3:C:100:THR:HG22	3:C:101:LEU:N	2.25	0.51
4:D:118:THR:CB	4:D:121:LYS:HD2	2.41	0.51
7:G:1:MET:O	7:G:3:PHE:CE1	2.64	0.51
16:T:26:DC:H2''	16:T:27:DA:C5'	2.41	0.51
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.10	0.50
1:A:1130:GLN:NE2	1:A:1134:ILE:HD11	2.26	0.50
1:A:315:LEU:HD13	1:A:319:GLY:O	2.11	0.50
2:B:1168:LEU:HD13	2:B:1208:MET:HE1	1.93	0.50
2:B:204:ILE:HG23	2:B:207:GLY:O	2.12	0.50
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.73	0.50
2:B:705:MET:H	2:B:710:LEU:CD1	2.24	0.50
5:E:17:ARG:CG	5:E:17:ARG:HH11	2.23	0.50
5:E:200:ARG:HH11	5:E:200:ARG:HG3	1.76	0.50
5:E:33:GLU:O	5:E:36:GLU:N	2.45	0.50
7:G:17:PHE:N	7:G:17:PHE:CD2	2.79	0.50
9:I:113:ASP:OD1	9:I:114:GLN:N	2.44	0.50
14:N:1:DA:H1'	14:N:2:DA:O5'	2.11	0.50
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.75	0.50
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.11	0.50
1:A:856:THR:HB	1:A:865:GLN:HB2	1.92	0.50
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.76	0.50
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.76	0.50
2:B:549:THR:O	2:B:628:THR:HG21	2.11	0.50
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.92	0.50
2:B:873:THR:HG22	2:B:874:PHE:N	2.25	0.50
3:C:179:GLU:HG2	3:C:180:TYR:N	2.26	0.50
4:D:201:LYS:O	4:D:202:ILE:CB	2.59	0.50
4:D:48:ILE:O	4:D:48:ILE:HG22	2.11	0.50
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.93	0.50
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.11	0.50
7:G:14:HIS:CD2	7:G:16:SER:CB	2.94	0.50
7:G:114:LEU:HB3	7:G:162:SER:CB	2.42	0.50
7:G:56:ILE:O	7:G:57:GLN:HB2	2.11	0.50
9:I:15:TYR:CD1	9:I:15:TYR:N	2.77	0.50
10:J:27:GLU:O	10:J:29:GLU:HG3	2.10	0.50
1:A:1368:MET:HE3	1:A:1368:MET:H	1.76	0.50
1:A:248:PRO:O	1:A:260:ASP:HB2	2.11	0.50
1:A:285:PRO:O	1:A:287:HIS:N	2.45	0.50
1:A:841:LEU:HD22	1:A:1371:LEU:HD22	1.94	0.50
1:A:942:PHE:CD2	1:A:943:LEU:HD23	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:GLN:HA	2:B:215:GLN:NE2	2.26	0.50
2:B:377:PHE:O	2:B:380:TYR:N	2.44	0.50
3:C:32:SER:OG	11:K:45:LEU:HD13	2.12	0.50
5:E:147:HIS:HB3	5:E:150:VAL:CG2	2.32	0.50
5:E:165:LEU:HD22	5:E:170:LEU:HB2	1.93	0.50
6:F:72:LYS:CE	6:F:142:SER:HB3	2.42	0.50
8:H:14:GLU:HG2	8:H:15:VAL:N	2.26	0.50
3:C:10:ILE:CD1	11:K:108:GLU:HB3	2.37	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.46	0.50
2:B:334:ILE:HG22	2:B:334:ILE:O	2.10	0.50
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.47	0.50
6:F:72:LYS:O	6:F:73:ALA:HB2	2.12	0.50
8:H:12:VAL:HG13	8:H:26:ILE:HG21	1.93	0.50
11:K:87:LEU:O	11:K:87:LEU:HD12	2.11	0.50
16:T:20:DC:H2''	16:T:21:DC:C5'	2.40	0.50
1:A:332:LYS:HA	1:A:337:ARG:HD2	1.94	0.50
1:A:44:THR:O	1:A:45:GLN:HB2	2.10	0.50
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.59	0.50
1:A:1436:ILE:CG2	2:B:1142:GLY:HA2	2.42	0.50
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.77	0.50
2:B:249:ARG:CZ	2:B:418:LYS:HZ1	2.24	0.50
2:B:289:LEU:HD21	2:B:371:GLU:O	2.11	0.50
2:B:614:SER:HA	2:B:697:GLU:OE1	2.11	0.50
4:D:134:THR:O	4:D:136:GLY:N	2.45	0.50
4:D:193:THR:HG22	4:D:194:LEU:HD23	1.94	0.50
4:D:53:SER:HB3	4:D:152:SER:HB2	1.94	0.50
4:D:64:VAL:C	4:D:66:ARG:N	2.65	0.50
12:L:34:CYS:O	12:L:36:SER:N	2.44	0.50
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.77	0.50
1:A:255:SER:OG	2:B:918:ILE:HD13	2.12	0.50
1:A:343:LYS:HE3	2:B:1151:LEU:HA	1.94	0.50
1:A:390:GLN:HA	1:A:390:GLN:OE1	2.11	0.50
1:A:475:THR:HG23	1:A:476:SER:H	1.76	0.50
1:A:541:ILE:HD13	1:A:549:MET:CE	2.40	0.50
1:A:84:ILE:O	1:A:84:ILE:CG2	2.60	0.50
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.50
2:B:1001:PHE:O	2:B:1072:MET:HA	2.12	0.50
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.94	0.50
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	1.94	0.50
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.12	0.50
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:GLU:OE1	2:B:572:HIS:HE1	1.95	0.50
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.94	0.50
1:A:786:HIS:HD2	2:B:703:ILE:HB	1.71	0.50
2:B:821:GLN:HE22	2:B:851:PHE:N	2.00	0.50
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.26	0.50
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.94	0.50
3:C:201:TRP:CE3	3:C:202:PRO:HD2	2.45	0.50
4:D:46:GLU:O	4:D:47:LEU:O	2.29	0.50
6:F:97:ARG:HG2	6:F:130:ILE:HG23	1.93	0.50
7:G:160:ILE:HG22	7:G:161:GLY:H	1.75	0.50
7:G:80:LYS:HE2	7:G:80:LYS:H	1.77	0.50
7:G:1:MET:CE	7:G:80:LYS:O	2.54	0.50
1:A:403:LYS:O	1:A:403:LYS:HG3	2.10	0.50
2:B:360:PHE:CD2	2:B:360:PHE:C	2.85	0.50
2:B:542:MET:CE	2:B:743:ILE:HG13	2.42	0.50
2:B:777:ALA:CB	2:B:1093:GLN:HB3	2.42	0.50
6:F:82:THR:CG2	6:F:84:TYR:HB2	2.41	0.50
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.41	0.50
8:H:6:PHE:O	8:H:58:THR:HG23	2.11	0.50
9:I:56:ALA:O	9:I:57:GLY:C	2.49	0.50
3:C:235:VAL:HG12	10:J:13:VAL:HG23	1.93	0.50
1:A:110:CYS:SG	1:A:111:GLY:N	2.84	0.50
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.94	0.50
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.94	0.50
1:A:814:PHE:O	1:A:815:PHE:C	2.49	0.50
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.47	0.50
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.94	0.50
1:A:98:LYS:O	1:A:99:ILE:C	2.50	0.50
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.42	0.50
2:B:378:LEU:HD12	2:B:378:LEU:O	2.12	0.50
2:B:906:SER:O	2:B:941:LEU:HD23	2.11	0.50
4:D:118:THR:CG2	4:D:121:LYS:HD2	2.42	0.50
4:D:50:LEU:HD12	4:D:55:ALA:HA	1.93	0.50
5:E:109:ILE:HG22	5:E:109:ILE:O	2.12	0.50
11:K:53:ASP:C	11:K:55:LYS:N	2.58	0.50
1:A:1013:ASP:O	1:A:1015:VAL:N	2.41	0.50
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.93	0.50
1:A:180:LYS:HZ1	1:A:294:SER:HB3	1.77	0.50
1:A:475:THR:CG2	1:A:476:SER:H	2.25	0.50
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.94	0.50
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:ILE:CD1	2:B:327:ARG:H	2.25	0.50
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.23	0.50
2:B:882:THR:HB	2:B:934:LYS:O	2.12	0.50
4:D:120:GLU:O	4:D:120:GLU:HG2	2.11	0.50
5:E:93:MET:CE	5:E:120:ALA:HB1	2.42	0.50
3:C:166:GLU:CG	11:K:10:PHE:HZ	2.24	0.50
15:P:2:A:O2'	15:P:3:G:H5'	2.12	0.50
1:A:1170:ILE:HG22	1:A:1174:PHE:CE1	2.47	0.49
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.41	0.49
1:A:1388:GLY:O	1:A:1391:ARG:N	2.41	0.49
1:A:1441:PHE:C	1:A:1441:PHE:CD1	2.86	0.49
1:A:226:GLU:O	1:A:226:GLU:HG2	2.10	0.49
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.77	0.49
1:A:38:PRO:HG2	1:A:39:GLU:OE1	2.11	0.49
1:A:639:PRO:HG2	1:A:640:GLN:N	2.25	0.49
1:A:982:THR:HG22	1:A:984:LYS:H	1.76	0.49
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.27	0.49
2:B:288:ALA:CA	2:B:330:ALA:HB1	2.42	0.49
2:B:377:PHE:C	2:B:379:GLY:N	2.65	0.49
2:B:470:LYS:C	2:B:472:ALA:H	2.16	0.49
2:B:549:THR:H	2:B:628:THR:HG23	1.76	0.49
4:D:173:HIS:O	4:D:175:PHE:N	2.45	0.49
5:E:124:VAL:HB	5:E:125:PRO:CD	2.43	0.49
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.12	0.49
11:K:50:LEU:C	11:K:52:ASN:H	2.14	0.49
1:A:873:MET:C	1:A:1058:VAL:HG23	2.32	0.49
1:A:1211:GLN:O	1:A:1212:VAL:C	2.51	0.49
1:A:1402:PHE:CZ	1:A:1403:GLU:HG3	2.47	0.49
1:A:445:ASN:CB	1:A:455:MET:HG2	2.41	0.49
1:A:607:ILE:HG12	1:A:612:ILE:HA	1.94	0.49
2:B:980:PHE:C	2:B:1095:LEU:HD13	2.32	0.49
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.24	0.49
3:C:242:GLN:C	3:C:244:VAL:N	2.66	0.49
4:D:145:MET:O	4:D:149:THR:HB	2.12	0.49
8:H:40:LEU:CD2	8:H:142:LEU:HD21	2.42	0.49
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.75	0.49
12:L:44:ASP:O	12:L:45:ALA:HB3	2.11	0.49
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.12	0.49
1:A:1064:VAL:O	1:A:1067:LEU:HB3	2.12	0.49
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.64	0.49
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:CG1	1:A:297:GLN:NE2	2.75	0.49
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.93	0.49
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.12	0.49
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.49
2:B:660:LYS:HD3	2:B:679:TYR:CE2	2.48	0.49
9:I:80:SER:HB2	9:I:103:CYS:SG	2.53	0.49
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.42	0.49
1:A:1135:ARG:HH21	1:A:1284:MET:HE2	1.78	0.49
1:A:64:ASN:O	1:A:65:LEU:C	2.51	0.49
2:B:400:HIS:ND1	2:B:517:THR:HG21	2.28	0.49
2:B:446:LEU:O	2:B:447:ALA:HB3	2.12	0.49
2:B:806:THR:H	2:B:809:MET:HG3	1.76	0.49
3:C:111:THR:C	3:C:112:ASN:HD22	2.15	0.49
3:C:119:VAL:HG12	3:C:120:ILE:H	1.76	0.49
3:C:170:TRP:O	3:C:171:GLY:C	2.51	0.49
4:D:205:ASP:O	4:D:208:GLU:HB3	2.12	0.49
5:E:22:MET:HB2	5:E:187:TYR:CE1	2.47	0.49
8:H:51:ALA:O	8:H:52:GLN:HB2	2.12	0.49
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.11	0.49
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.12	0.49
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.94	0.49
1:A:287:HIS:O	1:A:291:GLU:OE2	2.30	0.49
1:A:547:LEU:HD22	11:K:58:PHE:HE1	1.75	0.49
1:A:701:LEU:O	1:A:702:LEU:HG	2.13	0.49
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.95	0.49
1:A:903:ASN:ND2	1:A:904:THR:N	2.48	0.49
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.13	0.49
2:B:1159:ARG:NH1	2:B:1159:ARG:CB	2.66	0.49
2:B:1183:LYS:C	2:B:1185:CYS:H	2.15	0.49
2:B:708:GLU:HG3	2:B:709:ASP:H	1.77	0.49
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.12	0.49
5:E:116:ILE:HG22	5:E:120:ALA:HB3	1.94	0.49
7:G:101:VAL:CG1	7:G:102:GLN:N	2.75	0.49
7:G:122:ASN:OD1	7:G:125:SER:HB3	2.13	0.49
3:C:66:ARG:HH21	10:J:5:VAL:H	1.60	0.49
12:L:59:ALA:O	12:L:60:ARG:O	2.30	0.49
14:N:5:DA:C2	16:T:13:DA:C2	3.01	0.49
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.48	0.49
1:A:19:PHE:O	1:A:1416:ALA:HA	2.12	0.49
1:A:771:GLU:HA	1:A:1084:PHE:CE2	2.47	0.49
1:A:853:ASP:CG	1:A:855:THR:HG22	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.94	0.49
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.27	0.49
2:B:1130:PHE:O	2:B:1131:GLY:O	2.31	0.49
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.41	0.49
2:B:296:GLU:HA	2:B:299:GLU:HG3	1.94	0.49
2:B:578:THR:C	2:B:589:VAL:HG13	2.32	0.49
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.76	0.49
5:E:114:ASN:O	5:E:115:ASN:HB3	2.12	0.49
9:I:34:TYR:C	9:I:34:TYR:CD2	2.84	0.49
10:J:19:GLU:O	10:J:23:ASN:HB2	2.11	0.49
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.13	0.49
1:A:1407:GLU:N	1:A:1407:GLU:CD	2.65	0.49
1:A:1441:PHE:C	1:A:1441:PHE:HD1	2.16	0.49
1:A:40:THR:HG22	1:A:41:MET:HG3	1.94	0.49
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.95	0.49
4:D:144:THR:OG1	7:G:105:PRO:HD3	2.13	0.49
16:T:16:DT:H1'	16:T:17:DA:H5'	1.95	0.49
16:T:19:DG:H2'	16:T:20:DC:C6	2.48	0.49
1:A:1205:LYS:O	1:A:1206:ASP:O	2.30	0.49
1:A:1445:ILE:HG21	7:G:18:PHE:HE2	1.77	0.49
1:A:218:ASP:O	1:A:219:PHE:C	2.50	0.49
1:A:438:ASP:O	1:A:439:ASN:HB2	2.12	0.49
1:A:600:PRO:C	1:A:602:ASP:H	2.15	0.49
1:A:605:MET:HE2	1:A:612:ILE:HG23	1.94	0.49
2:B:1177:HIS:O	2:B:1179:GLN:N	2.43	0.49
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.42	0.49
2:B:542:MET:HE3	2:B:636:PRO:HG2	1.93	0.49
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.61	0.49
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.16	0.49
2:B:816:GLU:O	2:B:817:LEU:HD23	2.13	0.49
3:C:174:ALA:O	3:C:175:ALA:HB3	2.13	0.49
8:H:25:ARG:HA	8:H:41:ASP:HA	1.95	0.49
1:A:560:ILE:HG12	8:H:78:SER:HB2	1.94	0.49
1:A:1138:ILE:O	1:A:1275:GLY:HA2	2.13	0.49
1:A:381:THR:O	1:A:383:TYR:N	2.45	0.49
2:B:744:HIS:O	2:B:747:MET:HB2	2.13	0.49
2:B:876:LYS:HD2	2:B:893:LEU:O	2.13	0.49
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.76	0.49
6:F:81:THR:HB	6:F:136:ARG:HH11	1.78	0.49
7:G:87:VAL:HG21	7:G:103:VAL:HG11	1.94	0.49
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:LEU:N	1:A:1273:LEU:HD12	2.28	0.49
1:A:336:ILE:HD11	2:B:1203:LEU:HD11	1.94	0.49
1:A:34:LYS:H	1:A:34:LYS:HD3	1.78	0.49
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.48	0.49
1:A:754:SER:H	1:A:757:ASN:HD22	1.60	0.49
2:B:428:ILE:O	2:B:432:MET:HG3	2.13	0.49
2:B:768:THR:O	2:B:771:SER:HB2	2.13	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.61	0.49
5:E:195:VAL:HG12	5:E:196:VAL:N	2.28	0.49
7:G:38:CYS:SG	7:G:157:ILE:HG13	2.52	0.49
1:A:512:VAL:HG13	1:A:512:VAL:O	2.12	0.48
1:A:573:SER:O	1:A:576:GLN:HB2	2.13	0.48
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.94	0.48
1:A:527:THR:HG21	1:A:650:GLN:HG3	1.94	0.48
1:A:814:PHE:O	1:A:817:ALA:N	2.45	0.48
2:B:1023:VAL:O	2:B:1026:LEU:N	2.45	0.48
2:B:1135:ARG:O	2:B:1136:ASP:C	2.51	0.48
2:B:879:ARG:NH2	2:B:885:MET:HE3	2.28	0.48
2:B:976:ILE:HG12	2:B:993:THR:HG23	1.93	0.48
3:C:34:ARG:HG2	3:C:35:ARG:N	2.27	0.48
4:D:70:PHE:O	4:D:74:GLN:HG3	2.13	0.48
9:I:106:CYS:SG	9:I:108:HIS:N	2.85	0.48
9:I:108:HIS:CG	9:I:109:ILE:H	2.31	0.48
1:A:1434:ALA:O	1:A:1436:ILE:N	2.45	0.48
1:A:92:HIS:CB	1:A:236:LEU:HD21	2.37	0.48
1:A:265:LYS:HE2	1:A:322:VAL:CG2	2.43	0.48
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.95	0.48
1:A:417:TYR:O	1:A:418:SER:C	2.50	0.48
1:A:713:SER:O	1:A:717:ASN:ND2	2.47	0.48
1:A:72:GLU:O	1:A:73:GLY:O	2.30	0.48
2:B:1130:PHE:CD2	2:B:1130:PHE:O	2.66	0.48
2:B:172:ILE:HG22	2:B:173:MET:N	2.29	0.48
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
2:B:825:VAL:CG1	2:B:826:ALA:N	2.76	0.48
6:F:73:ALA:HA	6:F:143:PHE:HE1	1.78	0.48
7:G:145:VAL:HG12	7:G:146:LYS:H	1.77	0.48
8:H:58:THR:HB	8:H:143:LEU:HB2	1.95	0.48
1:A:873:MET:C	1:A:1058:VAL:CG2	2.81	0.48
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.26	0.48
1:A:1336:MET:HG3	1:A:1341:ILE:HA	1.95	0.48
1:A:135:PHE:HB2	1:A:223:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:O	1:A:428:TYR:C	2.52	0.48
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.96	0.48
2:B:125:SER:HB2	2:B:170:LEU:O	2.12	0.48
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.43	0.48
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.41	0.48
11:K:10:PHE:HD2	11:K:10:PHE:N	2.10	0.48
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.96	0.48
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.95	0.48
1:A:600:PRO:HG2	1:A:601:LYS:H	1.77	0.48
1:A:699:ALA:CB	1:A:701:LEU:HG	2.42	0.48
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.81	0.48
2:B:980:PHE:CA	2:B:1095:LEU:HD13	2.43	0.48
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.77	0.48
2:B:29:ASP:O	2:B:31:TRP:N	2.46	0.48
2:B:167:ILE:HA	2:B:450:ALA:HB2	1.96	0.48
2:B:616:ILE:HD13	2:B:625:LYS:CB	2.43	0.48
2:B:58:THR:HG22	2:B:62:ILE:HD11	1.95	0.48
2:B:812:LEU:C	2:B:814:PHE:N	2.66	0.48
2:B:976:ILE:HA	2:B:990:ILE:CG2	2.43	0.48
6:F:85:MET:HG2	6:F:89:GLU:HB2	1.95	0.48
7:G:145:VAL:CG1	7:G:146:LYS:H	2.26	0.48
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.43	0.48
11:K:68:PHE:N	11:K:68:PHE:CD2	2.76	0.48
12:L:27:LEU:HB3	12:L:37:LYS:HD3	1.96	0.48
1:A:1154:TYR:CE2	1:A:1156:PRO:HD3	2.49	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.51	0.48
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.13	0.48
1:A:147:VAL:O	1:A:149:GLU:HG3	2.13	0.48
1:A:608:ILE:HG13	1:A:613:ILE:CD1	2.44	0.48
1:A:822:GLU:O	1:A:825:ILE:HB	2.13	0.48
2:B:296:GLU:C	2:B:299:GLU:HB2	2.34	0.48
3:C:80:LEU:HD11	3:C:95:CYS:HA	1.96	0.48
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.47	0.48
2:B:797:TYR:O	10:J:1:MET:HG2	2.13	0.48
11:K:6:ARG:O	11:K:9:LEU:HG	2.13	0.48
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.47	0.48
1:A:1280:GLU:O	1:A:1281:ARG:O	2.32	0.48
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.96	0.48
1:A:305:ASP:CG	1:A:326:ARG:HD3	2.34	0.48
1:A:438:ASP:OD1	1:A:462:VAL:HG23	2.14	0.48
1:A:548:ASN:HD21	11:K:47:ARG:NH2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLN:HG2	1:A:654:ASN:HD21	1.79	0.48
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.48	0.48
2:B:310:MET:O	2:B:313:MET:HB2	2.14	0.48
2:B:866:TYR:C	2:B:868:MET:N	2.66	0.48
3:C:44:LEU:HD13	3:C:129:ILE:CD1	2.41	0.48
5:E:32:GLN:HE21	5:E:36:GLU:HG3	1.78	0.48
7:G:117:GLN:C	7:G:119:LEU:H	2.16	0.48
7:G:129:SER:HB2	7:G:137:ILE:O	2.13	0.48
10:J:23:ASN:C	10:J:25:LEU:N	2.67	0.48
14:N:1:DA:C1'	14:N:2:DA:H5'	2.42	0.48
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.41	0.48
1:A:108:MET:O	1:A:110:CYS:N	2.47	0.48
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.12	0.48
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.49	0.48
1:A:853:ASP:OD1	1:A:855:THR:N	2.46	0.48
2:B:1198:TYR:C	2:B:1198:TYR:CD2	2.87	0.48
2:B:526:GLU:HB2	2:B:752:ALA:HB3	1.94	0.48
4:D:176:GLU:C	4:D:178:ALA:N	2.67	0.48
5:E:149:LEU:O	5:E:151:PRO:HD3	2.13	0.48
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.74	0.48
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.96	0.48
10:J:45:CYS:O	10:J:48:ARG:HG3	2.13	0.48
1:A:265:LYS:HE2	1:A:322:VAL:HG21	1.95	0.48
2:B:1100:ASP:OD2	11:K:1:MET:CB	2.62	0.48
2:B:822:ASN:O	10:J:48:ARG:NH1	2.46	0.48
2:B:827:ILE:O	2:B:827:ILE:HG22	2.14	0.48
7:G:51:TYR:HD2	7:G:52:ASP:N	2.11	0.48
9:I:58:VAL:CG1	9:I:62:ILE:HG21	2.43	0.48
11:K:11:LEU:N	11:K:11:LEU:HD22	2.29	0.48
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.95	0.48
1:A:565:ILE:HG22	1:A:569:LYS:O	2.14	0.48
2:B:99:LYS:HB3	2:B:100:PRO:CD	2.44	0.48
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.67	0.48
3:C:148:ARG:HG2	3:C:149:LYS:H	1.78	0.48
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.44	0.48
8:H:15:VAL:HA	8:H:26:ILE:HG12	1.95	0.48
9:I:100:PHE:N	9:I:100:PHE:HD1	2.12	0.48
12:L:30:ILE:HG22	12:L:31:CYS:H	1.79	0.48
14:N:2:DA:H1'	14:N:3:DC:H5''	1.95	0.48
16:T:26:DC:H2'	16:T:27:DA:C8	2.49	0.48
1:A:1004:ASN:O	1:A:1008:GLN:CG	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:HE21	1:A:1134:ILE:CD1	2.26	0.48
1:A:264:PHE:O	1:A:267:ALA:N	2.47	0.48
1:A:591:PHE:HA	1:A:595:THR:CG2	2.42	0.48
1:A:726:ARG:HH12	13:M:5:GLY:HA3	1.79	0.48
1:A:910:PRO:HB3	1:A:916:GLY:HA3	1.96	0.48
2:B:1047:PHE:CD1	2:B:1047:PHE:N	2.80	0.48
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.47	0.48
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.95	0.48
4:D:131:GLU:O	4:D:132:GLN:HG2	2.13	0.48
4:D:137:ASN:HD22	4:D:137:ASN:C	2.18	0.48
5:E:48:ASP:CG	5:E:49:SER:N	2.63	0.48
6:F:111:LEU:C	6:F:113:GLY:H	2.18	0.48
8:H:59:ILE:O	8:H:60:ALA:HB3	2.14	0.48
9:I:16:PRO:HB3	9:I:27:PHE:CD2	2.49	0.48
11:K:40:HIS:O	11:K:41:THR:C	2.52	0.48
1:A:100:LYS:HG3	1:A:181:LEU:HD22	1.95	0.47
1:A:1114:PRO:O	1:A:1115:SER:O	2.32	0.47
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.44	0.47
1:A:22:PHE:HB2	2:B:1211:ASN:ND2	2.29	0.47
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.28	0.47
1:A:639:PRO:CG	1:A:640:GLN:H	2.25	0.47
2:B:1122:ARG:HB3	16:T:22:BRU:OP1	2.14	0.47
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.14	0.47
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.44	0.47
2:B:603:LEU:CD1	2:B:608:ASP:HB2	2.40	0.47
2:B:580:VAL:CG1	2:B:624:LEU:HB3	2.37	0.47
2:B:614:SER:HB2	2:B:694:ASP:OD1	2.14	0.47
4:D:40:HIS:CE1	4:D:41:GLN:HG2	2.50	0.47
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.49	0.47
1:A:1100:ARG:NH1	1:A:1111:MET:HE3	2.28	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.39	0.47
1:A:12:ARG:HG3	2:B:1192:TYR:CD2	2.49	0.47
1:A:1334:ASP:O	1:A:1335:ILE:C	2.52	0.47
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.96	0.47
1:A:982:THR:H	1:A:985:ASP:CG	2.16	0.47
2:B:309:GLN:O	2:B:312:GLU:HB3	2.14	0.47
2:B:752:ALA:O	2:B:755:ILE:HG13	2.15	0.47
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.95	0.47
5:E:85:GLU:O	5:E:87:SER:N	2.39	0.47
7:G:99:PHE:HE2	7:G:115:MET:HE3	1.78	0.47
10:J:32:GLU:CD	10:J:32:GLU:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:CD1	11:K:88:LYS:HA	2.44	0.47
16:T:16:DT:H1'	16:T:17:DA:C5'	2.44	0.47
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.62	0.47
1:A:1260:LEU:HG	1:A:1260:LEU:O	2.15	0.47
1:A:370:ILE:HD12	1:A:468:PHE:HE2	1.77	0.47
1:A:401:GLY:O	1:A:435:HIS:CD2	2.68	0.47
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.96	0.47
2:B:212:LEU:HD13	2:B:412:LEU:HD12	1.95	0.47
2:B:299:GLU:CD	2:B:572:HIS:HE1	2.17	0.47
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.48	0.47
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.97	0.47
2:B:579:ARG:O	2:B:623:GLU:HA	2.13	0.47
2:B:667:GLN:O	2:B:668:ASP:CG	2.52	0.47
6:F:76:LYS:O	6:F:79:ARG:HD3	2.13	0.47
7:G:27:LYS:CD	7:G:54:ILE:HD12	2.44	0.47
9:I:49:ILE:HG22	9:I:49:ILE:O	2.14	0.47
1:A:698:GLN:NE2	9:I:99:LEU:HD21	2.29	0.47
11:K:47:ARG:HD2	11:K:51:LEU:HD21	1.96	0.47
1:A:1121:GLU:O	1:A:1122:PRO:C	2.53	0.47
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.49	0.47
1:A:1447:GLU:O	1:A:1451:VAL:HG23	2.13	0.47
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.96	0.47
1:A:262:LEU:C	1:A:264:PHE:N	2.68	0.47
1:A:350:ARG:HD2	2:B:1128:LEU:CD2	2.45	0.47
1:A:3:GLY:O	1:A:4:GLN:HB2	2.15	0.47
1:A:565:ILE:O	1:A:570:PRO:HA	2.14	0.47
1:A:826:ASP:C	1:A:828:ALA:N	2.67	0.47
1:A:851:HIS:HB2	1:A:855:THR:HG23	1.96	0.47
2:B:1201:LYS:CE	2:B:1205:GLN:OE1	2.62	0.47
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.78	0.47
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.96	0.47
2:B:96:TYR:CD1	2:B:96:TYR:N	2.83	0.47
8:H:98:TYR:HD1	8:H:99:GLY:H	1.56	0.47
1:A:709:THR:HG23	9:I:94:ASP:HA	1.96	0.47
8:H:82:PRO:HG2	11:K:54:ARG:HD2	1.95	0.47
16:T:13:DA:H1'	16:T:14:DG:H5'	1.95	0.47
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.14	0.47
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.28	0.47
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.35	0.47
1:A:144:THR:O	1:A:146:MET:HG3	2.14	0.47
1:A:354:SER:HA	1:A:482:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.96	0.47
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.47	0.47
2:B:253:THR:CG2	2:B:254:LEU:N	2.77	0.47
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.78	0.47
2:B:659:ALA:HA	2:B:662:MET:HE2	1.95	0.47
2:B:736:THR:O	2:B:736:THR:HG22	2.14	0.47
2:B:860:MET:CB	2:B:965:LYS:HG2	2.42	0.47
3:C:168:ALA:C	3:C:170:TRP:H	2.18	0.47
4:D:195:ILE:HG22	4:D:195:ILE:O	2.14	0.47
5:E:128:PRO:HA	5:E:129:PRO:C	2.34	0.47
5:E:153:HIS:O	5:E:154:ILE:CG1	2.54	0.47
8:H:32:THR:HG22	8:H:33:GLN:OE1	2.13	0.47
8:H:4:THR:HA	8:H:60:ALA:HB2	1.96	0.47
10:J:27:GLU:C	10:J:29:GLU:N	2.68	0.47
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.96	0.47
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.96	0.47
1:A:1239:ARG:NH2	1:A:1241:ARG:HH22	2.03	0.47
1:A:252:PHE:O	1:A:253:ASN:CB	2.59	0.47
1:A:180:LYS:HZ3	1:A:294:SER:HB3	1.79	0.47
1:A:355:GLY:HA2	1:A:470:LEU:O	2.14	0.47
1:A:55:ASP:O	1:A:57:ARG:N	2.46	0.47
1:A:771:GLU:HA	1:A:1084:PHE:CZ	2.50	0.47
1:A:845:LEU:O	1:A:846:GLU:C	2.53	0.47
1:A:903:ASN:HD22	1:A:904:THR:H	1.58	0.47
2:B:1152:MET:HE3	2:B:1157:ALA:HA	1.97	0.47
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.15	0.47
3:C:183:TRP:CE2	3:C:207:CYS:HB3	2.50	0.47
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.96	0.47
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.95	0.47
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.45	0.47
1:A:761:MET:HA	1:A:804:TYR:HB2	1.96	0.47
2:B:224:GLN:O	2:B:238:ALA:HA	2.15	0.47
3:C:138:GLU:OE1	3:C:138:GLU:N	2.46	0.47
5:E:82:PHE:CD1	5:E:82:PHE:N	2.83	0.47
7:G:149:GLY:O	7:G:159:ALA:HB1	2.15	0.47
8:H:135:LEU:HD13	8:H:137:GLN:HE22	1.76	0.47
1:A:157:ASP:C	1:A:159:THR:H	2.16	0.47
1:A:541:ILE:HD12	1:A:577:ILE:CD1	2.39	0.47
1:A:67:CYS:O	1:A:68:GLN:CB	2.63	0.47
1:A:746:MET:HE1	2:B:1014:PRO:O	2.14	0.47
1:A:982:THR:HB	1:A:985:ASP:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ILE:HG22	2:B:355:ILE:O	2.15	0.47
2:B:361:LEU:N	2:B:362:PRO:CD	2.77	0.47
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.29	0.47
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.50	0.47
1:A:567:LYS:HE3	8:H:46:LEU:HD13	1.97	0.47
9:I:54:GLU:OE2	9:I:118:ARG:NH1	2.43	0.47
1:A:1005:GLU:O	1:A:1006:ILE:C	2.54	0.47
1:A:1127:ASP:CB	1:A:1130:GLN:HB3	2.42	0.47
1:A:1283:VAL:CG1	1:A:1284:MET:H	2.28	0.47
1:A:1319:VAL:H	1:A:1322:ILE:HD11	1.80	0.47
1:A:492:PRO:O	1:A:493:GLN:NE2	2.48	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.47
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.96	0.47
1:A:63:ARG:HA	1:A:74:MET:SD	2.55	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.96	0.47
2:B:125:SER:HB3	2:B:171:PRO:HA	1.96	0.47
2:B:464:GLY:HA2	2:B:479:VAL:O	2.15	0.47
2:B:556:THR:C	2:B:558:LEU:H	2.18	0.47
3:C:100:THR:OG1	3:C:121:VAL:CG2	2.62	0.47
3:C:142:VAL:H	10:J:16:ASP:HB3	1.79	0.47
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.47
5:E:60:PHE:CD2	5:E:60:PHE:C	2.87	0.47
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.96	0.47
1:A:166:GLY:O	1:A:167:CYS:SG	2.72	0.47
1:A:567:LYS:HB3	8:H:95:TYR:C	2.36	0.47
1:A:665:GLY:O	1:A:667:GLY:N	2.48	0.47
1:A:67:CYS:O	1:A:68:GLN:HB2	2.15	0.47
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.45	0.47
1:A:930:ASP:O	1:A:931:GLU:C	2.53	0.47
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.97	0.47
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.97	0.47
2:B:637:LEU:O	2:B:690:VAL:HG13	2.15	0.47
2:B:801:LYS:O	10:J:52:THR:CG2	2.56	0.47
3:C:39:ALA:HA	3:C:164:ALA:CB	2.39	0.47
7:G:27:LYS:CG	7:G:54:ILE:HD12	2.44	0.47
7:G:51:TYR:CD2	7:G:52:ASP:N	2.83	0.47
8:H:109:LYS:HB2	8:H:111:LEU:HD12	1.97	0.47
10:J:13:VAL:C	10:J:14:VAL:CG2	2.82	0.47
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.49	0.47
1:A:1265:ASN:O	1:A:1268:LEU:N	2.47	0.47
1:A:1339:LEU:HD23	5:E:144:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:O	1:A:1388:GLY:N	2.48	0.47
1:A:309:ALA:O	1:A:311:GLN:N	2.46	0.47
1:A:785:PRO:CB	2:B:703:ILE:HD12	2.45	0.47
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.96	0.47
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.70	0.47
9:I:55:THR:O	9:I:56:ALA:O	2.32	0.47
10:J:44:TYR:N	10:J:44:TYR:CD2	2.82	0.47
12:L:53:HIS:O	12:L:55:ILE:HD13	2.15	0.47
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.80	0.47
1:A:1014:ALA:O	1:A:1015:VAL:HG23	2.14	0.46
1:A:1289:ARG:HH12	1:A:1326:ARG:NH1	2.13	0.46
1:A:1340:GLY:O	1:A:1341:ILE:C	2.53	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.97	0.46
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.45	0.46
2:B:1010:LEU:HD22	2:B:1092:TYR:CE1	2.50	0.46
2:B:777:ALA:HB1	2:B:1093:GLN:HB3	1.97	0.46
2:B:1201:LYS:HG2	2:B:1202:LEU:N	2.28	0.46
2:B:185:THR:H	2:B:188:ASP:HB2	1.80	0.46
2:B:204:ILE:HG22	2:B:204:ILE:O	2.14	0.46
2:B:228:LYS:O	2:B:229:ALA:O	2.32	0.46
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.15	0.46
2:B:473:MET:O	2:B:475:SER:N	2.40	0.46
2:B:847:ASP:C	2:B:849:GLY:N	2.67	0.46
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.97	0.46
6:F:74:ILE:HG22	6:F:74:ILE:O	2.15	0.46
7:G:119:LEU:HD12	7:G:131:GLN:O	2.15	0.46
7:G:112:LYS:NZ	7:G:120:THR:HG22	2.30	0.46
1:A:1028:THR:HG22	1:A:1032:LEU:HD12	1.98	0.46
1:A:12:ARG:HB2	2:B:1218:THR:HG21	1.97	0.46
1:A:1325:THR:CG2	1:A:1325:THR:O	2.62	0.46
1:A:182:VAL:HG12	1:A:183:GLY:N	2.30	0.46
1:A:68:GLN:C	1:A:70:CYS:H	2.19	0.46
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.97	0.46
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	1.97	0.46
2:B:196:PRO:HG2	2:B:197:PHE:H	1.80	0.46
2:B:230:ALA:N	2:B:231:PRO:HD2	2.30	0.46
2:B:370:PHE:O	2:B:371:GLU:C	2.54	0.46
2:B:705:MET:HA	2:B:705:MET:CE	2.45	0.46
2:B:873:THR:HB	2:B:915:THR:OG1	2.15	0.46
2:B:969:ARG:HG2	2:B:970:THR:N	2.30	0.46
4:D:134:THR:C	4:D:136:GLY:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD12	8:H:124:ARG:O	2.14	0.46
8:H:40:LEU:HD12	8:H:41:ASP:N	2.30	0.46
10:J:23:ASN:O	10:J:25:LEU:N	2.47	0.46
10:J:2:ILE:HG23	10:J:3:VAL:H	1.80	0.46
1:A:548:ASN:ND2	11:K:47:ARG:HH21	2.13	0.46
11:K:63:VAL:O	11:K:63:VAL:HG23	2.15	0.46
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.50	0.46
1:A:474:VAL:HG22	1:A:474:VAL:O	2.15	0.46
1:A:551:TYR:HE2	11:K:62:LYS:HG2	1.80	0.46
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.19	0.46
2:B:604:ARG:HA	2:B:609:ILE:HG13	1.98	0.46
2:B:880:THR:HB	2:B:934:LYS:HD2	1.97	0.46
2:B:831:SER:CB	2:B:994:TYR:OH	2.64	0.46
3:C:119:VAL:CG1	3:C:120:ILE:N	2.78	0.46
3:C:141:GLY:HA2	10:J:16:ASP:HB3	1.97	0.46
3:C:175:ALA:CB	10:J:43:ARG:NH2	2.72	0.46
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.96	0.46
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.29	0.46
6:F:75:PRO:C	6:F:77:ASP:N	2.69	0.46
1:A:1059:HIS:ND1	6:F:86:THR:HA	2.29	0.46
10:J:30:LEU:CD1	10:J:38:ARG:HH12	2.28	0.46
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.30	0.46
3:C:52:GLU:HA	12:L:64:LEU:CD2	2.45	0.46
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.61	0.46
1:A:219:PHE:HE1	1:A:230:ARG:NH2	2.12	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
1:A:853:ASP:C	1:A:853:ASP:OD1	2.53	0.46
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.28	0.46
2:B:408:LEU:O	2:B:412:LEU:HG	2.14	0.46
2:B:418:LYS:HB3	2:B:422:LYS:HZ2	1.80	0.46
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.30	0.46
2:B:881:ASN:HB2	2:B:933:SER:N	2.31	0.46
2:B:996:ARG:HH12	3:C:174:ALA:H	1.63	0.46
3:C:16:ASP:O	3:C:17:ASN:ND2	2.48	0.46
3:C:205:LYS:HG2	3:C:205:LYS:O	2.16	0.46
5:E:120:ALA:O	5:E:122:LYS:N	2.48	0.46
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.45	0.46
8:H:128:ASN:O	8:H:131:ASN:ND2	2.48	0.46
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.49	0.46
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.50	0.46
1:A:321:PRO:O	1:A:322:VAL:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:MET:CE	2:B:1087:PHE:HB2	2.46	0.46
2:B:288:ALA:N	2:B:330:ALA:HB1	2.30	0.46
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.15	0.46
2:B:545:ILE:HG22	2:B:546:SER:O	2.16	0.46
2:B:619:ILE:O	2:B:621:GLU:N	2.47	0.46
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.48	0.46
3:C:10:ILE:H	3:C:10:ILE:HG13	1.45	0.46
3:C:56:THR:HG21	3:C:145:CYS:SG	2.55	0.46
3:C:183:TRP:O	3:C:185:LYS:N	2.49	0.46
3:C:186:LEU:N	3:C:186:LEU:HD12	2.31	0.46
4:D:55:ALA:O	4:D:59:ILE:HG13	2.15	0.46
5:E:45:LYS:HG2	5:E:46:TYR:CE1	2.51	0.46
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.97	0.46
10:J:6:ARG:HA	10:J:12:LYS:O	2.15	0.46
1:A:1006:ILE:HD12	5:E:167:ARG:CG	2.45	0.46
1:A:108:MET:C	1:A:110:CYS:N	2.69	0.46
1:A:1142:THR:HA	1:A:1273:LEU:HD13	1.98	0.46
1:A:574:GLY:O	1:A:575:LYS:C	2.54	0.46
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.30	0.46
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.50	0.46
2:B:1189:ILE:CG2	2:B:1190:ASP:N	2.78	0.46
2:B:1161:HIS:CE1	2:B:1193:GLN:HB2	2.50	0.46
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.03	0.46
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.30	0.46
2:B:556:THR:C	2:B:558:LEU:N	2.69	0.46
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.81	0.46
2:B:653:VAL:HA	2:B:689:LEU:HD22	1.98	0.46
3:C:27:LEU:O	3:C:28:ALA:C	2.54	0.46
4:D:218:GLU:O	4:D:219:THR:C	2.53	0.46
4:D:40:HIS:ND1	4:D:40:HIS:C	2.68	0.46
5:E:179:GLN:O	5:E:182:ASP:HB2	2.15	0.46
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.50	0.46
10:J:14:VAL:HG12	10:J:14:VAL:O	2.16	0.46
10:J:48:ARG:C	10:J:48:ARG:HD2	2.36	0.46
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.81	0.46
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.45	0.46
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.97	0.46
1:A:466:SER:HA	11:K:2:ASN:HD22	1.79	0.46
1:A:498:ARG:O	1:A:501:LEU:HB2	2.16	0.46
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.73	0.46
1:A:741:ASN:C	1:A:741:ASN:HD22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:CE	1:A:843:LYS:NZ	2.78	0.46
1:A:913:LEU:HD21	1:A:919:ILE:HD12	1.97	0.46
1:A:939:ASP:O	1:A:942:PHE:N	2.48	0.46
2:B:121:ASN:OD1	2:B:963:PHE:HZ	1.99	0.46
2:B:208:SER:OG	2:B:210:LYS:NZ	2.48	0.46
2:B:20:ASP:O	2:B:22:SER:N	2.47	0.46
2:B:313:MET:O	2:B:316:PRO:HD2	2.15	0.46
2:B:549:THR:N	2:B:628:THR:HG23	2.31	0.46
3:C:17:ASN:O	3:C:18:VAL:HG23	2.15	0.46
5:E:72:PHE:CD1	5:E:72:PHE:N	2.84	0.46
6:F:97:ARG:HA	6:F:100:GLN:HG3	1.98	0.46
7:G:102:GLN:HG3	7:G:106:MET:O	2.16	0.46
12:L:30:ILE:O	12:L:56:LEU:HD22	2.15	0.46
16:T:13:DA:H2"	16:T:14:DG:O5'	2.14	0.46
16:T:21:DC:H2"	16:T:22:BRU:H5"	1.97	0.46
1:A:1116:LEU:HD23	1:A:1308:THR:HG21	1.98	0.46
1:A:765:VAL:HG21	1:A:808:LEU:HD11	1.98	0.46
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.98	0.46
2:B:830:TYR:CZ	2:B:1000:PRO:HB3	2.51	0.46
2:B:1220:ARG:NH1	2:B:1220:ARG:CB	2.77	0.46
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.96	0.46
6:F:95:GLY:O	6:F:98:ALA:HB3	2.16	0.46
7:G:111:THR:C	7:G:113:HIS:N	2.68	0.46
1:A:1151:GLU:HA	9:I:44:TYR:O	2.16	0.46
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.97	0.46
1:A:112:LYS:HG2	1:A:113:LEU:N	2.31	0.46
1:A:443:LEU:O	1:A:489:LEU:HD12	2.16	0.46
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.97	0.46
1:A:842:VAL:C	1:A:844:ALA:N	2.68	0.46
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.97	0.46
2:B:287:ARG:NH1	2:B:324:ILE:O	2.48	0.46
3:C:10:ILE:HG22	3:C:11:ARG:O	2.16	0.46
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.31	0.46
4:D:118:THR:HG21	4:D:121:LYS:HD2	1.98	0.46
4:D:27:LEU:HD13	4:D:173:HIS:HD2	1.81	0.46
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.98	0.46
8:H:4:THR:HA	8:H:60:ALA:CB	2.45	0.46
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.51	0.46
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.31	0.46
1:A:359:LEU:O	1:A:360:GLU:C	2.53	0.46
1:A:770:VAL:O	1:A:772:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.99	0.46
2:B:248:SER:O	2:B:249:ARG:HB2	2.15	0.46
2:B:473:MET:C	2:B:475:SER:H	2.18	0.46
2:B:52:ASN:O	2:B:56:ASP:HB2	2.16	0.46
2:B:705:MET:HB3	2:B:706:GLN:H	1.54	0.46
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.97	0.46
5:E:55:ARG:O	5:E:57:MET:N	2.49	0.46
8:H:110:ASP:N	8:H:110:ASP:OD1	2.49	0.46
10:J:56:LEU:O	10:J:59:LYS:N	2.49	0.46
10:J:7:CYS:SG	10:J:49:MET:CE	3.04	0.46
11:K:22:ASP:O	11:K:31:VAL:HG13	2.16	0.46
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.34	0.46
1:A:296:LEU:O	1:A:300:VAL:HG23	2.15	0.45
1:A:623:GLY:C	1:A:625:SER:H	2.18	0.45
2:B:728:ARG:HH12	2:B:1047:PHE:HA	1.81	0.45
2:B:118:ARG:NH2	2:B:194:GLU:HG2	2.32	0.45
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.45
2:B:516:ASN:O	2:B:518:HIS:N	2.49	0.45
2:B:609:ILE:O	2:B:609:ILE:HG13	2.16	0.45
2:B:992:ILE:CG1	2:B:993:THR:H	2.27	0.45
2:B:996:ARG:NH2	3:C:175:ALA:N	2.51	0.45
3:C:209:TYR:N	3:C:209:TYR:CD1	2.84	0.45
5:E:116:ILE:HB	5:E:121:MET:CE	2.46	0.45
5:E:202:SER:C	5:E:204:THR:H	2.19	0.45
7:G:99:PHE:CE2	7:G:115:MET:HE3	2.51	0.45
11:K:6:ARG:O	11:K:8:GLU:N	2.49	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.25	0.45
1:A:1436:ILE:HG22	1:A:1436:ILE:O	2.15	0.45
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.96	0.45
1:A:20:GLY:C	1:A:21:LEU:HD23	2.36	0.45
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.52	0.45
1:A:260:ASP:OD1	1:A:261:ASP:N	2.49	0.45
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.51	0.45
1:A:528:LEU:HD21	1:A:749:ALA:O	2.16	0.45
1:A:595:THR:O	1:A:596:THR:HG23	2.16	0.45
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.97	0.45
1:A:64:ASN:O	1:A:66:LYS:N	2.49	0.45
2:B:1200:ALA:O	2:B:1201:LYS:C	2.54	0.45
2:B:324:ILE:HG23	2:B:329:THR:HB	1.97	0.45
2:B:288:ALA:O	2:B:331:LEU:HD11	2.16	0.45
2:B:360:PHE:O	2:B:361:LEU:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:MET:C	2:B:554:ILE:N	2.69	0.45
2:B:542:MET:CE	2:B:636:PRO:HG2	2.45	0.45
1:A:801:GLU:OE1	2:B:729:ILE:HD12	2.16	0.45
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.45	0.45
5:E:143:ASN:ND2	5:E:145:THR:OG1	2.48	0.45
5:E:151:PRO:HB3	5:E:200:ARG:HB3	1.98	0.45
5:E:55:ARG:C	5:E:57:MET:N	2.69	0.45
7:G:153:GLN:CG	7:G:154:VAL:HG23	2.38	0.45
8:H:112:ILE:HG22	8:H:113:ALA:H	1.81	0.45
1:A:1026:LEU:HA	1:A:1031:VAL:CG2	2.46	0.45
1:A:1169:ILE:HD13	1:A:1229:SER:HB3	1.98	0.45
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.97	0.45
1:A:391:LEU:HD23	1:A:400:PRO:O	2.16	0.45
1:A:44:THR:HG22	1:A:44:THR:O	2.16	0.45
1:A:569:LYS:HB3	1:A:571:LEU:HD11	1.98	0.45
1:A:529:CYS:HA	1:A:749:ALA:HB1	1.99	0.45
1:A:826:ASP:C	1:A:828:ALA:H	2.18	0.45
1:A:971:PHE:N	1:A:971:PHE:CD1	2.83	0.45
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.85	0.45
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.99	0.45
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.34	0.45
2:B:758:PHE:C	2:B:760:ASP:N	2.70	0.45
2:B:980:PHE:HA	2:B:1095:LEU:HD13	1.98	0.45
3:C:251:LEU:C	3:C:251:LEU:HD12	2.37	0.45
4:D:134:THR:C	4:D:136:GLY:H	2.19	0.45
4:D:51:ASN:HB2	4:D:182:SER:HB3	1.98	0.45
9:I:109:ILE:HG22	9:I:109:ILE:O	2.17	0.45
14:N:10:DA:H2"	14:N:11:DG:OP2	2.16	0.45
1:A:1114:PRO:HB2	1:A:1311:VAL:CG2	2.46	0.45
1:A:1333:ILE:HD13	1:A:1381:LEU:CD1	2.46	0.45
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.45	0.45
1:A:34:LYS:HB2	1:A:36:ARG:NH2	2.20	0.45
1:A:367:PRO:O	1:A:368:LYS:C	2.54	0.45
1:A:396:PRO:HB3	1:A:403:LYS:HB2	1.97	0.45
1:A:754:SER:O	1:A:755:PHE:C	2.55	0.45
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.16	0.45
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.37	0.45
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.30	0.45
2:B:464:GLY:C	2:B:465:ASN:HD22	2.20	0.45
2:B:582:VAL:HG23	2:B:626:ILE:CD1	2.45	0.45
2:B:661:LEU:HD23	2:B:679:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:SER:O	2:B:68:THR:C	2.55	0.45
2:B:604:ARG:HH11	2:B:691:GLU:HG2	1.81	0.45
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.50	0.45
2:B:879:ARG:NE	2:B:879:ARG:HA	2.30	0.45
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.51	0.45
9:I:58:VAL:HG12	9:I:58:VAL:O	2.15	0.45
1:A:1313:LEU:C	1:A:1315:GLU:N	2.70	0.45
1:A:1373:ASP:C	1:A:1376:THR:HG22	2.37	0.45
1:A:42:ASP:OD1	1:A:45:GLN:O	2.34	0.45
1:A:674:PRO:HA	1:A:677:ARG:NH1	2.32	0.45
1:A:756:ILE:O	1:A:759:ALA:HB3	2.16	0.45
1:A:982:THR:N	1:A:985:ASP:HB2	2.31	0.45
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.31	0.45
2:B:114:PRO:O	2:B:116:GLU:N	2.49	0.45
2:B:185:THR:O	2:B:186:GLU:C	2.55	0.45
2:B:486:TYR:N	2:B:486:TYR:CD2	2.83	0.45
4:D:170:THR:HB	4:D:172:LEU:HG	1.97	0.45
4:D:54:GLU:O	4:D:58:VAL:HG23	2.15	0.45
5:E:17:ARG:NH1	5:E:17:ARG:CG	2.80	0.45
7:G:1:MET:HE2	7:G:3:PHE:CE1	2.43	0.45
8:H:17:PRO:O	8:H:19:ARG:N	2.49	0.45
8:H:83:GLN:C	8:H:85:GLY:H	2.20	0.45
9:I:51:ASN:HD21	9:I:118:ARG:CZ	2.29	0.45
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.98	0.45
1:A:1048:ASN:O	1:A:1049:ILE:C	2.55	0.45
1:A:519:PRO:HD3	1:A:631:HIS:CG	2.51	0.45
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.47	0.45
1:A:961:ARG:HH11	1:A:961:ARG:HG3	1.80	0.45
1:A:960:ILE:CA	1:A:963:ILE:HG22	2.45	0.45
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.82	0.45
2:B:1132:GLU:O	2:B:1135:ARG:N	2.49	0.45
2:B:367:LEU:HD12	2:B:370:PHE:CE1	2.51	0.45
2:B:589:VAL:CG1	2:B:590:HIS:N	2.61	0.45
2:B:731:VAL:HG12	2:B:732:SER:N	2.31	0.45
1:A:598:LEU:CA	8:H:122:LEU:HD13	2.46	0.45
16:T:12:DT:H2"	16:T:13:DA:OP2	2.17	0.45
1:A:1343:ALA:HB1	5:E:149:LEU:HB2	1.99	0.45
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.16	0.45
1:A:326:ARG:HH22	1:A:330:LYS:HE3	1.81	0.45
1:A:940:ARG:NH1	1:A:940:ARG:HG2	2.32	0.45
2:B:1110:PRO:HG2	2:B:1119:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:CD	2:B:1193:GLN:NE2	2.78	0.45
1:A:782:ARG:NH2	2:B:699:GLU:O	2.47	0.45
2:B:796:LEU:O	2:B:797:TYR:C	2.55	0.45
2:B:821:GLN:NE2	2:B:850:LEU:HD12	2.32	0.45
3:C:133:ILE:CD1	3:C:237:SER:N	2.77	0.45
3:C:17:ASN:H	3:C:240:VAL:HG11	1.80	0.45
4:D:161:GLY:O	4:D:165:GLN:HG3	2.16	0.45
7:G:137:ILE:HG21	7:G:143:ILE:HD11	1.98	0.45
11:K:79:GLU:O	11:K:81:TYR:N	2.50	0.45
12:L:55:ILE:O	12:L:56:LEU:HB2	2.16	0.45
1:A:262:LEU:O	1:A:264:PHE:N	2.50	0.45
1:A:379:VAL:HG22	1:A:431:LYS:CG	2.42	0.45
1:A:381:THR:C	1:A:383:TYR:H	2.20	0.45
1:A:87:ALA:O	1:A:88:LYS:HG2	2.17	0.45
2:B:121:ASN:HA	2:B:207:GLY:CA	2.47	0.45
2:B:46:GLN:HG3	2:B:47:GLN:N	2.24	0.45
2:B:797:TYR:HB3	2:B:798:TYR:HD2	1.79	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.99	0.45
4:D:34:GLN:C	4:D:36:LYS:N	2.70	0.45
5:E:40:GLU:C	5:E:42:PHE:H	2.20	0.45
5:E:94:LYS:HG3	5:E:98:ILE:HD11	1.99	0.45
7:G:145:VAL:HG22	7:G:163:ILE:HG23	1.99	0.45
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.98	0.45
9:I:68:LEU:HB3	9:I:84:VAL:CG2	2.46	0.45
10:J:8:PHE:H	10:J:49:MET:HE1	1.82	0.45
1:A:100:LYS:HG3	1:A:181:LEU:CD2	2.47	0.45
1:A:1100:ARG:HH12	1:A:1111:MET:HE3	1.82	0.45
1:A:150:THR:O	1:A:150:THR:HG22	2.17	0.45
1:A:157:ASP:C	1:A:159:THR:N	2.71	0.45
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.45
1:A:546:VAL:O	1:A:550:LEU:HG	2.17	0.45
1:A:648:ASN:O	1:A:649:ILE:C	2.55	0.45
1:A:665:GLY:O	1:A:666:ILE:C	2.54	0.45
1:A:744:LYS:HG2	1:A:748:MET:CE	2.47	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.16	0.45
2:B:1003:ALA:O	3:C:177:GLU:HA	2.17	0.45
2:B:566:LEU:O	2:B:567:GLU:C	2.55	0.45
2:B:641:GLU:C	2:B:643:ASP:N	2.71	0.45
2:B:70:ILE:O	2:B:70:ILE:HG22	2.17	0.45
2:B:782:LEU:CD1	2:B:788:ARG:NH1	2.76	0.45
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:PHE:C	3:C:20:PHE:CD1	2.90	0.45
8:H:139:ASN:O	8:H:140:ALA:CB	2.61	0.45
2:B:800:GLN:CG	10:J:52:THR:HG22	2.42	0.45
14:N:1:DA:C2	16:T:17:DA:N1	2.85	0.45
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.32	0.45
1:A:597:LEU:N	1:A:597:LEU:CD1	2.78	0.45
1:A:860:LEU:HB3	1:A:862:ASN:OD1	2.17	0.45
2:B:1010:LEU:HD23	2:B:1092:TYR:CE1	2.52	0.45
2:B:234:ILE:HD12	2:B:234:ILE:N	2.31	0.45
2:B:265:SER:O	2:B:266:ALA:HB2	2.17	0.45
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.45
2:B:562:GLY:O	2:B:590:HIS:ND1	2.50	0.45
2:B:992:ILE:CG1	2:B:993:THR:N	2.78	0.45
2:B:831:SER:HG	2:B:994:TYR:HE1	1.62	0.45
3:C:11:ARG:O	3:C:12:GLU:C	2.55	0.45
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.99	0.45
5:E:59:SER:OG	5:E:81:GLU:HG3	2.17	0.45
8:H:108:SER:O	8:H:109:LYS:C	2.56	0.45
8:H:11:GLN:C	8:H:28:ALA:HB1	2.36	0.45
11:K:51:LEU:HD22	11:K:51:LEU:H	1.82	0.45
11:K:85:ASP:O	11:K:88:LYS:N	2.50	0.45
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.44
1:A:260:ASP:CG	1:A:261:ASP:N	2.71	0.44
1:A:416:ARG:C	1:A:417:TYR:CD2	2.91	0.44
1:A:53:LEU:O	1:A:54:ASN:C	2.55	0.44
1:A:828:ALA:HB1	2:B:530:GLY:CA	2.42	0.44
2:B:244:LEU:O	2:B:249:ARG:HG2	2.17	0.44
2:B:662:MET:HA	2:B:665:GLU:HB2	1.99	0.44
2:B:956:THR:HG22	2:B:957:ASN:O	2.17	0.44
3:C:147:LEU:CD2	3:C:147:LEU:N	2.75	0.44
3:C:233:GLU:OE1	10:J:12:LYS:HE2	2.17	0.44
5:E:134:THR:C	5:E:135:PHE:HD1	2.20	0.44
5:E:155:ARG:O	5:E:156:LEU:HG	2.16	0.44
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.98	0.44
1:A:537:ARG:NH2	8:H:122:LEU:HD12	2.25	0.44
9:I:10:CYS:O	9:I:11:ASN:C	2.55	0.44
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.46	0.44
16:T:23:DG:H2'	16:T:24:DG:C8	2.52	0.44
1:A:1005:GLU:HG3	1:A:1009:ASN:HD21	1.80	0.44
1:A:688:LYS:C	1:A:690:VAL:H	2.18	0.44
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD12	1:A:914:GLU:H	1.82	0.44
1:A:901:LEU:N	1:A:926:GLN:NE2	2.62	0.44
1:A:974:ASP:C	1:A:976:THR:H	2.20	0.44
2:B:302:CYS:SG	2:B:311:LEU:HD21	2.57	0.44
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.99	0.44
2:B:758:PHE:N	2:B:759:PRO:CD	2.81	0.44
2:B:799:PRO:O	2:B:800:GLN:HG3	2.17	0.44
2:B:868:MET:O	2:B:870:ILE:HG13	2.17	0.44
2:B:908:GLU:O	2:B:909:ASP:C	2.55	0.44
3:C:113:VAL:HG23	3:C:145:CYS:O	2.17	0.44
5:E:122:LYS:O	5:E:123:LEU:HD23	2.18	0.44
7:G:126:ASN:HD22	7:G:128:PRO:HD3	1.82	0.44
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.70	0.44
1:A:1070:GLN:O	1:A:1072:ILE:N	2.50	0.44
1:A:1315:GLU:C	1:A:1317:MET:H	2.19	0.44
1:A:200:ARG:HH11	1:A:200:ARG:HB3	1.82	0.44
1:A:433:GLU:OE1	2:B:1108:ARG:NH1	2.49	0.44
1:A:464:PRO:O	1:A:465:TYR:O	2.36	0.44
1:A:560:ILE:HG12	1:A:560:ILE:H	1.35	0.44
1:A:648:ASN:C	1:A:650:GLN:N	2.69	0.44
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.98	0.44
1:A:858:ASN:ND2	1:A:860:LEU:N	2.59	0.44
1:A:962:ARG:O	1:A:965:GLN:N	2.51	0.44
2:B:1152:MET:HE1	2:B:1157:ALA:HA	1.97	0.44
2:B:169:ARG:HB3	2:B:169:ARG:NH1	2.17	0.44
2:B:322:PHE:O	2:B:322:PHE:CD1	2.70	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.50	0.44
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.33	0.44
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.46	0.44
4:D:66:ARG:C	4:D:68:ARG:N	2.71	0.44
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.82	0.44
7:G:22:MET:O	7:G:23:LYS:C	2.56	0.44
8:H:19:ARG:C	8:H:20:TYR:HD2	2.21	0.44
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.99	0.44
16:T:24:DG:H2''	16:T:25:DT:H5'	1.99	0.44
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.53	0.44
1:A:1101:LEU:HD12	1:A:1101:LEU:O	2.17	0.44
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.18	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.48	0.44
1:A:1389:PHE:C	1:A:1391:ARG:H	2.20	0.44
1:A:252:PHE:O	1:A:256:GLN:NE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:O	1:A:314:ALA:HB3	2.16	0.44
1:A:738:LYS:C	1:A:740:LEU:H	2.20	0.44
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.00	0.44
2:B:90:ILE:HA	2:B:133:LYS:O	2.17	0.44
2:B:383:ASN:C	2:B:387:LEU:HD13	2.38	0.44
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.43	0.44
2:B:758:PHE:HB2	2:B:1024:ALA:CB	2.41	0.44
4:D:40:HIS:ND1	4:D:41:GLN:N	2.64	0.44
5:E:13:TRP:O	5:E:16:PHE:HB3	2.18	0.44
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.53	0.44
7:G:166:ASP:O	7:G:168:LEU:HG	2.17	0.44
8:H:91:ASP:O	8:H:93:TYR:N	2.41	0.44
1:A:1213:GLY:O	1:A:1214:GLU:C	2.53	0.44
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.18	0.44
2:B:212:LEU:HD12	2:B:409:ALA:HB1	1.98	0.44
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.82	0.44
2:B:525:ALA:O	2:B:768:THR:HG23	2.17	0.44
2:B:563:MET:HE3	2:B:580:VAL:CB	2.44	0.44
2:B:752:ALA:O	2:B:755:ILE:CG1	2.65	0.44
2:B:758:PHE:C	2:B:760:ASP:H	2.20	0.44
2:B:882:THR:HG21	2:B:884:ARG:HB2	1.99	0.44
3:C:241:ASP:HB3	11:K:109:TRP:CZ2	2.52	0.44
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.18	0.44
1:A:1206:ASP:O	1:A:1207:LEU:HD23	2.17	0.44
1:A:152:VAL:CG1	1:A:153:PRO:CD	2.92	0.44
1:A:428:TYR:HD1	1:A:428:TYR:H	1.62	0.44
1:A:478:TYR:O	1:A:479:ASN:HB3	2.18	0.44
1:A:65:LEU:O	1:A:66:LYS:C	2.56	0.44
1:A:666:ILE:HD12	1:A:667:GLY:N	2.27	0.44
2:B:1012:ILE:HD13	2:B:1092:TYR:OH	2.18	0.44
2:B:449:ASN:O	2:B:451:LYS:N	2.44	0.44
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.99	0.44
2:B:863:GLU:HG2	2:B:872:GLU:HB2	1.98	0.44
4:D:212:LYS:O	4:D:214:LEU:N	2.51	0.44
5:E:55:ARG:C	5:E:57:MET:H	2.20	0.44
8:H:27:GLU:HA	8:H:38:LEU:O	2.18	0.44
8:H:91:ASP:C	8:H:93:TYR:H	2.21	0.44
9:I:50:THR:HG22	9:I:52:ILE:H	1.83	0.44
9:I:61:ASP:C	9:I:63:GLY:H	2.21	0.44
16:T:8:DC:C2'	16:T:9:DA:OP2	2.63	0.44
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.99	0.44
1:A:1329:THR:CG2	1:A:1331:SER:H	1.98	0.44
1:A:715:GLU:O	1:A:717:ASN:N	2.50	0.44
2:B:176:SER:O	2:B:182:SER:HB3	2.18	0.44
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.52	0.44
2:B:578:THR:O	2:B:589:VAL:HG13	2.17	0.44
2:B:755:ILE:HG22	2:B:809:MET:HE1	2.00	0.44
2:B:857:ARG:O	2:B:967:ARG:HA	2.17	0.44
2:B:120:ARG:NH2	2:B:956:THR:HB	2.33	0.44
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.44
6:F:79:ARG:HG2	6:F:144:GLU:OE1	2.17	0.44
6:F:73:ALA:O	6:F:74:ILE:HB	2.18	0.44
9:I:14:LEU:HD13	9:I:28:GLU:N	2.33	0.44
1:A:935:GLN:NE2	1:A:1023:ARG:NH1	2.66	0.44
1:A:1166:ASP:O	1:A:1167:GLU:C	2.57	0.44
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.44
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.58	0.44
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.52	0.44
1:A:207:ILE:HG23	1:A:211:PHE:CE1	2.52	0.44
1:A:305:ASP:OD2	1:A:326:ARG:HD3	2.18	0.44
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	2.00	0.44
1:A:894:GLU:O	1:A:898:ARG:HB3	2.18	0.44
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.86	0.44
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	2.00	0.44
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.48	0.44
2:B:299:GLU:OE1	2:B:572:HIS:CE1	2.71	0.44
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.99	0.44
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.51	0.44
4:D:144:THR:HG22	4:D:144:THR:O	2.17	0.44
8:H:92:ASP:C	8:H:93:TYR:CD1	2.92	0.44
14:N:9:DG:C2	16:T:9:DA:C2	3.06	0.44
15:P:4:A:H2'	15:P:5:C:C6	2.53	0.44
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.45	0.44
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	2.18	0.44
1:A:1280:GLU:O	1:A:1282:VAL:HG23	2.18	0.44
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.33	0.44
1:A:261:ASP:O	1:A:264:PHE:HB2	2.18	0.44
1:A:477:PRO:CG	1:A:521:MET:HG2	2.48	0.44
1:A:62:ASP:O	1:A:63:ARG:HB2	2.18	0.44
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.99	0.44
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1172:ILE:O	2:B:1172:ILE:CG2	2.58	0.44
2:B:408:LEU:O	2:B:411:PRO:HD2	2.18	0.44
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.45	0.44
3:C:168:ALA:O	3:C:170:TRP:N	2.50	0.44
3:C:173:ALA:O	3:C:174:ALA:HB3	2.18	0.44
3:C:248:ILE:HG23	11:K:98:LEU:HD22	2.00	0.44
4:D:124:GLU:C	4:D:126:ILE:H	2.22	0.44
4:D:53:SER:HB3	4:D:152:SER:CA	2.47	0.44
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.53	0.44
10:J:1:MET:N	10:J:56:LEU:HB2	2.33	0.44
10:J:7:CYS:CB	10:J:49:MET:HE3	2.48	0.44
11:K:13:GLY:O	11:K:14:GLU:C	2.56	0.44
11:K:47:ARG:O	11:K:51:LEU:HD22	2.18	0.44
1:A:1107:VAL:CG1	1:A:1333:ILE:HD11	2.47	0.43
1:A:1271:ILE:HG22	1:A:1271:ILE:O	2.18	0.43
1:A:311:GLN:CB	1:A:312:PRO:CD	2.96	0.43
1:A:443:LEU:HA	1:A:443:LEU:HD22	1.79	0.43
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.43
1:A:548:ASN:HD21	11:K:47:ARG:CZ	2.31	0.43
1:A:629:LEU:HD23	1:A:629:LEU:C	2.38	0.43
1:A:91:PHE:H	1:A:297:GLN:NE2	2.10	0.43
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.33	0.43
2:B:294:ASP:C	2:B:296:GLU:N	2.72	0.43
2:B:502:ILE:HG12	2:B:535:LEU:HD13	1.99	0.43
2:B:616:ILE:HG13	2:B:697:GLU:HA	2.00	0.43
3:C:60:ASP:HB3	12:L:67:PHE:CZ	2.53	0.43
4:D:49:ALA:HB2	4:D:174:PRO:O	2.18	0.43
4:D:176:GLU:C	4:D:178:ALA:H	2.21	0.43
5:E:161:LYS:HG3	5:E:195:VAL:HG21	2.00	0.43
6:F:123:LYS:HB2	6:F:123:LYS:HE3	1.82	0.43
11:K:78:THR:HG22	11:K:79:GLU:H	1.81	0.43
12:L:43:THR:O	12:L:43:THR:HG22	2.18	0.43
12:L:48:CYS:O	12:L:50:ASP:N	2.42	0.43
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.51	0.43
1:A:264:PHE:C	1:A:266:LEU:N	2.72	0.43
1:A:332:LYS:CA	1:A:337:ARG:HD2	2.49	0.43
1:A:688:LYS:C	1:A:690:VAL:N	2.71	0.43
1:A:763:ALA:C	1:A:803:SER:HB3	2.38	0.43
1:A:886:ILE:HG22	1:A:887:GLY:N	2.33	0.43
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.82	0.43
2:B:547:VAL:HG13	2:B:548:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:MET:CE	2:B:601:ARG:HG3	2.47	0.43
2:B:845:SER:O	2:B:850:LEU:HB3	2.18	0.43
3:C:238:ILE:HA	3:C:239:PRO:HD3	1.88	0.43
6:F:85:MET:SD	6:F:93:ILE:HD12	2.58	0.43
7:G:132:SER:HB3	7:G:135:ASP:N	2.31	0.43
8:H:123:MET:HG2	8:H:124:ARG:N	2.33	0.43
8:H:19:ARG:O	8:H:20:TYR:HD2	2.01	0.43
10:J:13:VAL:C	10:J:14:VAL:HG23	2.38	0.43
10:J:9:SER:OG	10:J:48:ARG:NH2	2.51	0.43
16:T:16:DT:H6	16:T:16:DT:H2'	1.55	0.43
1:A:1385:THR:O	1:A:1387:HIS:N	2.51	0.43
1:A:39:GLU:O	1:A:53:LEU:CB	2.66	0.43
1:A:548:ASN:ND2	11:K:47:ARG:NH2	2.65	0.43
2:B:363:HIS:C	2:B:365:THR:H	2.21	0.43
2:B:576:ASP:CB	2:B:622:LYS:NZ	2.80	0.43
2:B:777:ALA:HA	2:B:1095:LEU:HA	2.00	0.43
2:B:879:ARG:NH2	2:B:885:MET:CE	2.82	0.43
3:C:181:ASP:O	3:C:181:ASP:CG	2.57	0.43
5:E:116:ILE:HG22	5:E:117:THR:N	2.32	0.43
7:G:117:GLN:O	7:G:119:LEU:N	2.51	0.43
11:K:31:VAL:CG1	11:K:32:VAL:N	2.80	0.43
12:L:55:ILE:O	12:L:56:LEU:CB	2.66	0.43
12:L:60:ARG:HG2	12:L:61:THR:N	2.30	0.43
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.52	0.43
1:A:135:PHE:HB2	1:A:223:GLY:N	2.34	0.43
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.00	0.43
2:B:547:VAL:H	2:B:612:GLU:CD	2.21	0.43
3:C:29:MET:CE	11:K:98:LEU:HG	2.48	0.43
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.40	0.43
3:C:88:CYS:O	3:C:88:CYS:SG	2.75	0.43
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.78	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.00	0.43
7:G:111:THR:C	7:G:113:HIS:H	2.21	0.43
7:G:12:THR:HG22	7:G:67:SER:HB3	2.01	0.43
8:H:10:PHE:N	8:H:10:PHE:CD1	2.86	0.43
1:A:1332:PHE:O	1:A:1333:ILE:C	2.56	0.43
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.51	0.43
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.54	0.43
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.96	0.43
1:A:838:GLN:O	1:A:842:VAL:HG23	2.19	0.43
2:B:1120:GLU:CG	2:B:1121:GLY:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.02	0.43
2:B:539:LEU:HD22	2:B:543:SER:OG	2.19	0.43
2:B:637:LEU:HA	2:B:743:ILE:HD11	2.00	0.43
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.62	0.43
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.48	0.43
4:D:128:VAL:C	4:D:130:LEU:N	2.71	0.43
4:D:49:ALA:CB	4:D:174:PRO:O	2.65	0.43
6:F:124:GLU:O	6:F:130:ILE:HG13	2.18	0.43
6:F:82:THR:HG22	6:F:84:TYR:HB2	2.01	0.43
7:G:143:ILE:CG2	7:G:145:VAL:HG23	2.45	0.43
7:G:22:MET:O	7:G:25:TYR:N	2.51	0.43
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.54	0.43
8:H:12:VAL:HB	8:H:52:GLN:H	1.83	0.43
1:A:1135:ARG:HH21	1:A:1284:MET:CE	2.31	0.43
1:A:1187:GLN:O	1:A:1243:VAL:HG23	2.19	0.43
1:A:1193:LEU:HD22	1:A:1260:LEU:HD11	2.00	0.43
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.82	0.43
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.19	0.43
2:B:1224:PHE:CZ	5:E:171:LYS:HG3	2.53	0.43
2:B:169:ARG:HH11	2:B:169:ARG:CB	2.20	0.43
2:B:388:CYS:C	2:B:390:LEU:N	2.70	0.43
2:B:516:ASN:ND2	2:B:516:ASN:H	2.07	0.43
2:B:838:SER:HA	2:B:989:THR:O	2.19	0.43
2:B:956:THR:HG22	2:B:957:ASN:N	2.34	0.43
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.48	0.43
4:D:192:LYS:HE3	4:D:207:LEU:HD23	2.00	0.43
14:N:5:DA:H2"	14:N:6:DC:O5'	2.18	0.43
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.49	0.43
1:A:211:PHE:HA	1:A:214:ILE:CD1	2.49	0.43
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.83	0.43
1:A:336:ILE:HG21	1:A:1401:SER:HA	2.00	0.43
1:A:40:THR:C	1:A:41:MET:HG3	2.38	0.43
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.31	0.43
2:B:116:GLU:O	2:B:117:ALA:C	2.56	0.43
2:B:418:LYS:HD3	2:B:422:LYS:HZ1	1.83	0.43
2:B:552:MET:HA	2:B:555:ILE:HB	2.00	0.43
2:B:612:GLU:O	2:B:612:GLU:HG2	2.18	0.43
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.49	0.43
3:C:75:MET:CB	3:C:128:ASN:HB3	2.38	0.43
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.74	0.43
3:C:97:VAL:HG12	3:C:99:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:ILE:HG22	5:E:213:ILE:O	2.19	0.43
4:D:190:GLU:HG3	7:G:167:TYR:CD2	2.54	0.43
8:H:3:ASN:O	8:H:60:ALA:HB1	2.18	0.43
10:J:56:LEU:O	10:J:58:GLU:N	2.51	0.43
11:K:60:ALA:O	11:K:73:LEU:HD12	2.19	0.43
1:A:1057:VAL:HG12	1:A:1058:VAL:O	2.19	0.43
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.65	0.43
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.54	0.43
1:A:608:ILE:O	1:A:610:GLY:N	2.52	0.43
1:A:709:THR:HG22	1:A:711:ARG:N	2.25	0.43
1:A:779:PHE:CE2	2:B:517:THR:HA	2.54	0.43
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.67	0.43
1:A:455:MET:HE1	2:B:1134:GLU:HB3	2.00	0.43
2:B:1202:LEU:CD2	2:B:1206:GLU:CD	2.87	0.43
2:B:325:GLN:O	2:B:326:ASP:HB3	2.19	0.43
2:B:345:LYS:C	2:B:347:LYS:N	2.70	0.43
2:B:682:SER:O	2:B:686:ASN:ND2	2.51	0.43
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.53	0.43
2:B:773:MET:SD	2:B:987:LYS:HB3	2.58	0.43
3:C:29:MET:HA	11:K:45:LEU:CD1	2.49	0.43
6:F:83:PRO:HA	6:F:146:TRP:CZ3	2.53	0.43
9:I:98:VAL:HG11	9:I:113:ASP:HB2	2.01	0.43
1:A:547:LEU:HB3	11:K:58:PHE:HE1	1.84	0.43
12:L:32:ALA:H	12:L:55:ILE:HG13	1.83	0.43
1:A:1042:PHE:CD2	1:A:1046:LEU:HD11	2.54	0.43
1:A:86:LEU:CG	1:A:237:THR:O	2.66	0.43
1:A:504:LEU:HD11	6:F:91:ALA:HB1	2.01	0.43
1:A:605:MET:HG2	1:A:621:THR:HG23	2.00	0.43
1:A:780:VAL:O	1:A:782:ARG:HG2	2.19	0.43
1:A:825:ILE:O	1:A:829:VAL:HG23	2.18	0.43
2:B:487:THR:CG2	2:B:488:TYR:N	2.81	0.43
2:B:530:GLY:O	2:B:531:GLN:C	2.56	0.43
2:B:558:LEU:C	2:B:560:GLU:N	2.63	0.43
2:B:812:LEU:C	2:B:814:PHE:H	2.21	0.43
5:E:24:LYS:HB2	5:E:24:LYS:HE3	1.82	0.43
7:G:30:LEU:HD22	7:G:72:VAL:HG11	2.01	0.43
4:D:175:PHE:CZ	7:G:85:GLU:HG3	2.41	0.43
8:H:113:ALA:HA	8:H:125:LEU:O	2.19	0.43
8:H:42:ILE:CG2	8:H:43:ASN:N	2.81	0.43
10:J:36:LEU:CD1	10:J:47:ARG:NH1	2.82	0.43
16:T:17:DA:H3'	16:T:17:DA:P	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.19	0.43
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.54	0.43
1:A:779:PHE:O	1:A:780:VAL:C	2.55	0.43
1:A:858:ASN:C	1:A:860:LEU:H	2.23	0.43
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.54	0.43
2:B:1108:ARG:O	2:B:1108:ARG:CG	2.67	0.43
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.36	0.43
2:B:324:ILE:HG12	2:B:329:THR:HG21	2.01	0.43
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.84	0.43
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.49	0.43
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.53	0.43
3:C:128:ASN:O	3:C:129:ILE:HB	2.17	0.43
5:E:137:GLU:C	5:E:139:ALA:H	2.22	0.43
7:G:126:ASN:HA	7:G:127:PRO:HA	1.73	0.43
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.98	0.43
10:J:56:LEU:O	10:J:57:ILE:C	2.56	0.43
11:K:58:PHE:HE2	11:K:74:ARG:HD3	1.84	0.43
2:B:902:GLY:O	12:L:65:VAL:HG11	2.19	0.43
16:T:17:DA:C8	16:T:18:DC:C5	3.05	0.43
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.82	0.42
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.18	0.42
1:A:834:THR:CG2	1:A:835:GLY:N	2.81	0.42
1:A:882:SER:HA	1:A:952:ALA:O	2.19	0.42
2:B:1100:ASP:OD2	11:K:1:MET:HB2	2.19	0.42
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.33	0.42
2:B:882:THR:HG21	2:B:935:ARG:CA	2.49	0.42
3:C:70:ILE:HG12	3:C:142:VAL:HG11	2.01	0.42
3:C:33:LEU:HG	3:C:37:MET:HE2	2.01	0.42
4:D:47:LEU:HD12	4:D:48:ILE:H	1.82	0.42
11:K:24:ASP:OD1	11:K:26:LYS:HB2	2.18	0.42
1:A:1325:THR:HG22	1:A:1325:THR:O	2.18	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.79	0.42
1:A:614:PHE:CB	8:H:122:LEU:HD21	2.49	0.42
1:A:663:SER:OG	1:A:664:THR:N	2.52	0.42
1:A:709:THR:CG2	9:I:94:ASP:HA	2.49	0.42
1:A:75:ASN:O	1:A:76:GLU:CB	2.67	0.42
1:A:760:GLN:HG2	1:A:765:VAL:O	2.19	0.42
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.54	0.42
2:B:388:CYS:O	2:B:390:LEU:N	2.52	0.42
2:B:417:PHE:O	2:B:420:LEU:HB2	2.19	0.42
2:B:595:ARG:O	2:B:596:LEU:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:LEU:HD11	2:B:684:LEU:HD11	2.00	0.42
2:B:705:MET:H	2:B:710:LEU:HD12	1.83	0.42
4:D:66:ARG:O	4:D:70:PHE:HB2	2.19	0.42
8:H:5:LEU:HD22	8:H:133:ASN:O	2.19	0.42
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	2.01	0.42
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.82	0.42
1:A:1385:THR:C	1:A:1387:HIS:N	2.71	0.42
1:A:253:ASN:O	1:A:254:GLU:HG3	2.19	0.42
1:A:355:GLY:N	1:A:482:PHE:CZ	2.87	0.42
1:A:470:LEU:O	1:A:470:LEU:HD12	2.19	0.42
1:A:590:ARG:NH2	1:A:620:LYS:CB	2.62	0.42
2:B:183:GLU:O	2:B:184:ALA:C	2.58	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.42
2:B:916:THR:HG22	2:B:918:ILE:HG13	2.00	0.42
2:B:997:GLU:H	2:B:997:GLU:CD	2.21	0.42
3:C:116:LYS:HB3	3:C:140:ASN:HA	2.01	0.42
3:C:69:LEU:N	3:C:69:LEU:HD12	2.34	0.42
4:D:170:THR:HG21	4:D:172:LEU:HD11	2.00	0.42
4:D:51:ASN:O	4:D:52:LEU:O	2.38	0.42
5:E:143:ASN:O	5:E:146:HIS:HB2	2.20	0.42
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.33	0.42
7:G:160:ILE:CG2	7:G:161:GLY:N	2.81	0.42
10:J:3:VAL:HG22	10:J:53:HIS:CE1	2.54	0.42
3:C:166:GLU:C	11:K:6:ARG:NH1	2.72	0.42
1:A:145:LYS:C	1:A:146:MET:HG3	2.39	0.42
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.54	0.42
1:A:376:TYR:HA	1:A:377:PRO:HD2	1.87	0.42
1:A:67:CYS:O	1:A:67:CYS:SG	2.78	0.42
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.54	0.42
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.76	0.42
2:B:1176:ASN:C	2:B:1178:ASN:N	2.66	0.42
2:B:240:ILE:HG21	2:B:381:MET:CE	2.49	0.42
2:B:289:LEU:CD1	2:B:375:ALA:HB2	2.49	0.42
3:C:100:THR:HG21	3:C:102:GLN:NE2	2.34	0.42
3:C:123:ASN:ND2	3:C:125:MET:SD	2.92	0.42
3:C:17:ASN:O	3:C:18:VAL:CG2	2.67	0.42
8:H:26:ILE:CG2	8:H:27:GLU:N	2.82	0.42
8:H:40:LEU:HB2	8:H:123:MET:HE2	2.01	0.42
8:H:76:THR:HG22	8:H:76:THR:O	2.19	0.42
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.85	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.85	0.42
11:K:76:GLN:HE21	11:K:76:GLN:HB3	1.53	0.42
1:A:1123:GLY:O	1:A:1124:HIS:C	2.57	0.42
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.77	0.42
1:A:1336:MET:HE1	1:A:1381:LEU:HG	2.00	0.42
1:A:770:VAL:HG12	1:A:771:GLU:N	2.34	0.42
2:B:1071:VAL:O	2:B:1072:MET:HG2	2.19	0.42
2:B:1181:GLU:HB3	2:B:1182:CYS:H	1.70	0.42
2:B:186:GLU:HG2	10:J:62:ARG:HH22	1.85	0.42
2:B:408:LEU:HD13	2:B:545:ILE:CD1	2.49	0.42
2:B:593:PRO:O	2:B:594:ALA:C	2.57	0.42
2:B:640:VAL:O	2:B:650:GLU:O	2.37	0.42
2:B:639:ILE:HD12	2:B:688:GLY:O	2.20	0.42
2:B:843:GLN:O	2:B:846:ILE:HB	2.19	0.42
2:B:874:PHE:HA	2:B:913:GLY:O	2.18	0.42
2:B:945:GLU:O	2:B:946:ASN:CB	2.68	0.42
2:B:969:ARG:HG2	2:B:970:THR:H	1.84	0.42
3:C:220:ASP:OD1	3:C:220:ASP:C	2.58	0.42
4:D:128:VAL:O	4:D:132:GLN:HG3	2.19	0.42
4:D:210:ILE:HG13	4:D:210:ILE:H	1.66	0.42
5:E:154:ILE:HG22	5:E:155:ARG:O	2.20	0.42
6:F:125:LEU:HA	6:F:130:ILE:HD11	2.02	0.42
8:H:102:TYR:N	8:H:102:TYR:CD2	2.87	0.42
10:J:21:TYR:C	10:J:23:ASN:H	2.23	0.42
15:P:8:G:O2'	15:P:9:G:H5'	2.19	0.42
1:A:1169:ILE:O	1:A:1169:ILE:HG22	2.20	0.42
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.42
1:A:90:VAL:O	1:A:235:ILE:HG23	2.19	0.42
2:B:1157:ALA:O	2:B:1158:PHE:CB	2.65	0.42
2:B:1159:ARG:HD3	2:B:1193:GLN:NE2	2.35	0.42
2:B:195:CYS:HB2	2:B:784:ASN:OD1	2.19	0.42
2:B:295:GLY:CA	2:B:298:LEU:HD23	2.48	0.42
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.55	0.42
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.08	0.42
2:B:792:MET:CE	2:B:857:ARG:NH2	2.83	0.42
3:C:161:LYS:HB3	3:C:162:GLY:H	1.64	0.42
2:B:1080:LYS:HG3	3:C:180:TYR:CE2	2.55	0.42
4:D:192:LYS:HD2	4:D:199:ASN:HA	2.00	0.42
5:E:124:VAL:C	5:E:126:SER:H	2.23	0.42
5:E:186:LEU:O	5:E:189:GLY:N	2.44	0.42
3:C:66:ARG:HH11	10:J:2:ILE:HG21	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:GLU:O	10:J:33:GLY:C	2.58	0.42
10:J:44:TYR:HA	10:J:47:ARG:CB	2.33	0.42
16:T:14:DG:H2"	16:T:15:DT:OP2	2.19	0.42
1:A:20:GLY:HA2	1:A:1413:GLY:O	2.19	0.42
1:A:458:HIS:CE1	1:A:507:VAL:CG2	3.03	0.42
1:A:605:MET:HG2	1:A:621:THR:HG21	2.01	0.42
2:B:1162:ILE:HA	2:B:1168:LEU:O	2.19	0.42
2:B:170:LEU:HD12	2:B:171:PRO:N	2.35	0.42
2:B:23:ALA:O	2:B:654:ARG:CD	2.67	0.42
2:B:834:ASN:CA	2:B:838:SER:O	2.67	0.42
2:B:857:ARG:HH11	2:B:945:GLU:CD	2.23	0.42
2:B:955:THR:N	2:B:963:PHE:O	2.51	0.42
2:B:975:GLN:HB3	2:B:975:GLN:HE21	1.59	0.42
3:C:146:LYS:HB2	10:J:57:ILE:HD11	2.02	0.42
3:C:236:GLY:O	3:C:237:SER:C	2.58	0.42
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.42
5:E:90:VAL:O	5:E:90:VAL:HG22	2.20	0.42
6:F:73:ALA:O	6:F:74:ILE:CB	2.67	0.42
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.20	0.42
9:I:26:LEU:HD13	9:I:35:VAL:HG11	2.01	0.42
9:I:65:ASP:HA	9:I:66:PRO:HD2	1.86	0.42
9:I:90:GLN:HE21	9:I:92:ARG:HD3	1.85	0.42
10:J:44:TYR:CA	10:J:47:ARG:HB2	2.32	0.42
1:A:1220:PHE:CG	1:A:1224:LEU:HD23	2.55	0.42
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.19	0.42
1:A:1444:MET:O	6:F:133:VAL:N	2.51	0.42
1:A:305:ASP:OD1	1:A:306:ASN:N	2.52	0.42
1:A:881:GLN:NE2	1:A:959:ASN:HA	2.35	0.42
2:B:1002:THR:HG22	2:B:1087:PHE:HE1	1.83	0.42
2:B:1106:ARG:CG	2:B:1107:ALA:N	2.83	0.42
1:A:350:ARG:HB3	2:B:1128:LEU:HD21	2.02	0.42
2:B:710:LEU:CD2	2:B:733:HIS:HB3	2.49	0.42
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.54	0.42
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.19	0.42
10:J:3:VAL:HA	10:J:4:PRO:HD3	1.78	0.42
12:L:47:ARG:HB3	12:L:48:CYS:H	1.70	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.83	0.42
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.68	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.65	0.42
1:A:343:LYS:HE3	2:B:1151:LEU:HB3	2.02	0.42
1:A:577:ILE:HA	1:A:580:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HG	1:A:613:ILE:HD12	2.01	0.42
1:A:818:MET:HG2	2:B:514:LEU:HG	2.02	0.42
1:A:915:SER:O	1:A:919:ILE:HB	2.20	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.02	0.42
2:B:1125:ASP:O	2:B:1126:GLY:O	2.37	0.42
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.30	0.42
3:C:168:ALA:C	3:C:170:TRP:N	2.72	0.42
3:C:189:THR:CG2	3:C:190:ASP:N	2.82	0.42
3:C:33:LEU:CD1	3:C:37:MET:HE2	2.48	0.42
5:E:161:LYS:HD2	5:E:195:VAL:HG23	2.01	0.42
5:E:91:LYS:O	5:E:93:MET:N	2.53	0.42
6:F:74:ILE:HD12	6:F:143:PHE:O	2.19	0.42
8:H:118:PHE:O	8:H:120:GLY:N	2.53	0.42
16:T:26:DC:H2'	16:T:27:DA:H8	1.85	0.42
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.01	0.42
1:A:1349:TYR:CD2	1:A:1350:LYS:N	2.88	0.42
1:A:343:LYS:HE3	2:B:1151:LEU:CB	2.50	0.42
1:A:39:GLU:OE1	1:A:39:GLU:N	2.53	0.42
1:A:456:MET:HE1	1:A:474:VAL:HG23	2.02	0.42
1:A:590:ARG:O	1:A:591:PHE:CB	2.66	0.42
1:A:90:VAL:HG12	1:A:91:PHE:H	1.85	0.42
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.50	0.42
2:B:124:TYR:HE2	2:B:179:CYS:SG	2.42	0.42
2:B:189:LEU:O	2:B:191:LYS:N	2.52	0.42
2:B:25:ILE:HD11	2:B:654:ARG:N	2.34	0.42
2:B:547:VAL:HG12	2:B:612:GLU:CD	2.39	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.73	0.42
2:B:542:MET:HE3	2:B:743:ILE:HG13	2.01	0.42
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.64	0.42
3:C:166:GLU:O	11:K:6:ARG:NH1	2.53	0.42
7:G:43:GLY:HA3	7:G:80:LYS:HB3	2.02	0.42
2:B:954:VAL:O	12:L:55:ILE:O	2.37	0.42
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.49	0.41
1:A:182:VAL:CG2	1:A:201:VAL:HG13	2.50	0.41
1:A:602:ASP:O	1:A:616:VAL:HG23	2.20	0.41
2:B:303:TYR:N	2:B:303:TYR:CD2	2.87	0.41
2:B:310:MET:HE3	2:B:387:LEU:HD12	2.01	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.23	0.41
2:B:466:TRP:HA	2:B:466:TRP:HE3	1.82	0.41
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.55	0.41
2:B:936:ASP:C	2:B:936:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:PHE:HE1	3:C:230:MET:HE1	1.85	0.41
3:C:73:GLN:HE21	3:C:74:SER:N	2.14	0.41
8:H:130:ARG:N	8:H:130:ARG:HD2	2.24	0.41
8:H:5:LEU:N	8:H:60:ALA:HB2	2.35	0.41
9:I:28:GLU:HB2	9:I:29:CYS:H	1.69	0.41
10:J:53:HIS:CD2	10:J:53:HIS:C	2.94	0.41
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.20	0.41
1:A:111:GLY:O	1:A:214:ILE:HA	2.20	0.41
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.35	0.41
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.35	0.41
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.20	0.41
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.43	0.41
1:A:588:LEU:O	1:A:606:LEU:HD12	2.20	0.41
1:A:466:SER:O	2:B:1099:VAL:HG11	2.20	0.41
2:B:564:GLU:HA	2:B:565:PRO:HD2	1.87	0.41
2:B:593:PRO:O	2:B:596:LEU:N	2.54	0.41
2:B:616:ILE:H	2:B:616:ILE:HD12	1.83	0.41
2:B:871:THR:CG2	2:B:872:GLU:N	2.83	0.41
3:C:221:TYR:CD1	3:C:222:LYS:N	2.87	0.41
4:D:119:ARG:HD3	4:D:221:TYR:HD2	1.86	0.41
5:E:137:GLU:O	5:E:139:ALA:N	2.53	0.41
5:E:190:LEU:C	5:E:191:LYS:HG3	2.40	0.41
7:G:153:GLN:O	7:G:154:VAL:O	2.37	0.41
8:H:138:GLU:O	8:H:139:ASN:C	2.59	0.41
8:H:40:LEU:HD21	8:H:142:LEU:HD21	2.01	0.41
9:I:25:LEU:HB3	9:I:38:ALA:HB2	2.03	0.41
1:A:302:THR:CG2	1:A:303:TYR:N	2.71	0.41
1:A:495:GLU:HB3	6:F:99:LEU:CB	2.49	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.02	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.78	0.41
2:B:1066:SER:O	2:B:1067:ARG:HD3	2.20	0.41
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.35	0.41
2:B:797:TYR:C	2:B:798:TYR:CD2	2.78	0.41
5:E:28:TYR:C	5:E:65:THR:HG23	2.41	0.41
7:G:112:LYS:HA	7:G:115:MET:SD	2.61	0.41
10:J:12:LYS:O	10:J:14:VAL:HG23	2.20	0.41
14:N:5:DA:H1'	14:N:6:DC:H5'	2.02	0.41
1:A:1102:LYS:O	1:A:1103:GLU:C	2.59	0.41
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.74	0.41
1:A:896:ARG:O	1:A:1029:ARG:HB3	2.20	0.41
2:B:128:LEU:N	2:B:128:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:ALA:HB2	2:B:738:PHE:HD2	1.77	0.41
3:C:260:LEU:O	3:C:261:ALA:C	2.59	0.41
7:G:49:LEU:O	7:G:50:ASP:C	2.58	0.41
7:G:4:ILE:O	7:G:4:ILE:HG22	2.19	0.41
8:H:84:ALA:CA	8:H:87:ARG:HD2	2.50	0.41
9:I:82:GLU:OE2	9:I:104:LEU:HD12	2.19	0.41
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.02	0.41
1:A:1139:GLU:HB2	1:A:1282:VAL:CG2	2.50	0.41
1:A:1364:ASN:O	1:A:1365:TYR:C	2.59	0.41
1:A:423:ASP:HB3	1:A:424:ILE:H	1.60	0.41
1:A:1063:MET:HG3	2:B:1139:ILE:O	2.20	0.41
2:B:1130:PHE:CE1	2:B:1150:ARG:HG3	2.54	0.41
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.41
2:B:1116:ARG:NE	2:B:1198:TYR:CE1	2.89	0.41
2:B:180:TYR:HD1	2:B:180:TYR:H	1.59	0.41
2:B:615:MET:O	2:B:697:GLU:HG3	2.21	0.41
2:B:912:ILE:CG2	2:B:913:GLY:N	2.83	0.41
2:B:956:THR:HG22	2:B:957:ASN:H	1.86	0.41
4:D:24:ALA:C	4:D:26:THR:N	2.71	0.41
6:F:100:GLN:O	6:F:105:ALA:HB2	2.21	0.41
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.85	0.41
1:A:1059:HIS:CE1	6:F:155:LEU:HD21	2.54	0.41
8:H:109:LYS:HD2	8:H:111:LEU:CD1	2.50	0.41
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.56	0.41
9:I:4:PHE:CD1	9:I:4:PHE:C	2.94	0.41
1:A:1197:LEU:HD11	1:A:1238:ILE:CD1	2.50	0.41
1:A:1295:THR:OG1	1:A:1295:THR:O	2.37	0.41
1:A:16:GLU:CG	1:A:1418:LEU:HD11	2.47	0.41
1:A:151:ASP:HA	1:A:162:VAL:O	2.21	0.41
1:A:150:THR:OG1	1:A:166:GLY:HA2	2.21	0.41
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.51	0.41
2:B:231:PRO:O	2:B:232:SER:HB2	2.20	0.41
2:B:293:PRO:HD2	2:B:296:GLU:OE1	2.19	0.41
2:B:547:VAL:N	2:B:612:GLU:OE2	2.53	0.41
2:B:781:PHE:O	2:B:782:LEU:HD23	2.20	0.41
2:B:797:TYR:CE1	2:B:854:LEU:HD23	2.53	0.41
2:B:880:THR:CB	2:B:934:LYS:HD2	2.51	0.41
3:C:108:GLU:O	3:C:109:SER:CB	2.68	0.41
3:C:8:VAL:HG12	3:C:9:LYS:N	2.36	0.41
5:E:12:LEU:HD12	5:E:12:LEU:O	2.21	0.41
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:SER:O	5:E:159:ASP:N	2.54	0.41
7:G:139:ILE:H	7:G:139:ILE:HG13	1.73	0.41
8:H:48:PRO:O	8:H:49:VAL:CG2	2.69	0.41
8:H:62:SER:O	8:H:63:LEU:O	2.39	0.41
8:H:81:PRO:HB3	8:H:82:PRO:HD2	2.03	0.41
11:K:49:GLU:OE1	11:K:97:LYS:HE3	2.20	0.41
1:A:119:ASN:O	1:A:122:MET:HB3	2.21	0.41
1:A:23:SER:HA	1:A:233:TRP:CD1	2.56	0.41
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.86	0.41
1:A:289:ILE:O	1:A:292:ALA:N	2.45	0.41
1:A:316:GLN:O	1:A:317:LYS:C	2.59	0.41
1:A:41:MET:N	1:A:41:MET:CE	2.83	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.80	0.41
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.41
2:B:377:PHE:C	2:B:379:GLY:H	2.23	0.41
2:B:381:MET:C	2:B:383:ASN:N	2.72	0.41
2:B:710:LEU:O	2:B:711:GLU:OE2	2.38	0.41
2:B:825:VAL:O	2:B:1087:PHE:HD2	2.04	0.41
4:D:30:GLY:H	7:G:82:PHE:HE2	1.69	0.41
5:E:33:GLU:C	5:E:35:VAL:H	2.24	0.41
6:F:73:ALA:O	6:F:74:ILE:HG13	2.21	0.41
8:H:58:THR:CG2	8:H:59:ILE:N	2.82	0.41
9:I:50:THR:CG2	9:I:51:ASN:H	2.29	0.41
10:J:8:PHE:N	10:J:49:MET:HE1	2.36	0.41
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.01	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.59	0.41
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.03	0.41
1:A:599:SER:HA	1:A:600:PRO:HD2	1.91	0.41
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.88	0.41
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.17	0.41
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.32	0.41
2:B:621:GLU:O	2:B:622:LYS:HB2	2.21	0.41
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.55	0.41
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.51	0.41
2:B:973:ILE:HG22	2:B:974:PRO:O	2.20	0.41
2:B:839:MET:HE2	2:B:980:PHE:CD1	2.56	0.41
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.49	0.41
2:B:1069:PHE:O	3:C:201:TRP:HH2	2.03	0.41
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.21	0.41
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.56	0.41
12:L:43:THR:C	12:L:45:ALA:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:HD2	1:A:1033:GLN:NE2	2.36	0.41
1:A:1070:GLN:O	1:A:1071:SER:C	2.57	0.41
1:A:106:VAL:HG12	1:A:107:CYS:N	2.36	0.41
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.20	0.41
1:A:365:GLY:HA2	1:A:461:LYS:O	2.21	0.41
1:A:567:LYS:HD3	8:H:95:TYR:HA	2.02	0.41
1:A:590:ARG:HD3	1:A:604:GLY:CA	2.51	0.41
1:A:605:MET:CE	1:A:612:ILE:HG23	2.50	0.41
1:A:666:ILE:CD1	1:A:667:GLY:N	2.82	0.41
1:A:741:ASN:ND2	1:A:741:ASN:C	2.74	0.41
1:A:93:VAL:HG23	1:A:304:MET:HE3	2.02	0.41
2:B:1197:PRO:HG2	2:B:1200:ALA:HB3	2.03	0.41
2:B:128:LEU:HD11	2:B:170:LEU:HB3	2.03	0.41
2:B:377:PHE:O	2:B:379:GLY:N	2.53	0.41
2:B:605:ARG:NH1	2:B:639:ILE:HG21	2.36	0.41
2:B:703:ILE:HG21	2:B:742:GLU:OE1	2.21	0.41
2:B:878:GLN:O	2:B:879:ARG:O	2.39	0.41
3:C:186:LEU:N	3:C:186:LEU:CD1	2.84	0.41
4:D:46:GLU:C	4:D:47:LEU:O	2.59	0.41
5:E:154:ILE:H	5:E:196:VAL:HG13	1.86	0.41
5:E:22:MET:HE3	5:E:26:ARG:NE	2.32	0.41
7:G:40:GLY:HA2	7:G:157:ILE:HD11	2.02	0.41
8:H:107:VAL:HG21	8:H:126:GLU:OE2	2.21	0.41
9:I:40:SER:OG	9:I:41:PRO:HD2	2.20	0.41
9:I:51:ASN:ND2	9:I:118:ARG:CZ	2.84	0.41
9:I:8:ARG:HG3	9:I:8:ARG:H	1.58	0.41
9:I:90:GLN:HE21	9:I:92:ARG:CD	2.34	0.41
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.21	0.41
1:A:120:GLU:HA	1:A:123:ARG:HG3	2.03	0.41
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.50	0.41
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.44	0.41
1:A:383:TYR:N	1:A:383:TYR:CD2	2.87	0.41
1:A:53:LEU:O	1:A:54:ASN:O	2.39	0.41
1:A:755:PHE:O	1:A:756:ILE:C	2.58	0.41
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.02	0.41
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.21	0.41
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.21	0.41
2:B:521:LEU:HD13	2:B:633:VAL:HB	2.02	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.50	0.41
3:C:242:GLN:HA	3:C:245:VAL:HG23	2.03	0.41
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:107:VAL:HG12	6:F:108:PHE:N	2.35	0.41
6:F:132:LEU:HD23	6:F:132:LEU:HA	1.88	0.41
6:F:72:LYS:HD2	6:F:142:SER:HB3	2.03	0.41
1:A:1444:MET:CB	7:G:59:GLY:O	2.69	0.41
2:B:308:TRP:CH2	9:I:45:ARG:HD3	2.56	0.41
11:K:43:GLY:O	11:K:46:ILE:N	2.52	0.41
1:A:1345:ARG:HG3	1:A:1372:VAL:HG12	2.03	0.41
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.02	0.41
1:A:496:GLU:O	1:A:497:THR:C	2.59	0.41
1:A:550:LEU:CD1	1:A:560:ILE:HG22	2.51	0.41
1:A:687:LYS:O	1:A:690:VAL:HB	2.21	0.41
1:A:69:THR:O	1:A:69:THR:HG22	2.21	0.41
2:B:104:GLU:OE1	12:L:54:ARG:NH2	2.54	0.41
2:B:411:PRO:O	2:B:414:ALA:CB	2.66	0.41
2:B:582:VAL:CG2	2:B:626:ILE:HG21	2.45	0.41
2:B:899:ILE:CD1	2:B:911:ILE:HG23	2.40	0.41
4:D:183:LEU:HD23	4:D:183:LEU:HA	1.86	0.41
4:D:34:GLN:O	4:D:36:LYS:N	2.53	0.41
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.03	0.41
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.51	0.41
1:A:1445:ILE:HA	6:F:132:LEU:HD23	2.03	0.41
8:H:59:ILE:CG2	8:H:60:ALA:N	2.73	0.41
2:B:737:THR:HG22	9:I:66:PRO:HA	1.98	0.41
10:J:18:TRP:HZ3	10:J:50:ILE:HG23	1.85	0.41
10:J:25:LEU:HD23	10:J:30:LEU:O	2.21	0.41
10:J:36:LEU:HD22	10:J:41:LEU:HD12	2.02	0.41
14:N:5:DA:C2	14:N:6:DC:C2	3.09	0.41
16:T:11:DG:H2''	16:T:12:DT:O5'	2.21	0.41
1:A:1004:ASN:OD1	1:A:1005:GLU:N	2.54	0.40
1:A:1016:THR:O	1:A:1017:LEU:C	2.59	0.40
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.50	0.40
1:A:534:LEU:HG	1:A:534:LEU:O	2.20	0.40
1:A:889:SER:HA	1:A:1297:GLU:N	2.36	0.40
1:A:881:GLN:NE2	1:A:958:VAL:O	2.54	0.40
2:B:1002:THR:CG2	2:B:1006:ILE:O	2.69	0.40
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.78	0.40
2:B:230:ALA:N	2:B:231:PRO:CD	2.84	0.40
2:B:292:ILE:HD11	2:B:327:ARG:N	2.35	0.40
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.21	0.40
2:B:576:ASP:HB3	2:B:622:LYS:HZ1	1.83	0.40
2:B:806:THR:HB	2:B:809:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.49	0.40
2:B:882:THR:HG22	2:B:884:ARG:HB2	2.03	0.40
3:C:252:GLN:HG3	11:K:95:ILE:HG23	2.02	0.40
5:E:147:HIS:HD2	5:E:149:LEU:H	1.68	0.40
5:E:211:TYR:CD1	5:E:211:TYR:N	2.90	0.40
6:F:111:LEU:C	6:F:113:GLY:N	2.75	0.40
6:F:123:LYS:C	6:F:125:LEU:N	2.74	0.40
1:A:1152:ILE:O	9:I:43:VAL:HB	2.21	0.40
11:K:43:GLY:O	11:K:45:LEU:N	2.54	0.40
3:C:29:MET:HE2	11:K:98:LEU:HG	2.03	0.40
12:L:30:ILE:O	12:L:56:LEU:CA	2.68	0.40
1:A:1161:THR:CG2	1:A:1162:VAL:H	2.35	0.40
1:A:1444:MET:HE3	1:A:1444:MET:HB2	1.77	0.40
1:A:164:ARG:HG3	1:A:165:GLY:N	2.36	0.40
1:A:447:GLN:NE2	16:T:20:DC:C4'	2.84	0.40
1:A:482:PHE:O	2:B:989:THR:CG2	2.62	0.40
1:A:546:VAL:HG21	1:A:572:TRP:CD2	2.56	0.40
1:A:668:ASP:OD1	1:A:741:ASN:ND2	2.54	0.40
1:A:768:GLN:OE1	1:A:816:HIS:HA	2.21	0.40
2:B:1197:PRO:O	2:B:1200:ALA:N	2.50	0.40
2:B:234:ILE:CG2	2:B:237:VAL:HG23	2.46	0.40
2:B:304:ASP:O	2:B:306:ASN:N	2.54	0.40
2:B:596:LEU:O	2:B:596:LEU:HD12	2.21	0.40
2:B:594:ALA:CA	2:B:617:ARG:HH12	2.34	0.40
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.49	0.40
2:B:906:SER:HA	2:B:946:ASN:HB2	2.03	0.40
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.90	0.40
3:C:58:LEU:N	3:C:58:LEU:HD22	2.35	0.40
4:D:25:ALA:C	4:D:27:LEU:H	2.24	0.40
7:G:23:LYS:O	7:G:27:LYS:HG3	2.20	0.40
1:A:567:LYS:NZ	8:H:95:TYR:CE1	2.88	0.40
9:I:103:CYS:C	9:I:105:SER:H	2.25	0.40
9:I:55:THR:O	9:I:56:ALA:C	2.60	0.40
10:J:21:TYR:C	10:J:23:ASN:N	2.74	0.40
16:T:22:BRU:H2'	16:T:23:DG:H8	1.86	0.40
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.69	0.40
1:A:350:ARG:HA	1:A:487:MET:O	2.21	0.40
1:A:474:VAL:HG13	1:A:474:VAL:O	2.20	0.40
1:A:441:PRO:O	1:A:492:PRO:HG3	2.22	0.40
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.40
1:A:914:GLU:HB2	1:A:979:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.85	0.40
2:B:116:GLU:C	2:B:118:ARG:N	2.74	0.40
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.42	0.40
2:B:873:THR:CG2	2:B:874:PHE:N	2.85	0.40
3:C:84:ARG:CZ	11:K:11:LEU:HD11	2.51	0.40
3:C:81:GLU:O	3:C:95:CYS:HB2	2.21	0.40
4:D:118:THR:HB	4:D:121:LYS:HB2	2.03	0.40
4:D:170:THR:HG21	4:D:172:LEU:CD1	2.51	0.40
5:E:163:GLU:O	5:E:164:LEU:C	2.60	0.40
9:I:58:VAL:HG13	9:I:62:ILE:HD13	2.03	0.40
11:K:48:ALA:O	11:K:50:LEU:N	2.54	0.40
2:B:1204:PHE:O	2:B:1205:GLN:C	2.58	0.40
2:B:408:LEU:C	2:B:411:PRO:HD2	2.41	0.40
2:B:519:TRP:CD1	2:B:519:TRP:C	2.94	0.40
4:D:215:SER:HA	4:D:218:GLU:OE2	2.21	0.40
6:F:81:THR:HB	6:F:136:ARG:NH1	2.35	0.40
9:I:108:HIS:CG	9:I:109:ILE:N	2.89	0.40
1:A:1152:ILE:HD11	9:I:44:TYR:CD2	2.57	0.40
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	2.03	0.40
1:A:1061:GLY:CA	1:A:1437:GLY:HA2	2.52	0.40
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.50	0.40
1:A:1441:PHE:CE2	6:F:89:GLU:HA	2.57	0.40
1:A:16:GLU:HG2	1:A:1418:LEU:CD1	2.48	0.40
1:A:322:VAL:HG12	1:A:322:VAL:O	2.20	0.40
1:A:353:ILE:HG23	1:A:487:MET:HG3	1.99	0.40
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.85	0.40
1:A:588:LEU:O	1:A:606:LEU:HA	2.21	0.40
1:A:650:GLN:O	1:A:651:LYS:C	2.60	0.40
1:A:666:ILE:HG12	2:B:1030:LEU:HD22	2.02	0.40
2:B:1125:ASP:OD1	2:B:1125:ASP:O	2.39	0.40
2:B:1176:ASN:O	2:B:1178:ASN:N	2.55	0.40
2:B:324:ILE:HD13	2:B:329:THR:HG22	2.03	0.40
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.04	0.40
2:B:707:PRO:O	2:B:708:GLU:O	2.40	0.40
2:B:742:GLU:O	2:B:743:ILE:C	2.59	0.40
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.87	0.40
2:B:889:THR:HG22	2:B:890:TYR:N	2.37	0.40
4:D:53:SER:CB	4:D:152:SER:HB2	2.51	0.40
4:D:53:SER:HB3	4:D:152:SER:CB	2.50	0.40
5:E:151:PRO:CB	5:E:200:ARG:HB3	2.51	0.40
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1733 (81%)	984 (70%)	283 (20%)	141 (10%)	0	4
2	B	1088/1224 (89%)	740 (68%)	220 (20%)	128 (12%)	0	3
3	C	264/318 (83%)	187 (71%)	52 (20%)	25 (10%)	0	4
4	D	173/221 (78%)	116 (67%)	37 (21%)	20 (12%)	0	3
5	E	212/215 (99%)	150 (71%)	41 (19%)	21 (10%)	0	4
6	F	82/155 (53%)	58 (71%)	14 (17%)	10 (12%)	0	2
7	G	169/171 (99%)	126 (75%)	30 (18%)	13 (8%)	1	6
8	H	129/146 (88%)	95 (74%)	17 (13%)	17 (13%)	0	1
9	I	117/122 (96%)	74 (63%)	28 (24%)	15 (13%)	0	2
10	J	63/70 (90%)	38 (60%)	14 (22%)	11 (18%)	0	0
11	K	112/120 (93%)	86 (77%)	17 (15%)	9 (8%)	1	6
12	L	44/70 (63%)	19 (43%)	13 (30%)	12 (27%)	0	0
13	M	3/8 (38%)	3 (100%)	0	0	100	100
All	All	3864/4573 (84%)	2676 (69%)	766 (20%)	422 (11%)	0	3

All (422) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	57	ARG
1	A	67	CYS
1	A	71	GLN
1	A	73	GLY
1	A	74	MET

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Mol	Chain	Res	Type
1	A	93	VAL
1	A	131	SER
1	A	253	ASN
1	A	257	ARG
1	A	283	GLY
1	A	286	HIS
1	A	302	THR
1	A	303	TYR
1	A	311	GLN
1	A	312	PRO
1	A	335	ARG
1	A	364	VAL
1	A	410	GLY
1	A	424	ILE
1	A	465	TYR
1	A	525	GLN
1	A	567	LYS
1	A	597	LEU
1	A	598	LEU
1	A	775	ILE
1	A	1013	ASP
1	A	1016	THR
1	A	1036	ARG
1	A	1115	SER
1	A	1165	GLU
1	A	1206	ASP
1	A	1231	ASP
1	A	1233	ASP
1	A	1255	GLU
1	A	1281	ARG
1	A	1438	THR
2	B	106	ASP
2	B	108	VAL
2	B	229	ALA
2	B	266	ALA
2	B	282	ILE
2	B	333	PHE
2	B	334	ILE
2	B	365	THR
2	B	367	LEU
2	B	401	PHE
2	B	470	LYS

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Mol	Chain	Res	Type
2	B	620	ARG
2	B	629	ASP
2	B	641	GLU
2	B	708	GLU
2	B	713	ALA
2	B	731	VAL
2	B	813	LYS
2	B	869	SER
2	B	879	ARG
2	B	881	ASN
2	B	884	ARG
2	B	907	GLY
2	B	976	ILE
2	B	1046	PRO
2	B	1097	HIS
2	B	1100	ASP
2	B	1131	GLY
2	B	1155	SER
2	B	1156	ASP
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1182	CYS
3	C	108	GLU
3	C	109	SER
3	C	161	LYS
3	C	237	SER
4	D	5	THR
4	D	18	VAL
4	D	47	LEU
4	D	131	GLU
4	D	174	PRO
4	D	202	ILE
5	E	73	PRO
5	E	74	ASP
5	E	87	SER
5	E	106	GLN
6	F	73	ALA
6	F	74	ILE
7	G	52	ASP
7	G	118	ASP
7	G	123	ALA

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Mol	Chain	Res	Type
7	G	139	ILE
7	G	154	VAL
8	H	17	PRO
8	H	60	ALA
8	H	108	SER
8	H	128	ASN
8	H	140	ALA
9	I	20	LYS
9	I	50	THR
9	I	51	ASN
9	I	56	ALA
9	I	106	CYS
9	I	107	SER
10	J	2	ILE
10	J	32	GLU
10	J	42	LYS
10	J	64	ASN
11	K	7	PHE
11	K	54	ARG
12	L	35	SER
12	L	39	SER
12	L	42	ARG
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	35	ILE
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	69	THR
1	A	76	GLU
1	A	84	ILE
1	A	130	ASP
1	A	318	SER
1	A	415	LEU
1	A	423	ASP
1	A	466	SER
1	A	517	ASN
1	A	534	LEU
1	A	591	PHE
1	A	628	GLY

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Mol	Chain	Res	Type
1	A	672	ASP
1	A	699	ALA
1	A	716	ASP
1	A	771	GLU
1	A	846	GLU
1	A	847	ASP
1	A	852	TYR
1	A	854	ASN
1	A	972	HIS
1	A	1002	GLY
1	A	1014	ALA
1	A	1015	VAL
1	A	1120	LEU
1	A	1123	GLY
1	A	1212	VAL
1	A	1221	LYS
1	A	1261	LYS
1	A	1266	THR
1	A	1314	SER
1	A	1341	ILE
1	A	1405	THR
1	A	1421	CYS
2	B	21	GLU
2	B	30	SER
2	B	55	VAL
2	B	58	THR
2	B	68	THR
2	B	115	GLN
2	B	176	SER
2	B	186	GLU
2	B	206	ASN
2	B	219	ALA
2	B	259	TYR
2	B	260	GLY
2	B	264	SER
2	B	267	ARG
2	B	295	GLY
2	B	466	TRP
2	B	467	GLY
2	B	517	THR
2	B	530	GLY
2	B	557	PHE

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Mol	Chain	Res	Type
2	B	559	SER
2	B	575	PRO
2	B	642	ASP
2	B	705	MET
2	B	709	ASP
2	B	734	HIS
2	B	792	MET
2	B	883	LEU
2	B	888	GLY
2	B	946	ASN
2	B	1006	ILE
2	B	1069	PHE
2	B	1075	GLY
2	B	1126	GLY
2	B	1176	ASN
2	B	1186	ASP
2	B	1223	ASP
3	C	5	GLY
3	C	18	VAL
3	C	107	SER
3	C	110	THR
3	C	133	ILE
3	C	149	LYS
3	C	156	THR
3	C	173	ALA
3	C	184	ASN
4	D	16	LYS
4	D	52	LEU
4	D	120	GLU
4	D	198	LEU
4	D	213	GLU
4	D	219	THR
5	E	30	ILE
5	E	45	LYS
5	E	88	VAL
5	E	120	ALA
5	E	121	MET
5	E	130	ALA
5	E	138	ALA
6	F	154	ASP
7	G	50	ASP
8	H	18	GLY

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Mol	Chain	Res	Type
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	90	ALA
9	I	11	ASN
9	I	57	GLY
10	J	6	ARG
10	J	14	VAL
10	J	28	ASP
11	K	14	GLU
11	K	15	GLY
11	K	43	GLY
11	K	44	ASN
11	K	49	GLU
11	K	80	GLY
12	L	53	HIS
12	L	55	ILE
1	A	45	GLN
1	A	154	SER
1	A	197	PRO
1	A	263	THR
1	A	336	ILE
1	A	382	PRO
1	A	418	SER
1	A	609	ASP
1	A	666	ILE
1	A	776	ALA
1	A	871	ASP
1	A	885	THR
1	A	986	ILE
1	A	1004	ASN
1	A	1122	PRO
1	A	1124	HIS
1	A	1164	PRO
1	A	1224	LEU
1	A	1365	TYR
1	A	1366	ARG
1	A	1386	ARG
2	B	46	GLN
2	B	56	ASP
2	B	182	SER
2	B	262	GLU

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Mol	Chain	Res	Type
2	B	308	TRP
2	B	332	ASP
2	B	389	ALA
2	B	414	ALA
2	B	450	ALA
2	B	460	ALA
2	B	474	SER
2	B	531	GLN
2	B	591	ARG
2	B	610	ASN
2	B	711	GLU
2	B	842	ASN
2	B	848	ARG
2	B	909	ASP
2	B	951	GLN
2	B	1022	THR
2	B	1108	ARG
2	B	1121	GLY
2	B	1158	PHE
2	B	1178	ASN
2	B	1181	GLU
3	C	90	ASP
3	C	132	PRO
4	D	13	ARG
4	D	15	LEU
4	D	21	GLU
4	D	53	SER
4	D	177	VAL
5	E	3	GLN
5	E	41	ASP
5	E	51	GLY
6	F	81	THR
7	G	35	GLU
7	G	165	GLU
7	G	167	TYR
8	H	83	GLN
8	H	109	LYS
9	I	34	TYR
9	I	47	GLU
10	J	24	LEU
10	J	33	GLY
10	J	44	TYR

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Mol	Chain	Res	Type
11	K	78	THR
12	L	43	THR
12	L	49	LYS
1	A	5	GLN
1	A	44	THR
1	A	65	LEU
1	A	109	HIS
1	A	317	LYS
1	A	322	VAL
1	A	568	PRO
1	A	1071	SER
1	A	1114	PRO
1	A	1139	GLU
1	A	1167	GLU
1	A	1280	GLU
1	A	1324	PRO
1	A	1335	ILE
1	A	1378	GLN
1	A	1403	GLU
1	A	1411	GLU
2	B	114	PRO
2	B	190	TYR
2	B	263	GLY
2	B	305	VAL
2	B	680	THR
2	B	727	LYS
2	B	738	PHE
2	B	785	TYR
2	B	1116	ARG
2	B	1136	ASP
2	B	1177	HIS
3	C	148	ARG
3	C	153	LEU
5	E	56	LYS
5	E	59	SER
5	E	203	GLU
6	F	150	GLU
7	G	51	TYR
7	G	67	SER
8	H	92	ASP
9	I	9	ASP
9	I	86	PHE

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Mol	Chain	Res	Type
12	L	44	ASP
12	L	56	LEU
1	A	70	CYS
1	A	196	GLU
1	A	233	TRP
1	A	254	GLU
1	A	310	GLY
1	A	600	PRO
1	A	650	GLN
1	A	738	LYS
1	A	752	LYS
1	A	859	SER
1	A	958	VAL
1	A	979	SER
1	A	1062	GLU
1	A	1204	ASP
1	A	1398	MET
2	B	24	PRO
2	B	28	GLU
2	B	45	SER
2	B	184	ALA
2	B	436	VAL
2	B	469	GLN
2	B	594	ALA
2	B	1065	GLN
2	B	1183	LYS
2	B	1188	LYS
3	C	34	ARG
3	C	129	ILE
3	C	169	LYS
3	C	227	THR
3	C	240	VAL
5	E	86	PRO
5	E	192	ARG
6	F	106	PRO
6	F	111	LEU
6	F	151	LEU
7	G	17	PHE
7	G	128	PRO
8	H	12	VAL
8	H	95	TYR
8	H	119	GLY

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Mol	Chain	Res	Type
9	I	33	SER
1	A	4	GLN
1	A	148	CYS
1	A	651	LYS
1	A	1011	GLN
2	B	131	ASP
2	B	304	ASP
2	B	551	PRO
3	C	60	ASP
3	C	142	VAL
4	D	135	GLY
5	E	40	GLU
8	H	77	ARG
9	I	8	ARG
2	B	290	GLY
2	B	1017	ILE
4	D	196	PRO
6	F	109	VAL
9	I	75	CYS
1	A	519	PRO
1	A	756	ILE
3	C	171	GLY
10	J	57	ILE
1	A	244	PRO
1	A	1242	VAL
2	B	992	ILE
2	B	1099	VAL
5	E	38	PRO
6	F	105	ALA
1	A	231	PRO
2	B	464	GLY
2	B	636	PRO
2	B	977	GLY
1	A	377	PRO
1	A	1075	PRO
2	B	315	LYS
4	D	30	GLY

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1520 (82%)	1134 (91%)	107 (9%)	10	35
2	B	960/1061 (90%)	870 (91%)	90 (9%)	8	30
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	20
4	D	140/200 (70%)	125 (89%)	15 (11%)	6	24
5	E	196/197 (100%)	185 (94%)	11 (6%)	21	51
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	18
7	G	152/152 (100%)	142 (93%)	10 (7%)	16	46
8	H	117/128 (91%)	107 (92%)	10 (8%)	10	35
9	I	113/116 (97%)	103 (91%)	10 (9%)	10	33
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	20
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	12
13	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3428/4011 (86%)	3115 (91%)	313 (9%)	9	32

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	62	ASP
1	A	77	CYS
1	A	83	HIS
1	A	93	VAL
1	A	110	CYS
1	A	200	ARG
1	A	213	HIS
1	A	215	SER
1	A	236	LEU
1	A	243	PRO
1	A	261	ASP
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	335	ARG
1	A	344	ARG
1	A	369	SER
1	A	375	THR
1	A	385	ILE
1	A	389	THR
1	A	403	LYS
1	A	408	ASP
1	A	412	ARG
1	A	425	GLN
1	A	434	ARG
1	A	440	ASP
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	450	LEU
1	A	451	HIS
1	A	462	VAL
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	493	GLN
1	A	524	VAL
1	A	542	GLU
1	A	552	TRP
1	A	560	ILE
1	A	562	THR
1	A	597	LEU
1	A	618	GLU
1	A	626	ASN
1	A	635	ARG
1	A	650	GLN
1	A	666	ILE
1	A	676	MET
1	A	685	GLU
1	A	711	ARG
1	A	727	ASP
1	A	731	ARG
1	A	738	LYS
1	A	739	ASP
1	A	740	LEU

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Mol	Chain	Res	Type
1	A	741	ASN
1	A	764	CYS
1	A	774	ARG
1	A	821	ARG
1	A	839	ARG
1	A	858	ASN
1	A	886	ILE
1	A	903	ASN
1	A	918	GLU
1	A	929	LEU
1	A	940	ARG
1	A	998	LEU
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1128	GLN
1	A	1146	VAL
1	A	1166	ASP
1	A	1194	ARG
1	A	1214	GLU
1	A	1236	LEU
1	A	1242	VAL
1	A	1258	HIS
1	A	1264	GLU
1	A	1267	MET
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1303	GLU
1	A	1332	PHE
1	A	1336	MET
1	A	1364	ASN
1	A	1371	LEU
1	A	1385	THR
1	A	1393	ASN
1	A	1400	CYS

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Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1426	GLU
1	A	1432	GLN
1	A	1441	PHE
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
2	B	20	ASP
2	B	30	SER
2	B	57	TYR
2	B	169	ARG
2	B	175	ARG
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	235	SER
2	B	261	ARG
2	B	267	ARG
2	B	268	THR
2	B	286	PHE
2	B	299	GLU
2	B	303	TYR
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	427	ASP
2	B	446	LEU
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	513	GLN
2	B	516	ASN
2	B	518	HIS
2	B	557	PHE
2	B	572	HIS
2	B	591	ARG
2	B	603	LEU

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Mol	Chain	Res	Type
2	B	614	SER
2	B	616	ILE
2	B	629	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	664	THR
2	B	678	GLU
2	B	679	TYR
2	B	737	THR
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	797	TYR
2	B	798	TYR
2	B	805	THR
2	B	811	TYR
2	B	830	TYR
2	B	831	SER
2	B	835	GLN
2	B	845	SER
2	B	859	TYR
2	B	878	GLN
2	B	887	HIS
2	B	895	ASP
2	B	899	ILE
2	B	909	ASP
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	970	THR
2	B	999	MET
2	B	1002	THR
2	B	1021	MET
2	B	1022	THR
2	B	1045	SER
2	B	1046	PRO
2	B	1047	PHE
2	B	1069	PHE
2	B	1071	VAL
2	B	1084	GLN
2	B	1092	TYR

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Mol	Chain	Res	Type
2	B	1096	ARG
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1183	LYS
2	B	1185	CYS
2	B	1189	ILE
2	B	1192	TYR
2	B	1198	TYR
2	B	1218	THR
2	B	1220	ARG
2	B	1224	PHE
3	C	35	ARG
3	C	60	ASP
3	C	62	PHE
3	C	67	LEU
3	C	77	ILE
3	C	91	HIS
3	C	102	GLN
3	C	104	PHE
3	C	111	THR
3	C	112	ASN
3	C	121	VAL
3	C	133	ILE
3	C	136	ASP
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	163	ILE
3	C	166	GLU
3	C	170	TRP
3	C	193	TYR
3	C	194	GLU
3	C	209	TYR
3	C	233	GLU
3	C	235	VAL
3	C	251	LEU
3	C	262	LEU
3	C	268	ASP
4	D	28	GLN
4	D	40	HIS

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Mol	Chain	Res	Type
4	D	47	LEU
4	D	50	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	156	ASP
4	D	174	PRO
4	D	187	THR
4	D	193	THR
4	D	207	LEU
4	D	221	TYR
5	E	9	ILE
5	E	17	ARG
5	E	60	PHE
5	E	74	ASP
5	E	78	LEU
5	E	104	ASN
5	E	114	ASN
5	E	132	ILE
5	E	144	ILE
5	E	146	HIS
5	E	175	LEU
6	F	90	ARG
6	F	99	LEU
6	F	103	MET
6	F	111	LEU
6	F	116	ASP
6	F	119	ARG
6	F	138	LEU
6	F	140	ASP
6	F	143	PHE
7	G	1	MET
7	G	13	LEU
7	G	21	ARG
7	G	51	TYR
7	G	74	TYR
7	G	80	LYS
7	G	88	ASP
7	G	128	PRO
7	G	163	ILE

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Mol	Chain	Res	Type
7	G	171	ILE
8	H	10	PHE
8	H	17	PRO
8	H	33	GLN
8	H	56	THR
8	H	63	LEU
8	H	95	TYR
8	H	98	TYR
8	H	102	TYR
8	H	110	ASP
8	H	130	ARG
9	I	4	PHE
9	I	7	CYS
9	I	8	ARG
9	I	12	ASN
9	I	14	LEU
9	I	34	TYR
9	I	51	ASN
9	I	87	GLN
9	I	100	PHE
9	I	106	CYS
10	J	7	CYS
10	J	13	VAL
10	J	16	ASP
10	J	43	ARG
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	1	MET
11	K	10	PHE
11	K	25	THR
11	K	32	VAL
11	K	47	ARG
11	K	51	LEU
11	K	61	TYR
11	K	76	GLN
11	K	78	THR
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	55	ILE
12	L	63	ARG

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Mol	Chain	Res	Type
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	83	HIS
1	A	119	ASN
1	A	225	ASN
1	A	297	GLN
1	A	339	ASN
1	A	358	ASN
1	A	394	ASN
1	A	435	HIS
1	A	503	GLN
1	A	611	GLN
1	A	698	GLN
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	881	GLN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1218	GLN
1	A	1258	HIS
1	A	1265	ASN
1	A	1270	ASN
1	A	1278	ASN
1	A	1364	ASN
1	A	1387	HIS

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Mol	Chain	Res	Type
1	A	1390	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	383	ASN
2	B	449	ASN
2	B	465	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	572	HIS
2	B	706	GLN
2	B	744	HIS
2	B	763	GLN
2	B	821	GLN
2	B	822	ASN
2	B	835	GLN
2	B	842	ASN
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	24	ASN
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	167	HIS
4	D	39	ASN
4	D	137	ASN
4	D	138	ASN
4	D	143	ASN
4	D	165	GLN
4	D	173	HIS
4	D	179	GLN

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Mol	Chain	Res	Type
5	E	8	ASN
5	E	32	GLN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	126	ASN
8	H	128	ASN
8	H	137	GLN
8	H	139	ASN
9	I	12	ASN
9	I	46	HIS
9	I	51	ASN
9	I	60	GLN
9	I	90	GLN
10	J	53	HIS
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/11 (81%)	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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	TRX	M	4	13	14,16,17	1.18	1 (7%)	15,22,24	2.63	4 (26%)
13	ILX	M	3	13	8,9,10	1.35	1 (12%)	9,11,13	2.14	2 (22%)
13	CSX	M	8	13	3,6,7	1.01	0	1,6,8	1.64	0
16	BRU	T	22	15,16	15,21,22	1.70	3 (20%)	17,30,33	4.08	4 (23%)
13	HYP	M	2	13	6,8,9	0.89	0	5,10,12	1.70	2 (40%)

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	TRX	M	4	13	-	0/4/6/8	0/2/2/2
13	ILX	M	3	13	-	0/11/12/14	-
13	CSX	M	8	13	-	0/1/5/7	-
16	BRU	T	22	15,16	-	0/4/21/22	0/2/2/2
13	HYP	M	2	13	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	22	BRU	C4-C5	5.05	1.44	1.38
16	T	22	BRU	C4-N3	3.27	1.38	1.33
13	M	4	TRX	CZ3-CH2	3.06	1.44	1.38
13	M	3	ILX	CB-CA	-3.03	1.51	1.54
16	T	22	BRU	C6-C5	-2.04	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	22	BRU	C4-N3-C2	14.47	127.36	115.14
13	M	4	TRX	CB-CG-CD1	-7.20	119.07	127.97
16	T	22	BRU	C5-C4-N3	-6.94	115.34	123.64
13	M	3	ILX	CB-CA-C	-5.50	105.52	112.94
13	M	4	TRX	CB-CG-CD2	4.90	133.87	126.25
13	M	4	TRX	CZ2-CE2-CD2	3.01	125.04	121.16
16	T	22	BRU	C5-C6-N1	2.87	123.68	119.97
13	M	4	TRX	CH2-CZ2-CE2	-2.85	116.28	119.29
16	T	22	BRU	BR-C5-C6	2.82	123.74	117.31
13	M	2	HYP	OD1-CG-CD	-2.32	105.27	110.35
13	M	2	HYP	O-C-CA	-2.17	119.09	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	3	ILX	OG1-CG1-CB	2.02	114.59	109.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	4	TRX	1	0
13	M	3	ILX	1	0
16	T	22	BRU	4	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1418/1733 (81%)	-0.26	6 (0%) 92 92	37, 86, 139, 189	0
2	B	1106/1224 (90%)	-0.15	9 (0%) 86 85	37, 96, 148, 181	0
3	C	266/318 (83%)	-0.33	0 100 100	49, 83, 117, 141	0
4	D	177/221 (80%)	-0.24	0 100 100	66, 107, 145, 149	0
5	E	214/215 (99%)	-0.01	6 (2%) 53 51	66, 127, 171, 180	0
6	F	84/155 (54%)	-0.45	0 100 100	42, 70, 99, 108	0
7	G	171/171 (100%)	-0.21	0 100 100	70, 90, 126, 136	0
8	H	133/146 (91%)	0.25	5 (3%) 40 39	91, 125, 152, 168	0
9	I	119/122 (97%)	0.03	7 (5%) 22 23	84, 125, 158, 175	0
10	J	65/70 (92%)	-0.35	0 100 100	44, 76, 113, 128	0
11	K	114/120 (95%)	-0.34	0 100 100	56, 83, 109, 133	0
12	L	46/70 (65%)	0.50	5 (10%) 5 6	76, 152, 166, 169	0
13	M	4/8 (50%)	-0.51	0 100 100	88, 90, 91, 97	0
14	N	13/14 (92%)	0.64	1 (7%) 13 15	151, 178, 218, 221	0
15	P	10/11 (90%)	-0.35	0 100 100	89, 111, 162, 172	0
16	T	24/26 (92%)	0.19	3 (12%) 3 4	80, 159, 224, 233	0
All	All	3964/4624 (85%)	-0.19	42 (1%) 80 79	37, 93, 152, 233	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	6.8
1	A	1176	LEU	6.7
2	B	471	LYS	5.9
16	T	4	DA	5.3
2	B	883	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	882	THR	3.9
14	N	13	DT	3.7
1	A	1455	PRO	3.7
9	I	119	THR	3.6
2	B	470	LYS	3.2
5	E	51	GLY	3.0
9	I	116	ASN	2.9
16	T	7	DT	2.9
2	B	709	ASP	2.8
12	L	25	ALA	2.8
9	I	118	ARG	2.8
1	A	69	THR	2.8
12	L	26	THR	2.8
5	E	118	PRO	2.7
9	I	120	GLN	2.7
1	A	161	LEU	2.7
2	B	467	GLY	2.7
16	T	5	DG	2.6
8	H	86	ASP	2.5
5	E	110	PHE	2.5
2	B	432	MET	2.5
9	I	52	ILE	2.5
2	B	250	PHE	2.4
5	E	50	MET	2.4
9	I	117	LYS	2.3
1	A	1175	SER	2.3
8	H	113	ALA	2.3
8	H	139	ASN	2.2
5	E	44	ALA	2.2
8	H	123	MET	2.2
5	E	39	LEU	2.1
2	B	715	ALA	2.1
8	H	132	LEU	2.1
12	L	28	LYS	2.1
9	I	101	PHE	2.1
1	A	117	GLU	2.0
12	L	37	LYS	2.0

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

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. The B-factors column lists the minimum,

median, 95th 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	B-factors(Å ²)	Q<0.9
16	BRU	T	22	20/21	0.82	0.18	69,75,79,82	0
13	TRX	M	4	15/16	0.95	0.26	88,91,93,93	0
13	CSX	M	8	7/8	0.97	0.15	92,94,95,97	0
13	HYP	M	2	8/9	0.97	0.12	84,85,86,87	0
13	ILX	M	3	10/11	0.98	0.17	85,86,88,91	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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
17	ZN	I	1122	1/1	0.94	0.09	144,144,144,144	0
17	ZN	L	1071	1/1	0.95	0.09	107,107,107,107	0
17	ZN	A	2456	1/1	0.97	0.08	78,78,78,78	0
17	ZN	C	1269	1/1	0.99	0.13	67,67,67,67	0
17	ZN	B	2225	1/1	0.99	0.18	65,65,65,65	0
18	MG	A	2458	1/1	0.99	0.16	43,43,43,43	0
17	ZN	A	2457	1/1	0.99	0.14	53,53,53,53	0
17	ZN	I	1121	1/1	0.99	0.16	96,96,96,96	0
17	ZN	J	1066	1/1	0.99	0.21	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.