



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:39 pm BST

PDB ID : 1R5U
Title : RNA POLYMERASE II TFIIB COMPLEX
Authors : Bushnell, D.A.; Westover, K.D.; Davis, R.; Kornberg, R.D.
Deposited on : 2003-10-13
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

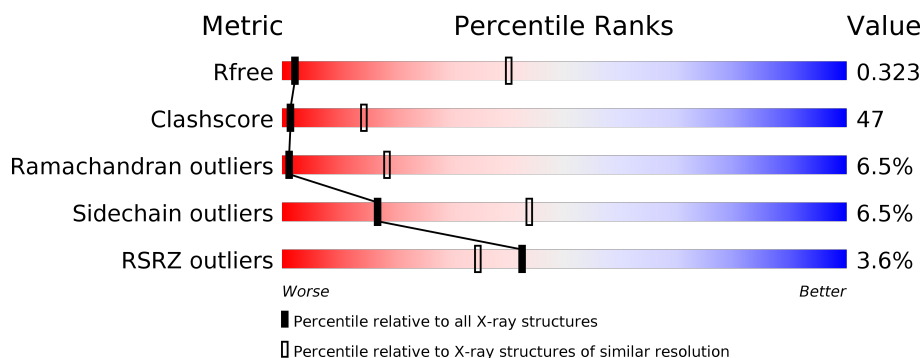
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	E	215	
5	F	155	
6	H	146	

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Mol	Chain	Length	Quality of chain
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	86	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ZN	I	203	-	-	-	X
12	ZN	I	204	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28300 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1380	Total	C	N	O	S	0	0	0
			10850	6847	1898	2044	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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 polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	118	Total	C	N	O	S	0	0	0
			967	594	178	185	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 11 is a protein called TRANSCRIPTION FACTOR II B (TFIIB).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	86	Total	C	N	O	0	0	0
			343	171	86	86			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0
12	M	1	Total 1	Zn 1	0	0

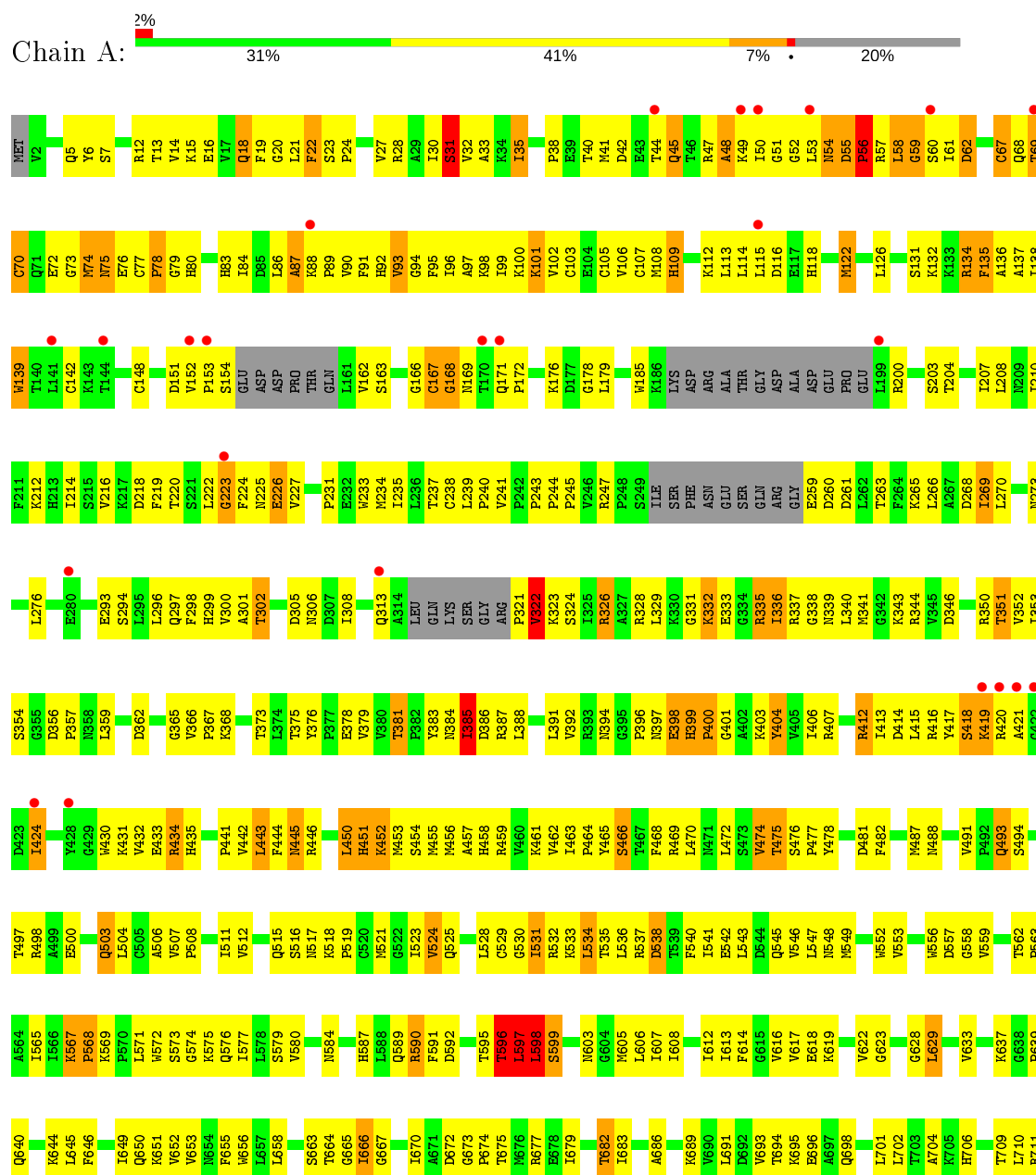
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

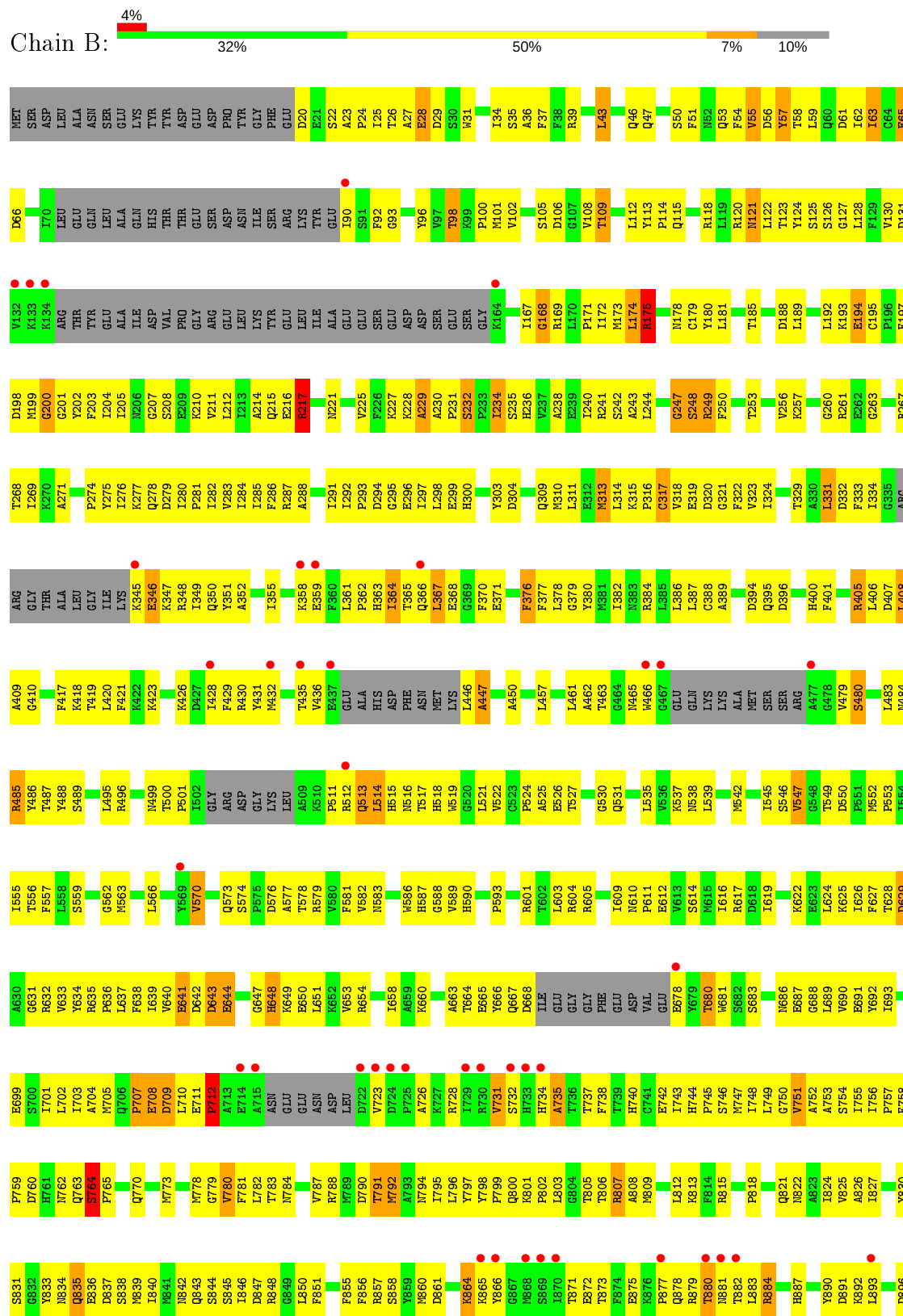
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

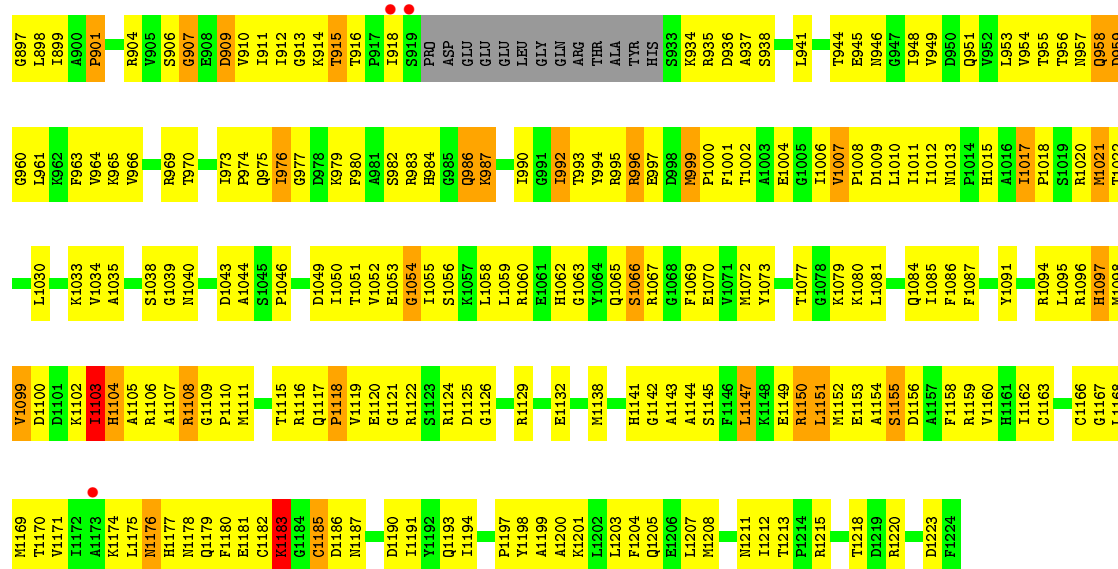
- Molecule 1: DNA-directed RNA polymerase II largest subunit



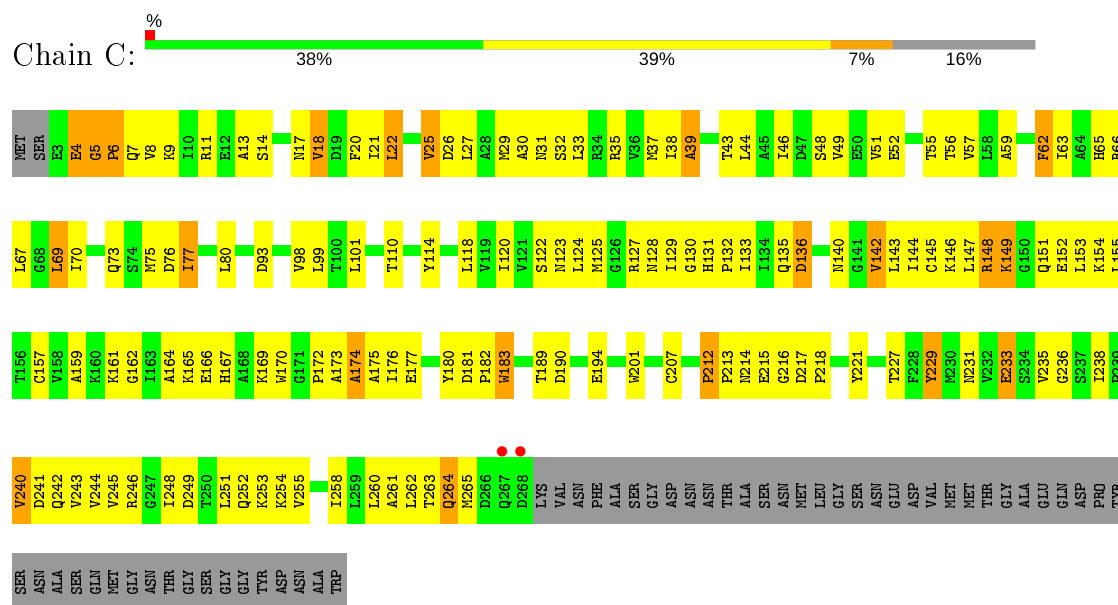


- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

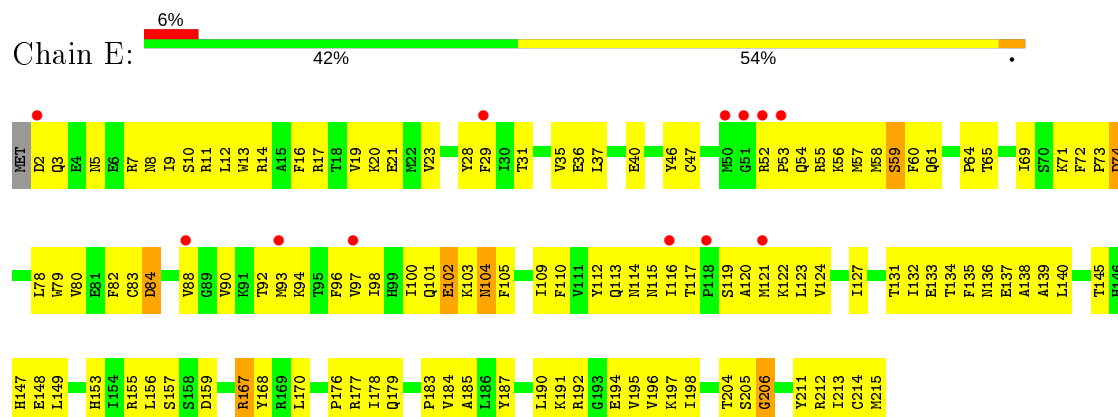




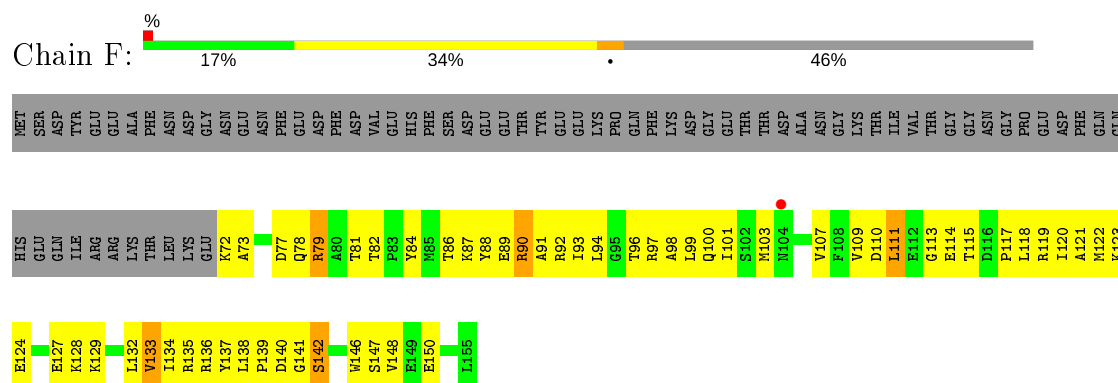
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



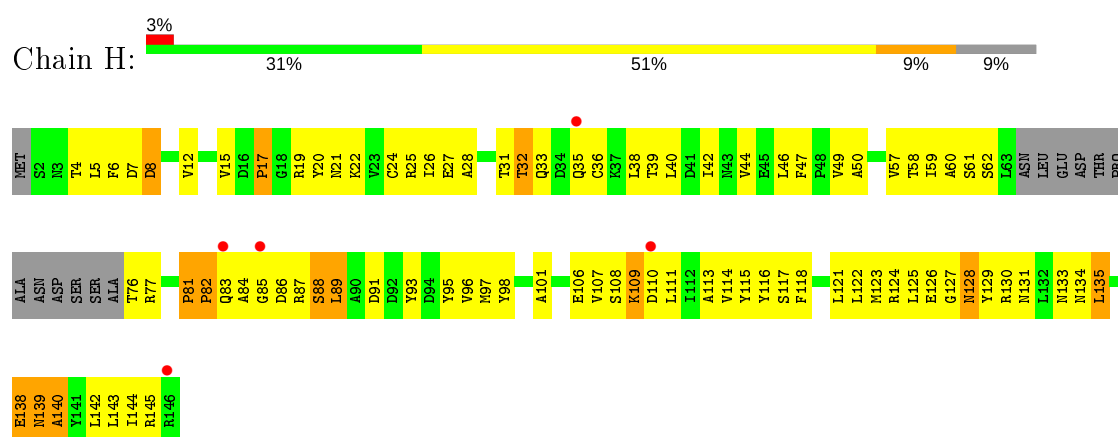
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



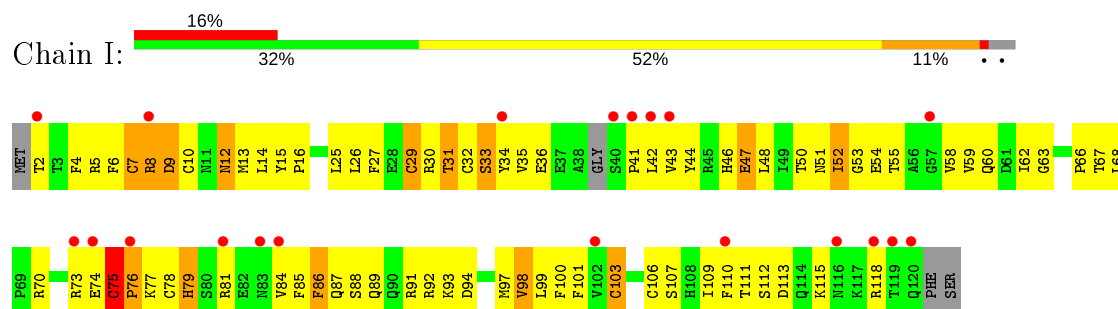
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



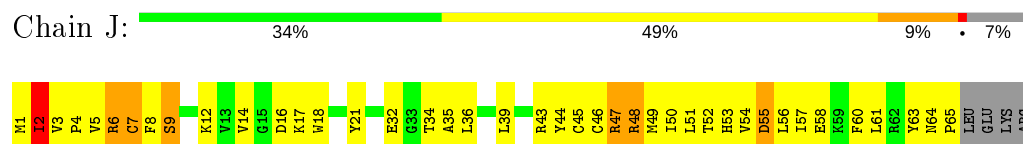
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

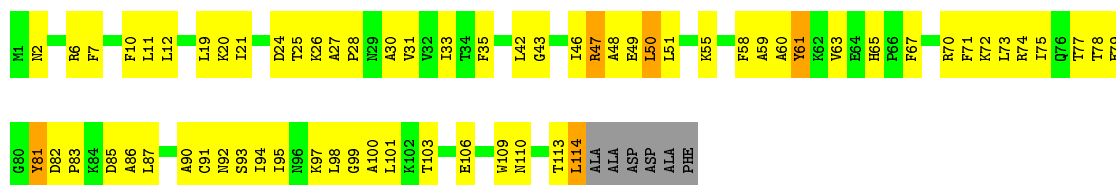


- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

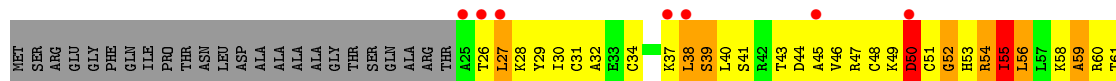


- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

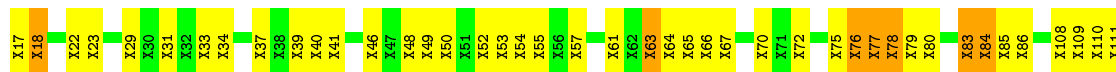




- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 11: TRANSCRIPTION FACTOR II B (TFIIB)



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	212.44Å 217.18Å 422.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 51.23 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-4.50) 99.2 (51.23-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.345 , 0.373 0.305 , 0.323	Depositor DCC
R_{free} test set	3333 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	1.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 177.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28300	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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

5.1 Standard geometry

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

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	0.48	3/11040 (0.0%)	0.73	15/14922 (0.1%)
2	B	0.49	2/8891 (0.0%)	0.72	3/11990 (0.0%)
3	C	0.48	0/2133	0.76	2/2891 (0.1%)
4	E	0.36	0/1788	0.65	0/2406
5	F	0.40	0/691	0.64	0/933
6	H	0.40	0/1086	0.73	0/1470
7	I	0.48	0/984	0.76	1/1323 (0.1%)
8	J	0.53	0/541	0.78	0/727
9	K	0.46	0/937	0.68	0/1265
10	L	0.49	0/366	0.78	0/485
All	All	0.47	5/28457 (0.0%)	0.73	21/38412 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
11	M	0	33
All	All	0	35

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1274	ARG	C-N	21.02	1.70	1.33
2	B	217	ARG	C-N	-14.21	1.01	1.34
1	A	1141	THR	C-N	10.82	1.58	1.34
2	B	1150	ARG	C-N	9.61	1.56	1.34
1	A	346	ASP	C-N	8.96	1.54	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	THR	O-C-N	-12.22	103.15	122.70
1	A	1274	ARG	O-C-N	-8.93	108.02	123.20
2	B	217	ARG	O-C-N	-8.89	108.48	122.70
1	A	1141	THR	CA-C-N	8.53	135.97	117.20
1	A	1141	THR	C-N-CA	8.49	142.94	121.70
1	A	1274	ARG	CA-C-N	7.13	130.46	116.20
1	A	1394	THR	O-C-N	-6.76	111.70	123.20
1	A	1392	SER	N-CA-C	6.32	128.06	111.00
3	C	39	ALA	N-CA-C	6.05	127.34	111.00
1	A	398	GLU	N-CA-C	-5.75	95.46	111.00
3	C	183	TRP	N-CA-C	-5.60	95.88	111.00
1	A	1394	THR	CA-C-N	5.46	127.13	116.20
1	A	1274	ARG	C-N-CA	5.42	133.69	122.30
2	B	647	GLY	N-CA-C	5.22	126.16	113.10
1	A	750	GLY	N-CA-C	-5.19	100.14	113.10
1	A	1403	GLU	N-CA-C	5.18	124.97	111.00
7	I	75	CYS	N-CA-C	-5.14	97.12	111.00
1	A	1394	THR	C-N-CA	5.08	132.98	122.30
1	A	452	LYS	N-CA-C	-5.06	97.33	111.00
1	A	466	SER	N-CA-C	5.01	124.54	111.00
2	B	712	PRO	N-CA-C	-5.01	99.07	112.10

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	217	ARG	Mainchain
2	B	405	ARG	Mainchain
11	M	108	UNK	Mainchain
11	M	109	UNK	Peptide
11	M	111	UNK	Mainchain
11	M	112	UNK	Mainchain,Peptide
11	M	116	UNK	Mainchain,Peptide
11	M	118	UNK	Peptide
11	M	18	UNK	Mainchain,Peptide
11	M	29	UNK	Mainchain
11	M	54	UNK	Mainchain
11	M	57	UNK	Mainchain,Peptide
11	M	61	UNK	Mainchain
11	M	63	UNK	Mainchain
11	M	66	UNK	Peptide

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Mol	Chain	Res	Type	Group
11	M	67	UNK	Mainchain,Peptide
11	M	70	UNK	Mainchain
11	M	72	UNK	Peptide
11	M	75	UNK	Mainchain
11	M	76	UNK	Mainchain
11	M	77	UNK	Mainchain,Peptide
11	M	78	UNK	Mainchain
11	M	83	UNK	Mainchain,Peptide
11	M	84	UNK	Mainchain,Peptide
11	M	85	UNK	Peptide
11	M	86	UNK	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10850	0	10952	1129	3
2	B	8721	0	8747	936	1
3	C	2095	0	2052	164	0
4	E	1752	0	1776	129	1
5	F	679	0	701	63	0
6	H	1068	0	1040	129	0
7	I	967	0	929	140	2
8	J	532	0	544	77	0
9	K	919	0	929	87	0
10	L	364	0	388	54	0
11	M	343	0	19	34	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	2	0
12	J	1	0	0	1	0
12	L	1	0	0	0	0
12	M	1	0	0	0	0
13	A	1	0	0	0	0
All	All	28300	0	28077	2624	4

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 47.

All (2624) 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:783:THR:HG21	1:A:815:PHE:CZ	1.39	1.57
1:A:783:THR:CG2	1:A:815:PHE:CZ	2.00	1.43
1:A:1274:ARG:C	1:A:1275:GLY:N	1.70	1.42
1:A:1147:THR:O	7:I:48:LEU:CD1	1.77	1.33
1:A:1151:GLU:CG	7:I:44:TYR:O	1.79	1.31
10:L:60:ARG:HG3	10:L:61:THR:H	1.05	1.19
1:A:822:GLU:HA	2:B:513:GLN:NE2	1.60	1.16
1:A:1153:TYR:CZ	7:I:42:LEU:HA	1.81	1.15
1:A:1149:ALA:HB1	7:I:46:HIS:H	1.09	1.14
2:B:345:LYS:HA	2:B:348:ARG:HE	1.11	1.14
1:A:783:THR:CG2	1:A:815:PHE:CE2	2.32	1.11
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.00	1.11
11:M:63:UNK:O	11:M:64:UNK:O	1.69	1.10
1:A:1151:GLU:HA	7:I:44:TYR:HB3	1.24	1.10
11:M:63:UNK:N	11:M:63:UNK:CA	2.15	1.10
1:A:1150:SER:O	7:I:44:TYR:CD2	2.05	1.09
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.18	1.09
2:B:512:ARG:HH21	2:B:535:LEU:HD11	1.17	1.09
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.65	1.09
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.33	1.09
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.27	1.09
1:A:1329:THR:HG22	1:A:1331:SER:H	1.16	1.08
1:A:810:PRO:HB3	2:B:519:TRP:HH2	1.12	1.08
1:A:775:ILE:HD12	1:A:815:PHE:HB3	1.36	1.07
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.36	1.07
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.33	1.07
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.38	1.06
1:A:855:THR:HG21	1:A:857:ARG:HE	1.12	1.06
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.34	1.05
2:B:708:GLU:HG3	2:B:709:ASP:H	1.17	1.05
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.18	1.05
7:I:111:THR:HG22	7:I:113:ASP:H	1.06	1.05
11:M:110:UNK:O	11:M:112:UNK:N	1.90	1.04
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.39	1.04
1:A:1151:GLU:HG2	7:I:44:TYR:O	0.86	1.04
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.22	1.02
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.41	1.02
11:M:41:UNK:CA	11:M:41:UNK:N	2.22	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.39	1.02
1:A:810:PRO:CB	2:B:519:TRP:HH2	1.72	1.02
9:K:113:THR:O	9:K:114:LEU:HB2	1.60	1.02
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	1.56	1.02
3:C:80:LEU:HD22	3:C:129:ILE:HD11	1.41	1.01
11:M:40:UNK:O	11:M:41:UNK:O	1.77	1.01
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.57	1.01
1:A:1150:SER:O	7:I:44:TYR:HD2	1.40	1.01
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.38	1.01
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.41	1.00
1:A:913:LEU:HD12	1:A:914:GLU:H	1.25	1.00
1:A:810:PRO:HB3	2:B:519:TRP:CH2	1.95	1.00
1:A:1147:THR:O	7:I:48:LEU:HD12	0.82	0.99
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.39	0.99
1:A:1149:ALA:HA	7:I:46:HIS:HB3	1.44	0.99
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.91	0.99
2:B:394:ASP:OD2	7:I:91:ARG:HG3	1.63	0.99
1:A:775:ILE:CD1	1:A:815:PHE:HB3	1.94	0.98
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.45	0.98
1:A:706:HIS:CD2	1:A:1135:ARG:CZ	2.46	0.97
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.47	0.96
2:B:174:LEU:O	2:B:175:ARG:HB2	1.64	0.96
1:A:706:HIS:CD2	1:A:1135:ARG:NH2	2.34	0.96
2:B:842:ASN:ND2	2:B:845:SER:H	1.62	0.96
1:A:567:LYS:HB3	6:H:96:VAL:H	1.26	0.96
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.43	0.96
3:C:167:HIS:CD2	3:C:169:LYS:H	1.83	0.96
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.47	0.96
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.46	0.95
11:M:22:UNK:O	11:M:23:UNK:O	1.82	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.81	0.95
1:A:783:THR:HG22	1:A:815:PHE:CZ	1.99	0.95
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.46	0.95
3:C:56:THR:HG22	3:C:57:VAL:H	1.28	0.95
11:M:40:UNK:C	11:M:41:UNK:CA	2.44	0.94
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.02	0.94
2:B:842:ASN:HD22	2:B:845:SER:H	1.17	0.93
11:M:39:UNK:C	11:M:41:UNK:N	2.08	0.93
1:A:1116:LEU:HD12	1:A:1329:THR:OG1	1.67	0.93
2:B:737:THR:HG21	7:I:66:PRO:O	1.68	0.93
2:B:955:THR:HG22	2:B:956:THR:H	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.48	0.93
1:A:1281:ARG:HD2	1:A:1309:ASP:OD2	1.68	0.93
1:A:783:THR:HG22	1:A:784:LEU:HG	1.48	0.93
2:B:1002:THR:HG22	2:B:1006:ILE:N	1.84	0.92
1:A:413:ILE:HG12	11:M:48:UNK:O	1.69	0.92
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.32	0.92
1:A:813:PHE:HE2	2:B:524:PRO:HG3	1.32	0.92
4:E:5:ASN:HD21	4:E:52:ARG:HG2	1.35	0.92
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.51	0.92
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.69	0.91
1:A:412:ARG:O	11:M:50:UNK:CA	2.13	0.91
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.35	0.91
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.50	0.91
1:A:1149:ALA:HB2	7:I:47:GLU:H	1.35	0.91
1:A:783:THR:CG2	1:A:815:PHE:HZ	1.61	0.91
10:L:60:ARG:HG3	10:L:61:THR:N	1.85	0.91
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.53	0.90
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.53	0.90
1:A:549:MET:SD	1:A:577:ILE:HD12	2.12	0.90
3:C:73:GLN:HE21	3:C:75:MET:H	1.14	0.90
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.54	0.90
1:A:1152:ILE:O	7:I:43:VAL:HG11	1.70	0.90
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	1.87	0.90
1:A:381:THR:HG22	1:A:383:TYR:H	1.35	0.90
1:A:61:ILE:HG22	1:A:62:ASP:H	1.37	0.90
2:B:955:THR:HG22	2:B:956:THR:N	1.85	0.90
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.53	0.90
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.87	0.89
7:I:111:THR:HG22	7:I:113:ASP:N	1.86	0.89
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	0.93	0.89
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.55	0.89
1:A:822:GLU:HA	2:B:513:GLN:HE22	1.30	0.89
3:C:167:HIS:HD2	3:C:169:LYS:H	0.90	0.89
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.08	0.89
1:A:1147:THR:C	7:I:48:LEU:HD12	1.91	0.89
2:B:956:THR:HA	2:B:961:LEU:O	1.71	0.89
1:A:816:HIS:CE1	2:B:764:SER:HB2	2.08	0.89
11:M:33:UNK:O	11:M:34:UNK:C	2.20	0.89
1:A:962:ARG:HA	1:A:965:GLN:HE21	1.38	0.89
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.54	0.89
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:CG2	2:B:956:THR:H	1.87	0.88
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.85	0.88
2:B:1110:PRO:HD3	11:M:39:UNK:O	1.72	0.87
2:B:345:LYS:CA	2:B:348:ARG:HE	1.87	0.87
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.40	0.87
11:M:63:UNK:O	11:M:64:UNK:C	2.23	0.87
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.72	0.87
2:B:744:HIS:HD2	2:B:746:SER:H	1.23	0.87
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.56	0.87
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.03	0.86
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.01	0.86
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.56	0.86
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.04	0.86
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.38	0.86
2:B:228:LYS:HD3	2:B:234:ILE:HD13	1.57	0.86
1:A:666:ILE:CD1	2:B:1030:LEU:HD13	2.04	0.86
2:B:512:ARG:HH21	2:B:535:LEU:CD1	1.88	0.86
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.56	0.86
1:A:605:MET:HE3	1:A:614:PHE:O	1.75	0.85
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.56	0.85
2:B:247:GLY:CA	2:B:418:LYS:HZ3	1.89	0.85
1:A:1039:LYS:O	1:A:1043:ASP:HB2	1.75	0.85
1:A:1149:ALA:HB1	7:I:46:HIS:N	1.91	0.85
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	1.91	0.84
2:B:1106:ARG:HH21	2:B:1109:GLY:H	1.23	0.84
5:F:147:SER:OG	5:F:150:GLU:HG3	1.78	0.84
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.57	0.84
4:E:2:ASP:O	4:E:3:GLN:HG2	1.78	0.84
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.08	0.84
1:A:417:TYR:O	1:A:418:SER:HB2	1.75	0.84
2:B:801:LYS:O	8:J:52:THR:HG23	1.75	0.84
2:B:1002:THR:CG2	2:B:1006:ILE:H	1.91	0.84
4:E:177:ARG:HD3	4:E:215:MET:SD	2.18	0.84
1:A:535:THR:HG21	1:A:617:VAL:H	1.43	0.84
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.11	0.84
11:M:110:UNK:C	11:M:112:UNK:N	2.36	0.84
6:H:125:LEU:HG	6:H:130:ARG:NH1	1.92	0.83
1:A:1153:TYR:CE2	7:I:42:LEU:HA	2.12	0.83
2:B:108:VAL:HG12	2:B:109:THR:H	1.42	0.83
9:K:12:LEU:HD12	9:K:12:LEU:H	1.42	0.83
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.59	0.83
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.61	0.83
8:J:46:CYS:HG	12:J:101:ZN:ZN	0.87	0.83
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.59	0.83
1:A:337:ARG:NH1	1:A:839:ARG:HH12	1.77	0.83
2:B:542:MET:HG3	2:B:747:MET:HE3	1.58	0.83
1:A:709:THR:HG21	7:I:93:LYS:O	1.77	0.82
2:B:912:ILE:O	2:B:938:SER:HB2	1.76	0.82
2:B:345:LYS:HA	2:B:348:ARG:NE	1.91	0.82
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.61	0.82
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.15	0.82
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.61	0.82
1:A:413:ILE:HA	11:M:49:UNK:C	1.90	0.82
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.41	0.82
6:H:93:TYR:HB3	6:H:144:ILE:O	1.80	0.82
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.44	0.82
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.62	0.82
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.61	0.82
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.62	0.82
3:C:11:ARG:NH2	3:C:229:TYR:HD2	1.77	0.81
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.62	0.81
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.60	0.81
1:A:885:THR:HG23	1:A:893:PHE:HE1	1.44	0.81
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.16	0.81
1:A:775:ILE:HD12	1:A:815:PHE:CB	2.10	0.81
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.63	0.81
1:A:1153:TYR:OH	7:I:42:LEU:HD13	1.79	0.81
1:A:413:ILE:HA	11:M:49:UNK:CA	2.10	0.81
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.60	0.81
2:B:1106:ARG:NH2	2:B:1109:GLY:H	1.79	0.81
2:B:1106:ARG:HE	2:B:1109:GLY:N	1.79	0.80
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.12	0.80
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.96	0.80
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.62	0.80
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.43	0.80
2:B:244:LEU:O	2:B:249:ARG:HG2	1.81	0.80
2:B:542:MET:HE3	2:B:747:MET:HG3	1.63	0.80
1:A:472:LEU:O	1:A:475:THR:HB	1.81	0.80
1:A:1153:TYR:HA	7:I:43:VAL:HG21	1.63	0.80
2:B:1106:ARG:HH21	2:B:1109:GLY:N	1.78	0.80
1:A:855:THR:HG21	1:A:857:ARG:NE	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.11	0.80
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.62	0.80
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.63	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.11	0.80
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.63	0.80
6:H:5:LEU:HD11	6:H:135:LEU:HG	1.63	0.79
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.17	0.79
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.64	0.79
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.28	0.79
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.12	0.79
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.63	0.79
7:I:50:THR:CG2	7:I:52:ILE:HG23	2.11	0.79
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.12	0.79
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.12	0.79
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.63	0.79
2:B:842:ASN:ND2	2:B:845:SER:N	2.31	0.79
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.64	0.79
1:A:1152:ILE:O	7:I:43:VAL:CG1	2.31	0.79
1:A:1151:GLU:HA	7:I:44:TYR:CB	2.10	0.79
2:B:487:THR:HG22	2:B:489:SER:H	1.48	0.79
3:C:56:THR:HG22	3:C:57:VAL:N	1.97	0.79
1:A:298:PHE:O	1:A:302:THR:HB	1.83	0.79
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.64	0.79
2:B:121:ASN:HD22	2:B:121:ASN:N	1.79	0.79
2:B:855:PHE:HZ	2:B:857:ARG:NH1	1.81	0.79
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.11	0.78
1:A:58:LEU:HD22	1:A:80:HIS:O	1.83	0.78
1:A:825:ILE:HD11	2:B:512:ARG:O	1.83	0.78
1:A:313:GLN:HB2	1:A:322:VAL:CG2	2.14	0.78
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.48	0.78
1:A:32:VAL:HG21	1:A:68:GLN:NE2	1.97	0.78
1:A:913:LEU:HD12	1:A:914:GLU:N	1.99	0.78
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.14	0.78
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.64	0.78
11:M:63:UNK:C	11:M:63:UNK:N	2.46	0.78
1:A:353:ILE:HD13	1:A:487:MET:CE	2.14	0.78
1:A:666:ILE:HD13	2:B:1030:LEU:HD22	1.65	0.78
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.49	0.78
2:B:583:ASN:HD21	2:B:628:THR:HB	1.49	0.78
6:H:40:LEU:HD23	6:H:42:ILE:HD11	1.65	0.78
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLU:CA	2:B:513:GLN:NE2	2.46	0.78
1:A:810:PRO:CB	2:B:519:TRP:CH2	2.60	0.78
1:A:70:CYS:O	1:A:72:GLU:HG2	1.84	0.77
1:A:313:GLN:HB2	1:A:322:VAL:HG23	1.64	0.77
1:A:742:ASN:HA	1:A:745:GLN:HB2	1.63	0.77
1:A:825:ILE:HG23	2:B:512:ARG:HD3	1.66	0.77
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	1.84	0.77
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.13	0.77
1:A:901:LEU:H	1:A:926:GLN:NE2	1.82	0.77
1:A:1150:SER:C	7:I:44:TYR:HD2	1.88	0.77
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.47	0.77
2:B:1166:CYS:O	2:B:1168:LEU:N	2.18	0.77
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.49	0.77
1:A:1281:ARG:O	1:A:1282:VAL:HG23	1.83	0.77
2:B:707:PRO:HG2	2:B:708:GLU:H	1.49	0.77
8:J:12:LYS:O	8:J:14:VAL:HG23	1.85	0.77
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.66	0.77
1:A:399:HIS:O	1:A:401:GLY:N	2.17	0.77
1:A:813:PHE:CE2	2:B:524:PRO:HG3	2.20	0.77
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.19	0.77
2:B:1106:ARG:HE	2:B:1109:GLY:H	1.29	0.77
2:B:496:ARG:NH1	2:B:539:LEU:HB2	1.99	0.77
3:C:124:LEU:O	3:C:127:ARG:HG2	1.85	0.76
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.67	0.76
1:A:40:THR:HG22	1:A:41:MET:HG3	1.64	0.76
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.65	0.76
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.50	0.76
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.85	0.76
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.51	0.76
1:A:265:LYS:NZ	1:A:323:LYS:H	1.84	0.76
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.68	0.76
3:C:167:HIS:HD2	3:C:169:LYS:N	1.76	0.76
3:C:165:LYS:O	9:K:6:ARG:NH1	2.17	0.76
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.51	0.76
1:A:223:GLY:O	1:A:1415:SER:HA	1.86	0.76
2:B:423:LYS:HA	2:B:426:LYS:HE2	1.68	0.76
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.68	0.76
1:A:768:GLN:CG	1:A:816:HIS:HA	2.16	0.76
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.16	0.76
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.21	0.76
1:A:95:PHE:O	1:A:99:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:THR:HG23	1:A:815:PHE:CE2	2.20	0.75
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.21	0.75
2:B:708:GLU:HG3	2:B:709:ASP:N	1.98	0.75
2:B:882:THR:HG22	2:B:884:ARG:H	1.51	0.75
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.15	0.75
1:A:1149:ALA:CB	7:I:47:GLU:H	1.99	0.75
1:A:41:MET:HA	1:A:49:LYS:HA	1.68	0.75
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.51	0.75
1:A:31:SER:CB	1:A:83:HIS:HB2	2.15	0.75
2:B:232:SER:OG	2:B:234:ILE:HD12	1.84	0.75
2:B:996:ARG:NH2	3:C:174:ALA:O	2.19	0.75
4:E:69:ILE:HG23	4:E:73:PRO:HA	1.67	0.75
5:F:111:LEU:N	5:F:111:LEU:HD12	2.02	0.75
10:L:38:LEU:O	10:L:39:SER:HB3	1.85	0.75
4:E:61:GLN:HE21	4:E:105:PHE:HE2	1.34	0.75
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.69	0.75
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.86	0.75
2:B:118:ARG:HH22	2:B:194:GLU:CD	1.90	0.75
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.68	0.75
2:B:842:ASN:HD22	2:B:845:SER:N	1.83	0.75
1:A:341:MET:HE1	1:A:1401:SER:HB2	1.69	0.74
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.27	0.74
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.03	0.74
1:A:24:PRO:HB3	1:A:237:THR:HB	1.67	0.74
1:A:710:LEU:H	1:A:710:LEU:HD12	1.52	0.74
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.68	0.74
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.22	0.74
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.68	0.74
2:B:770:GLN:HG2	2:B:983:ARG:O	1.86	0.74
1:A:1436:ILE:HG22	1:A:1437:GLY:H	1.52	0.74
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.68	0.74
1:A:535:THR:CG2	1:A:616:VAL:HA	2.17	0.74
6:H:89:LEU:C	6:H:91:ASP:H	1.90	0.74
1:A:534:LEU:O	1:A:574:GLY:HA3	1.88	0.74
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.17	0.74
4:E:124:VAL:HA	4:E:132:ILE:HD12	1.70	0.74
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.02	0.74
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.23	0.74
1:A:853:ASP:OD1	1:A:855:THR:HB	1.88	0.74
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.69	0.74
2:B:711:GLU:N	2:B:712:PRO:HD3	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.17	0.74
1:A:818:MET:HA	2:B:514:LEU:HB3	1.70	0.74
1:A:857:ARG:HD3	1:A:861:GLY:O	1.88	0.74
7:I:103:CYS:HG	12:I:204:ZN:ZN	0.97	0.74
2:B:46:GLN:HG3	2:B:47:GLN:N	2.03	0.74
1:A:1399:ARG:HB2	1:A:1408:ILE:HG21	1.70	0.74
2:B:1106:ARG:NE	2:B:1109:GLY:H	1.85	0.74
7:I:74:GLU:HB3	7:I:79:HIS:HA	1.70	0.73
1:A:75:ASN:O	1:A:76:GLU:HB3	1.88	0.73
9:K:65:HIS:HD2	9:K:67:PHE:H	1.35	0.73
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.71	0.73
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.69	0.73
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.70	0.73
2:B:542:MET:HE1	2:B:743:ILE:HG21	1.69	0.73
6:H:5:LEU:HB3	6:H:133:ASN:O	1.88	0.73
1:A:321:PRO:O	1:A:322:VAL:HB	1.87	0.73
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.73
2:B:234:ILE:H	2:B:234:ILE:HD12	1.53	0.73
1:A:1258:HIS:ND1	1:A:1262:LYS:HE3	2.04	0.73
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.70	0.73
6:H:35:GLN:HB3	6:H:111:LEU:HD21	1.70	0.73
2:B:363:HIS:O	2:B:364:ILE:HB	1.88	0.73
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.68	0.73
9:K:65:HIS:CD2	9:K:67:PHE:H	2.06	0.73
2:B:708:GLU:O	2:B:710:LEU:N	2.22	0.73
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.23	0.73
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.88	0.73
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.71	0.73
1:A:567:LYS:HB3	6:H:96:VAL:N	2.02	0.73
1:A:500:GLU:OE2	2:B:1145:SER:HB2	1.88	0.73
1:A:1149:ALA:HB2	7:I:47:GLU:N	2.03	0.73
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.70	0.72
2:B:955:THR:CG2	2:B:956:THR:N	2.49	0.72
1:A:1151:GLU:CA	7:I:44:TYR:HB3	2.11	0.72
1:A:417:TYR:O	1:A:418:SER:CB	2.36	0.72
1:A:48:ALA:O	1:A:49:LYS:HG3	1.89	0.72
1:A:925:LEU:O	1:A:929:LEU:HD23	1.88	0.72
2:B:58:THR:O	2:B:62:ILE:HG13	1.89	0.72
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.71	0.72
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.52	0.72
2:B:745:PRO:O	2:B:748:ILE:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:61:GLN:NE2	4:E:105:PHE:HE2	1.87	0.72
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.71	0.72
2:B:570:VAL:HB	2:B:573:GLN:CB	2.18	0.72
1:A:575:LYS:HB3	1:A:612:ILE:HG23	1.71	0.72
2:B:313:MET:CE	2:B:386:LEU:HD22	2.19	0.72
1:A:598:LEU:HD22	6:H:25:ARG:NH1	2.05	0.72
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.30	0.72
1:A:340:LEU:HD21	2:B:1200:ALA:HB2	1.72	0.72
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.70	0.72
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.71	0.72
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.69	0.72
2:B:636:PRO:O	2:B:637:LEU:HG	1.90	0.72
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.72	0.72
2:B:737:THR:HG23	7:I:66:PRO:CB	2.20	0.72
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.23	0.72
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.90	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.72
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.04	0.72
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.70	0.71
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.71	0.71
1:A:1390:ASN:ND2	1:A:1399:ARG:HA	2.05	0.71
1:A:1397:LEU:O	1:A:1400:CYS:HB2	1.89	0.71
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.38	0.71
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.72	0.71
1:A:337:ARG:NH1	1:A:839:ARG:NH1	2.37	0.71
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.54	0.71
2:B:555:ILE:HD13	2:B:587:HIS:CE1	2.26	0.71
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.25	0.71
10:L:47:ARG:HG2	10:L:52:GLY:HA2	1.72	0.71
9:K:55:LYS:HD3	9:K:78:THR:CB	2.20	0.71
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.38	0.71
1:A:44:THR:O	1:A:45:GLN:HB2	1.91	0.71
1:A:900:ASP:OD2	1:A:903:ASN:HB2	1.90	0.71
2:B:65:GLU:HG3	2:B:66:ASP:H	1.56	0.71
11:M:40:UNK:O	11:M:41:UNK:CA	2.36	0.71
1:A:675:THR:CB	1:A:736:ASN:HD21	2.04	0.71
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.06	0.71
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.73	0.71
1:A:1153:TYR:OH	7:I:42:LEU:CD1	2.39	0.70
1:A:367:PRO:HB3	1:A:466:SER:HA	1.74	0.70
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:60:ARG:CG	10:L:61:THR:H	1.94	0.70
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.26	0.70
2:B:792:MET:HA	2:B:856:PHE:O	1.91	0.70
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.57	0.70
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.31	0.70
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.56	0.70
9:K:55:LYS:HD3	9:K:78:THR:HB	1.72	0.70
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.72	0.70
1:A:351:THR:HG21	2:B:1103:ILE:HG23	1.71	0.70
1:A:567:LYS:HE3	6:H:46:LEU:CD1	2.22	0.70
2:B:1066:SER:O	2:B:1067:ARG:HD3	1.90	0.70
1:A:418:SER:HA	11:M:46:UNK:O	1.91	0.70
2:B:637:LEU:CD1	2:B:693:ILE:HD12	2.20	0.70
4:E:56:LYS:HG3	4:E:84:ASP:HB2	1.73	0.70
2:B:130:VAL:HG12	2:B:131:ASP:N	2.07	0.70
1:A:343:LYS:HE3	2:B:1151:LEU:O	1.92	0.70
2:B:378:LEU:O	2:B:382:ILE:HG13	1.92	0.69
1:A:1153:TYR:HA	7:I:43:VAL:CG2	2.21	0.69
6:H:36:CYS:SG	6:H:130:ARG:NH2	2.65	0.69
1:A:775:ILE:CD1	1:A:815:PHE:CB	2.67	0.69
2:B:54:PHE:HA	2:B:58:THR:HB	1.74	0.69
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.74	0.69
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.74	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.69
1:A:858:ASN:HD22	1:A:858:ASN:C	1.95	0.69
2:B:463:THR:CG2	2:B:465:ASN:HD22	2.05	0.69
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.08	0.69
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.93	0.69
1:A:763:ALA:O	1:A:803:SER:HB3	1.92	0.69
2:B:108:VAL:HG12	2:B:109:THR:N	2.06	0.69
2:B:955:THR:HG23	10:L:54:ARG:O	1.91	0.69
4:E:168:TYR:HB3	4:E:170:LEU:HD21	1.72	0.69
6:H:49:VAL:HG12	6:H:50:ALA:N	2.07	0.69
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.74	0.69
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.74	0.69
1:A:72:GLU:OE2	2:B:1175:LEU:HD12	1.92	0.69
2:B:542:MET:CE	2:B:747:MET:HG3	2.22	0.69
1:A:391:LEU:HD22	1:A:400:PRO:O	1.93	0.69
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.74	0.69
2:B:314:LEU:O	2:B:317:CYS:HB2	1.92	0.69
1:A:225:ASN:O	1:A:227:VAL:N	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:75:CYS:SG	7:I:103:CYS:SG	2.91	0.69
4:E:83:CYS:SG	4:E:88:VAL:HG22	2.32	0.68
1:A:584:ASN:O	1:A:637:LYS:HE3	1.92	0.68
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.74	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
3:C:254:LYS:HB3	9:K:42:LEU:HD11	1.75	0.68
1:A:1152:ILE:O	7:I:43:VAL:CB	2.41	0.68
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.21	0.68
1:A:535:THR:HG21	1:A:616:VAL:HA	1.75	0.68
1:A:599:SER:HB2	1:A:603:ASN:H	1.58	0.68
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.08	0.68
2:B:884:ARG:O	2:B:936:ASP:HB3	1.93	0.68
2:B:882:THR:HG21	2:B:935:ARG:HA	1.75	0.68
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.76	0.68
2:B:46:GLN:HG3	2:B:47:GLN:H	1.58	0.68
1:A:535:THR:HG21	1:A:617:VAL:N	2.08	0.68
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.75	0.68
2:B:976:ILE:O	2:B:990:ILE:HB	1.94	0.68
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.23	0.68
8:J:1:MET:H2	8:J:56:LEU:HB2	1.59	0.68
1:A:994:GLN:HE21	1:A:1019:CYS:HB3	1.59	0.68
2:B:842:ASN:ND2	2:B:844:SER:HB2	2.09	0.68
5:F:81:THR:HG21	5:F:136:ARG:CD	2.20	0.68
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.76	0.68
2:B:954:VAL:O	10:L:55:ILE:O	2.11	0.68
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.59	0.68
2:B:711:GLU:N	2:B:712:PRO:CD	2.57	0.67
4:E:127:ILE:O	4:E:127:ILE:HG13	1.93	0.67
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.07	0.67
2:B:864:LYS:HB3	2:B:872:GLU:H	1.59	0.67
7:I:53:GLY:O	7:I:89:GLN:HB2	1.94	0.67
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.29	0.67
6:H:7:ASP:O	6:H:8:ASP:HB2	1.92	0.67
1:A:351:THR:CG2	2:B:1103:ILE:HG23	2.24	0.67
2:B:280:ILE:HG22	2:B:285:ILE:HG13	1.76	0.67
2:B:986:GLN:HE22	2:B:1020:ARG:CZ	2.08	0.67
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.77	0.67
3:C:8:VAL:HG12	3:C:9:LYS:N	2.09	0.67
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.76	0.67
2:B:1039:GLY:HA2	8:J:51:LEU:HD21	1.77	0.67
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:HB2	1:A:565:ILE:O	1.94	0.67
1:A:814:PHE:O	1:A:817:ALA:HB3	1.95	0.67
1:A:525:GLN:CB	2:B:835:GLN:HG2	2.25	0.67
1:A:694:THR:O	1:A:698:GLN:HG3	1.94	0.67
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.07	0.67
2:B:514:LEU:HD12	2:B:515:HIS:N	2.09	0.67
2:B:22:SER:O	2:B:654:ARG:HD2	1.94	0.67
3:C:93:ASP:O	3:C:127:ARG:NH2	2.27	0.67
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.77	0.67
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.10	0.67
3:C:8:VAL:HG12	3:C:9:LYS:H	1.60	0.67
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.76	0.67
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.60	0.67
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.76	0.67
1:A:914:GLU:HB2	1:A:979:SER:O	1.95	0.67
2:B:957:ASN:O	2:B:959:ASP:N	2.29	0.67
3:C:80:LEU:HD22	3:C:129:ILE:CD1	2.21	0.67
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.28	0.66
1:A:590:ARG:HB3	1:A:605:MET:N	2.10	0.66
5:F:109:VAL:HG12	5:F:110:ASP:N	2.10	0.66
1:A:305:ASP:HB3	1:A:308:ILE:HD11	1.77	0.66
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.76	0.66
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.76	0.66
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.30	0.66
2:B:709:ASP:O	2:B:710:LEU:HD23	1.94	0.66
4:E:93:MET:HE2	4:E:120:ALA:HB1	1.76	0.66
9:K:47:ARG:NH1	9:K:47:ARG:HB3	2.09	0.66
1:A:751:SER:O	1:A:752:LYS:HG2	1.96	0.66
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.76	0.66
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.43	0.66
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.29	0.66
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.30	0.66
3:C:56:THR:HG21	3:C:145:CYS:SG	2.35	0.66
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.28	0.66
2:B:751:VAL:O	2:B:754:SER:HB2	1.95	0.66
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.77	0.66
10:L:45:ALA:O	10:L:46:VAL:HG23	1.95	0.66
2:B:649:LYS:HE2	2:B:738:PHE:O	1.96	0.66
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.77	0.66
1:A:1333:ILE:O	1:A:1336:MET:HB3	1.96	0.66
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.77	0.66
3:C:260:LEU:O	3:C:264:GLN:HG3	1.95	0.66
3:C:98:VAL:C	3:C:99:LEU:HD23	2.16	0.66
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.31	0.66
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.78	0.66
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.30	0.66
2:B:711:GLU:H	2:B:712:PRO:HD3	1.60	0.66
3:C:5:GLY:O	3:C:7:GLN:HG3	1.95	0.66
7:I:32:CYS:SG	7:I:33:SER:N	2.69	0.66
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.06	0.65
2:B:363:HIS:O	2:B:364:ILE:CB	2.44	0.65
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.77	0.65
4:E:176:PRO:O	4:E:212:ARG:HA	1.95	0.65
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.31	0.65
7:I:111:THR:HG21	7:I:113:ASP:HB2	1.78	0.65
1:A:1115:SER:HA	1:A:1308:THR:HG22	1.77	0.65
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.77	0.65
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.35	0.65
1:A:810:PRO:HG2	2:B:705:MET:SD	2.36	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.28	0.65
5:F:96:THR:O	5:F:100:GLN:HG3	1.97	0.65
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.62	0.65
1:A:741:ASN:HD22	1:A:741:ASN:C	1.99	0.65
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.79	0.65
4:E:124:VAL:HG22	4:E:132:ILE:HG21	1.79	0.65
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.31	0.65
1:A:1153:TYR:CE2	7:I:42:LEU:CA	2.69	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.65
1:A:715:GLU:O	1:A:719:VAL:HG23	1.96	0.65
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.27	0.65
1:A:329:LEU:HD23	1:A:335:ARG:HG3	1.78	0.65
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.31	0.65
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.78	0.65
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.78	0.65
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.62	0.65
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.97	0.65
2:B:128:LEU:HB3	2:B:167:ILE:O	1.95	0.65
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.65
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
2:B:1116:ARG:HD2	2:B:1198:TYR:CG	2.32	0.64
6:H:107:VAL:HG21	6:H:126:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:TYR:O	1:A:1037:LEU:N	2.30	0.64
2:B:349:ILE:O	2:B:352:ALA:HB3	1.96	0.64
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.27	0.64
2:B:805:THR:HG21	2:B:815:ARG:HE	1.62	0.64
10:L:51:CYS:O	10:L:53:HIS:N	2.28	0.64
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.27	0.64
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.12	0.64
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.31	0.64
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.26	0.64
1:A:994:GLN:HE22	1:A:1023:ARG:NE	1.95	0.64
1:A:306:ASN:HD21	1:A:324:SER:H	1.43	0.64
2:B:1051:THR:CG2	2:B:1053:GLU:H	1.93	0.64
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.28	0.64
2:B:1201:LYS:O	2:B:1205:GLN:HG3	1.98	0.64
1:A:381:THR:HG22	1:A:383:TYR:N	2.09	0.64
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.79	0.64
2:B:604:ARG:HG2	2:B:604:ARG:O	1.98	0.64
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.79	0.64
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.64
1:A:579:SER:OG	1:A:612:ILE:HG22	1.97	0.64
1:A:901:LEU:HA	1:A:907:THR:HG23	1.80	0.64
2:B:1170:THR:O	2:B:1170:THR:HG22	1.97	0.64
2:B:247:GLY:H	2:B:418:LYS:NZ	1.96	0.64
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.32	0.64
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.32	0.64
5:F:111:LEU:H	5:F:111:LEU:HD12	1.61	0.64
6:H:49:VAL:HG12	6:H:50:ALA:H	1.62	0.64
11:M:31:UNK:CA	11:M:114:UNK:O	2.45	0.64
5:F:86:THR:OG1	5:F:89:GLU:HG3	1.98	0.64
6:H:12:VAL:HA	6:H:28:ALA:CB	2.28	0.64
10:L:40:LEU:HD13	10:L:44:ASP:CG	2.19	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.81	0.63
2:B:525:ALA:O	2:B:527:THR:HG22	1.99	0.63
11:M:52:UNK:C	11:M:53:UNK:O	2.46	0.63
1:A:475:THR:HG22	1:A:476:SER:N	2.12	0.63
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.80	0.63
1:A:73:GLY:O	1:A:75:ASN:N	2.32	0.63
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.63
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.79	0.63
2:B:25:ILE:HG22	2:B:29:ASP:HB2	1.79	0.63
2:B:708:GLU:CG	2:B:709:ASP:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:CYS:HB2	7:I:29:CYS:HB2	1.81	0.63
1:A:354:SER:HA	1:A:482:PHE:CD2	2.34	0.63
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.62	0.63
2:B:914:LYS:HB3	2:B:937:ALA:O	1.99	0.63
4:E:96:PHE:O	4:E:100:ILE:HG13	1.99	0.63
1:A:337:ARG:NE	1:A:839:ARG:HH22	1.97	0.63
1:A:1150:SER:OG	7:I:44:TYR:CE2	2.51	0.63
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.79	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HG3	2.33	0.63
1:A:33:ALA:O	1:A:83:HIS:HB3	1.99	0.63
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.80	0.63
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.29	0.63
10:L:48:CYS:SG	10:L:49:LYS:N	2.70	0.63
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.80	0.63
2:B:1034:VAL:HG23	2:B:1059:LEU:HB2	1.80	0.63
7:I:29:CYS:HG	7:I:32:CYS:HG	1.44	0.63
1:A:328:ARG:O	1:A:335:ARG:HG2	1.99	0.63
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.80	0.63
3:C:22:LEU:HD22	3:C:25:VAL:CG2	2.25	0.63
6:H:31:THR:O	6:H:32:THR:CB	2.47	0.63
7:I:106:CYS:HG	12:I:204:ZN:ZN	1.12	0.63
8:J:9:SER:OG	8:J:48:ARG:NH2	2.30	0.63
10:L:55:ILE:HG13	10:L:56:LEU:H	1.63	0.63
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.79	0.63
5:F:97:ARG:O	5:F:101:ILE:HG13	1.99	0.63
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.14	0.63
2:B:1106:ARG:HD2	2:B:1126:GLY:O	1.99	0.63
2:B:221:ASN:OD1	2:B:242:SER:HA	1.98	0.63
2:B:247:GLY:N	2:B:418:LYS:NZ	2.47	0.63
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.34	0.63
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.29	0.63
1:A:108:MET:O	1:A:109:HIS:HB2	1.99	0.62
2:B:824:ILE:CG1	8:J:48:ARG:HH12	2.08	0.62
11:M:80:UNK:CA	11:M:83:UNK:O	2.47	0.62
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.34	0.62
1:A:418:SER:O	1:A:420:ARG:N	2.32	0.62
1:A:706:HIS:CG	1:A:1135:ARG:NH2	2.67	0.62
1:A:871:ASP:OD2	4:E:204:THR:HG23	1.99	0.62
2:B:512:ARG:NH2	2:B:535:LEU:HD11	2.02	0.62
2:B:405:ARG:HA	2:B:631:GLY:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:78:LEU:C	4:E:78:LEU:HD23	2.20	0.62
5:F:111:LEU:H	5:F:111:LEU:CD1	2.12	0.62
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.33	0.62
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	1.99	0.62
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.80	0.62
1:A:590:ARG:HB3	1:A:605:MET:H	1.64	0.62
1:A:915:SER:O	1:A:919:ILE:HG13	2.00	0.62
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.81	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.80	0.62
4:E:156:LEU:HD12	4:E:195:VAL:HG12	1.81	0.62
3:C:166:GLU:HA	9:K:6:ARG:HB3	1.82	0.62
1:A:381:THR:CG2	1:A:383:TYR:H	2.09	0.62
1:A:825:ILE:HG23	2:B:512:ARG:CD	2.28	0.62
4:E:178:ILE:HG23	4:E:214:CYS:HA	1.81	0.62
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.00	0.62
1:A:1054:LEU:O	1:A:1057:VAL:HG23	1.99	0.62
1:A:225:ASN:O	1:A:226:GLU:HG2	1.99	0.62
1:A:814:PHE:CE1	2:B:519:TRP:CA	2.83	0.62
2:B:549:THR:HB	2:B:628:THR:CG2	2.30	0.62
1:A:689:LYS:O	1:A:693:VAL:HG23	2.00	0.62
1:A:783:THR:HG22	1:A:815:PHE:CE2	2.21	0.62
2:B:542:MET:CG	2:B:747:MET:HE3	2.29	0.62
3:C:46:ILE:HA	3:C:159:ALA:HA	1.82	0.62
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.79	0.62
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.20	0.62
1:A:982:THR:HG22	1:A:984:LYS:H	1.64	0.62
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.34	0.61
2:B:1072:MET:HE3	2:B:1085:ILE:HD12	1.82	0.61
2:B:616:ILE:N	2:B:616:ILE:HD12	2.15	0.61
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.30	0.61
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.65	0.61
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.82	0.61
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.82	0.61
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.00	0.61
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.81	0.61
1:A:961:ARG:O	1:A:965:GLN:HG3	2.00	0.61
2:B:1116:ARG:NH1	2:B:1198:TYR:CD1	2.67	0.61
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.63	0.61
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.66	0.61
2:B:208:SER:OG	2:B:210:LYS:HD3	1.99	0.61
3:C:173:ALA:O	3:C:174:ALA:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:63:VAL:O	9:K:63:VAL:CG2	2.48	0.61
1:A:1212:VAL:O	1:A:1216:ILE:HG13	1.99	0.61
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.30	0.61
2:B:1187:ASN:OD1	2:B:1190:ASP:HB3	1.99	0.61
1:A:709:THR:HB	1:A:712:GLU:H	1.64	0.61
1:A:789:LYS:HG3	7:I:67:THR:HB	1.83	0.61
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.82	0.61
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.29	0.61
1:A:445:ASN:HB2	1:A:454:SER:O	2.00	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.01	0.61
2:B:446:LEU:O	2:B:447:ALA:CB	2.48	0.61
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.82	0.61
2:B:787:VAL:O	2:B:787:VAL:HG12	2.00	0.61
8:J:48:ARG:HE	8:J:49:MET:HE2	1.66	0.61
2:B:1169:MET:HE1	2:B:1201:LYS:O	2.01	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
3:C:49:VAL:HG21	3:C:67:LEU:HD12	1.83	0.61
1:A:148:CYS:O	1:A:168:GLY:HA2	2.00	0.61
2:B:686:ASN:C	2:B:688:GLY:H	2.04	0.61
4:E:93:MET:O	4:E:97:VAL:HG23	2.00	0.61
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.65	0.61
10:L:51:CYS:HB2	10:L:53:HIS:CD2	2.35	0.61
1:A:1192:LEU:HD22	1:A:1239:ARG:NH2	2.16	0.61
1:A:672:ASP:OD1	1:A:674:PRO:HD2	2.00	0.61
2:B:114:PRO:HB3	2:B:174:LEU:HD11	1.82	0.61
2:B:120:ARG:CG	2:B:955:THR:HG21	2.23	0.61
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.30	0.61
4:E:47:CYS:HA	4:E:53:PRO:HA	1.83	0.61
2:B:25:ILE:HG22	2:B:26:THR:H	1.65	0.61
5:F:101:ILE:HD12	5:F:121:ALA:HB2	1.82	0.61
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.83	0.61
10:L:26:THR:O	10:L:27:LEU:HB3	2.01	0.61
2:B:1102:LYS:O	2:B:1104:HIS:N	2.32	0.60
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.01	0.60
2:B:995:ARG:NH1	2:B:995:ARG:HB2	2.16	0.60
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.27	0.60
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.81	0.60
7:I:5:ARG:HD3	7:I:36:GLU:OE2	2.01	0.60
1:A:1152:ILE:O	7:I:43:VAL:HB	2.01	0.60
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.84	0.60
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:OD1	1:A:324:SER:HB3	2.01	0.60
2:B:1039:GLY:HA2	8:J:51:LEU:CD2	2.31	0.60
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.81	0.60
1:A:418:SER:O	1:A:419:LYS:C	2.39	0.60
1:A:663:SER:OG	1:A:664:THR:N	2.34	0.60
1:A:824:LEU:O	1:A:827:THR:HB	2.00	0.60
2:B:839:MET:HE3	2:B:1010:LEU:CD1	2.31	0.60
1:A:1158:PRO:HB3	1:A:1241:ARG:NH1	2.17	0.60
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.83	0.60
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.60
1:A:736:ASN:O	1:A:737:LEU:C	2.38	0.60
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.31	0.60
6:H:106:GLU:C	6:H:108:SER:H	2.02	0.60
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.04	0.60
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.31	0.60
1:A:704:ALA:HB2	1:A:710:LEU:CG	2.23	0.60
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.02	0.60
2:B:803:LEU:H	2:B:822:ASN:HD21	1.48	0.60
2:B:975:GLN:HG2	2:B:976:ILE:H	1.67	0.60
7:I:8:ARG:HG3	7:I:9:ASP:N	2.15	0.60
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.66	0.60
1:A:567:LYS:O	1:A:569:LYS:N	2.35	0.60
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.02	0.60
2:B:394:ASP:OD2	7:I:91:ARG:CG	2.45	0.60
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.01	0.60
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.32	0.60
1:A:219:PHE:O	1:A:222:LEU:N	2.33	0.60
1:A:567:LYS:CB	1:A:568:PRO:CD	2.67	0.60
1:A:549:MET:SD	1:A:577:ILE:CD1	2.87	0.60
2:B:121:ASN:ND2	2:B:121:ASN:N	2.50	0.60
1:A:231:PRO:HA	1:A:234:MET:HE2	1.83	0.60
2:B:1106:ARG:HH12	2:B:1118:PRO:HB3	1.67	0.60
2:B:429:PHE:HA	2:B:432:MET:HE2	1.84	0.60
8:J:1:MET:N	8:J:56:LEU:HB2	2.17	0.60
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.83	0.59
1:A:44:THR:O	1:A:44:THR:HG22	2.02	0.59
6:H:89:LEU:C	6:H:91:ASP:N	2.55	0.59
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.83	0.59
2:B:90:ILE:HD12	2:B:432:MET:SD	2.42	0.59
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.32	0.59
3:C:166:GLU:CG	9:K:10:PHE:HZ	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:139:ASN:O	6:H:140:ALA:HB2	2.02	0.59
9:K:90:ALA:O	9:K:94:ILE:HG13	2.01	0.59
1:A:166:GLY:O	1:A:167:CYS:HB3	2.02	0.59
1:A:322:VAL:O	1:A:323:LYS:HG3	2.01	0.59
4:E:78:LEU:HD23	4:E:79:TRP:N	2.16	0.59
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.84	0.59
6:H:84:ALA:HA	6:H:87:ARG:CG	2.32	0.59
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.68	0.59
1:A:469:ARG:NH2	2:B:976:ILE:HD13	2.18	0.59
7:I:15:TYR:O	7:I:27:PHE:HA	2.02	0.59
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.33	0.59
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.01	0.59
1:A:68:GLN:HE22	1:A:80:HIS:CB	2.15	0.59
2:B:913:GLY:HA2	2:B:938:SER:CB	2.32	0.59
4:E:29:PHE:HB2	4:E:65:THR:HG22	1.83	0.59
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.00	0.59
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.56	0.59
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.38	0.59
5:F:81:THR:HG22	5:F:82:THR:N	2.18	0.59
1:A:1390:ASN:HD22	1:A:1399:ARG:HA	1.67	0.59
1:A:742:ASN:CA	1:A:745:GLN:HB2	2.33	0.59
1:A:779:PHE:CZ	2:B:517:THR:HA	2.37	0.59
7:I:111:THR:CG2	7:I:113:ASP:HB2	2.33	0.59
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.83	0.59
6:H:109:LYS:NZ	6:H:109:LYS:HB2	2.18	0.59
1:A:1153:TYR:CZ	7:I:42:LEU:CA	2.72	0.59
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.03	0.59
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.33	0.59
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.37	0.59
1:A:783:THR:HG21	1:A:815:PHE:CE1	2.27	0.59
1:A:68:GLN:HE22	1:A:80:HIS:HB3	1.68	0.59
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.59
1:A:93:VAL:HG11	1:A:308:ILE:CD1	2.33	0.59
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.85	0.59
2:B:806:THR:HB	2:B:809:MET:HG3	1.85	0.59
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.43	0.59
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.59
2:B:642:ASP:O	2:B:644:GLU:N	2.36	0.59
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.18	0.59
6:H:81:PRO:CB	6:H:82:PRO:CD	2.81	0.59
1:A:1150:SER:OG	7:I:44:TYR:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.03	0.58
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.58
1:A:756:ILE:HG22	1:A:757:ASN:N	2.17	0.58
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.17	0.58
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.15	0.58
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.58
1:A:97:ALA:HA	1:A:100:LYS:HE3	1.84	0.58
1:A:225:ASN:HD22	1:A:227:VAL:HB	1.68	0.58
1:A:385:ILE:HG22	1:A:386:ASP:N	2.18	0.58
1:A:76:GLU:HG3	1:A:76:GLU:O	2.02	0.58
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.49	0.58
2:B:463:THR:HG22	2:B:465:ASN:HD22	1.66	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.85	0.58
3:C:148:ARG:HG3	8:J:61:LEU:O	2.03	0.58
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.33	0.58
5:F:127:GLU:O	5:F:129:LYS:HG3	2.03	0.58
7:I:16:PRO:HB3	7:I:27:PHE:CE2	2.38	0.58
1:A:31:SER:OG	1:A:83:HIS:HB2	2.02	0.58
7:I:85:PHE:CD1	7:I:99:LEU:HD22	2.37	0.58
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.33	0.58
2:B:955:THR:OG1	10:L:55:ILE:HA	2.04	0.58
1:A:840:ARG:HB3	1:A:1384:VAL:HG12	1.85	0.58
1:A:414:ASP:O	1:A:417:TYR:O	2.22	0.58
2:B:479:VAL:HG12	2:B:480:SER:N	2.17	0.58
4:E:5:ASN:ND2	4:E:52:ARG:HG2	2.12	0.58
6:H:123:MET:HE3	6:H:142:LEU:CD2	2.31	0.58
1:A:1115:SER:O	1:A:1329:THR:HG23	2.02	0.58
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.85	0.58
1:A:783:THR:HG22	1:A:815:PHE:HZ	1.44	0.58
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.35	0.58
2:B:46:GLN:O	2:B:408:LEU:HD23	2.03	0.58
4:E:156:LEU:HD12	4:E:195:VAL:CG1	2.33	0.58
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.04	0.58
1:A:151:ASP:HA	1:A:162:VAL:O	2.02	0.58
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.86	0.58
1:A:399:HIS:O	1:A:435:HIS:HD2	1.87	0.58
2:B:1171:VAL:CG1	2:B:1191:ILE:HD13	2.32	0.58
2:B:287:ARG:NH1	2:B:324:ILE:O	2.37	0.58
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.33	0.58
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.36	0.58
1:A:101:LYS:O	1:A:105:CYS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:GLU:O	1:A:1318:THR:HG23	2.04	0.58
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.86	0.58
2:B:519:TRP:C	2:B:519:TRP:CD1	2.76	0.58
2:B:666:TYR:C	2:B:668:ASP:H	2.06	0.58
2:B:806:THR:OG1	2:B:809:MET:HE3	2.04	0.58
3:C:244:VAL:O	3:C:248:ILE:HG13	2.03	0.58
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.04	0.58
1:A:225:ASN:ND2	1:A:227:VAL:HB	2.18	0.58
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.67	0.58
2:B:589:VAL:HG12	2:B:590:HIS:N	2.18	0.58
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.86	0.58
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.68	0.58
2:B:1116:ARG:CZ	2:B:1198:TYR:CE1	2.87	0.58
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.18	0.58
2:B:512:ARG:NH2	2:B:535:LEU:CD1	2.62	0.58
1:A:810:PRO:HB2	2:B:519:TRP:HH2	1.67	0.58
2:B:756:ILE:O	2:B:759:PRO:HD3	2.04	0.58
1:A:524:VAL:HG12	1:A:525:GLN:H	1.69	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.19	0.58
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.84	0.58
3:C:258:ILE:O	3:C:261:ALA:HB3	2.04	0.58
6:H:97:MET:HE2	6:H:142:LEU:HD23	1.86	0.58
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.69	0.58
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.86	0.58
1:A:1399:ARG:CB	1:A:1408:ILE:HD13	2.28	0.57
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.04	0.57
2:B:130:VAL:HG12	2:B:131:ASP:H	1.67	0.57
2:B:25:ILE:HG22	2:B:29:ASP:CB	2.34	0.57
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.69	0.57
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.84	0.57
1:A:41:MET:HB3	1:A:48:ALA:O	2.04	0.57
1:A:511:ILE:HA	1:A:521:MET:HE3	1.85	0.57
1:A:814:PHE:CZ	2:B:519:TRP:N	2.72	0.57
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.37	0.57
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.52	0.57
2:B:860:MET:HG2	2:B:861:ASP:N	2.18	0.57
1:A:1325:THR:O	4:E:148:GLU:HB2	2.04	0.57
4:E:157:SER:C	4:E:159:ASP:H	2.07	0.57
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.31	0.57
1:A:825:ILE:HD12	2:B:513:GLN:NE2	2.19	0.57
4:E:46:TYR:HA	4:E:57:MET:SD	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:N	5:F:111:LEU:CD1	2.67	0.57
6:H:97:MET:CE	6:H:142:LEU:HD23	2.35	0.57
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.86	0.57
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.44	0.57
1:A:882:SER:HA	1:A:952:ALA:O	2.04	0.57
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.20	0.57
3:C:55:THR:HB	3:C:152:GLU:H	1.70	0.57
5:F:111:LEU:C	5:F:113:GLY:H	2.07	0.57
10:L:70:ARG:HG2	10:L:70:ARG:HH11	1.66	0.57
1:A:443:LEU:HD13	1:A:455:MET:HE1	1.87	0.57
1:A:710:LEU:HD12	1:A:710:LEU:N	2.20	0.57
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.86	0.57
2:B:803:LEU:N	2:B:822:ASN:HD21	2.02	0.57
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.38	0.57
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.86	0.57
4:E:213:ILE:O	4:E:213:ILE:HG23	2.04	0.57
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.45	0.57
8:J:48:ARG:HE	8:J:49:MET:CE	2.16	0.57
9:K:65:HIS:HD2	9:K:67:PHE:N	2.02	0.57
1:A:1074:GLU:O	1:A:1076:ALA:N	2.37	0.57
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.39	0.57
1:A:57:ARG:O	1:A:68:GLN:HG3	2.03	0.57
5:F:87:LYS:HE2	5:F:88:TYR:CZ	2.39	0.57
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.04	0.57
1:A:537:ARG:HB2	6:H:20:TYR:CE2	2.39	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:HB2	2.34	0.57
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.39	0.57
1:A:401:GLY:C	1:A:435:HIS:CD2	2.79	0.57
2:B:1022:THR:HG23	2:B:1022:THR:O	2.05	0.57
6:H:82:PRO:O	6:H:83:GLN:HB2	2.04	0.57
6:H:89:LEU:HD22	6:H:91:ASP:OD2	2.05	0.57
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.85	0.57
9:K:47:ARG:HD3	9:K:59:ALA:O	2.03	0.57
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.39	0.57
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.35	0.57
1:A:1365:TYR:O	1:A:1366:ARG:C	2.43	0.57
1:A:260:ASP:OD1	1:A:261:ASP:N	2.37	0.57
1:A:76:GLU:O	1:A:76:GLU:CG	2.53	0.57
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.34	0.57
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.85	0.57
3:C:56:THR:CG2	3:C:57:VAL:H	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.86	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.53	0.57
1:A:577:ILE:O	1:A:580:VAL:HG23	2.04	0.57
1:A:901:LEU:H	1:A:926:GLN:HE21	1.50	0.57
2:B:243:ALA:HA	2:B:250:PHE:O	2.05	0.57
2:B:287:ARG:CG	2:B:292:ILE:HA	2.26	0.57
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.70	0.57
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.05	0.56
1:A:1300:LYS:NZ	1:A:1300:LYS:HB3	2.20	0.56
3:C:248:ILE:CD1	9:K:101:LEU:HD22	2.35	0.56
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.86	0.56
1:A:1444:MET:HE1	5:F:135:ARG:NE	2.20	0.56
2:B:57:TYR:HD1	2:B:57:TYR:N	2.03	0.56
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.56
4:E:46:TYR:CE2	4:E:58:MET:HA	2.40	0.56
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.40	0.56
10:L:32:ALA:HB3	10:L:55:ILE:CD1	2.26	0.56
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.20	0.56
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.41	0.56
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.85	0.56
2:B:958:GLN:O	2:B:960:GLY:N	2.33	0.56
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.02	0.56
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.06	0.56
1:A:1389:PHE:O	1:A:1392:SER:HB3	2.06	0.56
1:A:401:GLY:O	1:A:435:HIS:CD2	2.58	0.56
2:B:704:ALA:HB1	2:B:710:LEU:HD12	1.87	0.56
3:C:229:TYR:N	3:C:229:TYR:CD1	2.74	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.04	0.56
10:L:49:LYS:O	10:L:50:ASP:HB2	2.03	0.56
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.72	0.56
2:B:101:MET:HB2	2:B:169:ARG:HH12	1.69	0.56
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.05	0.56
2:B:1180:PHE:O	2:B:1181:GLU:HB2	2.05	0.56
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.05	0.56
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.40	0.56
6:H:89:LEU:HD22	6:H:91:ASP:CG	2.25	0.56
7:I:111:THR:HG22	7:I:112:SER:N	2.19	0.56
7:I:7:CYS:C	7:I:8:ARG:O	2.43	0.56
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.40	0.56
1:A:838:GLN:O	1:A:842:VAL:HG23	2.06	0.56
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLY:HA3	2:B:1086:PHE:CD1	2.41	0.56
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.87	0.56
3:C:145:CYS:SG	3:C:146:LYS:N	2.79	0.56
1:A:35:ILE:HG12	1:A:52:GLY:O	2.06	0.56
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.41	0.56
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.48	0.56
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.13	0.56
2:B:566:LEU:HD22	2:B:586:TRP:O	2.06	0.56
5:F:99:LEU:HD12	5:F:99:LEU:O	2.06	0.56
9:K:50:LEU:CD1	9:K:73:LEU:HD21	2.35	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
1:A:567:LYS:NZ	6:H:46:LEU:CB	2.67	0.56
1:A:885:THR:O	1:A:885:THR:HG22	2.05	0.56
2:B:744:HIS:CD2	2:B:746:SER:H	2.14	0.56
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.87	0.56
4:E:195:VAL:HG22	4:E:213:ILE:HB	1.88	0.56
6:H:106:GLU:C	6:H:108:SER:N	2.57	0.56
2:B:848:ARG:NH1	8:J:8:PHE:O	2.36	0.56
2:B:23:ALA:O	2:B:654:ARG:HB3	2.04	0.56
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.06	0.56
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.88	0.56
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.05	0.56
6:H:84:ALA:HA	6:H:87:ARG:HG3	1.88	0.56
1:A:1017:LEU:HD23	4:E:204:THR:O	2.06	0.56
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.54	0.56
1:A:1328:TYR:CG	1:A:1329:THR:N	2.74	0.56
1:A:50:ILE:C	1:A:52:GLY:H	2.09	0.56
2:B:34:ILE:O	2:B:37:PHE:HB3	2.06	0.56
2:B:429:PHE:HA	2:B:432:MET:CE	2.35	0.56
6:H:89:LEU:O	6:H:91:ASP:N	2.37	0.56
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.88	0.55
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.88	0.55
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.55
6:H:59:ILE:HG22	6:H:60:ALA:N	2.20	0.55
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.36	0.55
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.86	0.55
10:L:63:ARG:O	10:L:64:LEU:O	2.25	0.55
1:A:710:LEU:H	1:A:710:LEU:CD1	2.19	0.55
2:B:120:ARG:NH1	10:L:54:ARG:NH1	2.54	0.55
2:B:794:ASN:C	2:B:795:ILE:HD12	2.26	0.55
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:168:TYR:HB3	4:E:170:LEU:CD2	2.36	0.55
4:E:195:VAL:HG22	4:E:213:ILE:CB	2.36	0.55
1:A:1329:THR:HG22	1:A:1331:SER:N	2.01	0.55
1:A:511:ILE:HG12	1:A:521:MET:HE3	1.89	0.55
2:B:566:LEU:HD13	2:B:588:GLY:CA	2.36	0.55
2:B:864:LYS:HG3	2:B:865:LYS:N	2.21	0.55
2:B:120:ARG:HE	2:B:955:THR:CG2	2.20	0.55
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.41	0.55
1:A:672:ASP:HB3	1:A:675:THR:OG1	2.05	0.55
1:A:775:ILE:HD12	1:A:815:PHE:CG	2.41	0.55
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.37	0.55
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.89	0.55
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.55
5:F:94:LEU:HD21	5:F:122:MET:HA	1.89	0.55
8:J:21:TYR:HA	8:J:39:LEU:HD11	1.89	0.55
1:A:399:HIS:O	1:A:435:HIS:CD2	2.60	0.55
1:A:15:LYS:HD2	2:B:1220:ARG:HE	1.72	0.55
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.47	0.55
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.60	0.55
2:B:556:THR:HG22	2:B:557:PHE:N	2.20	0.55
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.47	0.55
10:L:26:THR:HG22	10:L:27:LEU:N	2.21	0.55
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.89	0.55
1:A:92:HIS:HD2	1:A:94:GLY:H	1.53	0.55
2:B:361:LEU:N	2:B:362:PRO:CD	2.69	0.55
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.89	0.55
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.37	0.55
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.07	0.55
1:A:122:MET:O	1:A:126:LEU:HG	2.07	0.55
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.89	0.55
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.41	0.55
7:I:7:CYS:O	7:I:8:ARG:O	2.24	0.55
1:A:216:VAL:O	1:A:219:PHE:HB2	2.06	0.55
1:A:845:LEU:N	1:A:845:LEU:HD23	2.22	0.55
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.70	0.55
3:C:37:MET:HG2	3:C:243:VAL:CG1	2.34	0.55
3:C:99:LEU:HD23	3:C:99:LEU:N	2.20	0.55
9:K:61:TYR:HA	9:K:72:LYS:O	2.06	0.55
1:A:515:GLN:HG3	1:A:516:SER:N	2.22	0.55
1:A:741:ASN:ND2	1:A:743:VAL:H	2.05	0.55
2:B:542:MET:HE1	2:B:743:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:THR:HG22	2:B:681:TRP:H	1.72	0.55
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.07	0.55
2:B:783:THR:HA	8:J:60:PHE:HE1	1.72	0.55
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.89	0.54
1:A:867:ILE:HG22	1:A:872:GLY:N	2.22	0.54
1:A:89:PRO:O	1:A:204:THR:HG21	2.07	0.54
2:B:1171:VAL:HG11	2:B:1191:ILE:HD13	1.88	0.54
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.91	0.54
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.07	0.54
2:B:479:VAL:HG12	2:B:480:SER:H	1.72	0.54
2:B:864:LYS:N	2:B:872:GLU:OE1	2.39	0.54
3:C:13:ALA:O	9:K:114:LEU:HD13	2.08	0.54
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.42	0.54
4:E:176:PRO:HD2	4:E:211:TYR:O	2.07	0.54
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.67	0.54
1:A:821:ARG:O	1:A:822:GLU:C	2.46	0.54
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.31	0.54
2:B:756:ILE:HG21	2:B:759:PRO:HB3	1.90	0.54
2:B:758:PHE:C	2:B:760:ASP:H	2.11	0.54
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.89	0.54
4:E:61:GLN:NE2	4:E:105:PHE:CE2	2.71	0.54
10:L:70:ARG:HG2	10:L:70:ARG:NH1	2.22	0.54
1:A:646:PHE:O	1:A:650:GLN:HG3	2.08	0.54
1:A:885:THR:O	1:A:940:ARG:HG3	2.07	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.42	0.54
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.23	0.54
1:A:1299:VAL:CG1	1:A:1300:LYS:H	2.20	0.54
1:A:533:LYS:O	1:A:535:THR:N	2.40	0.54
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.89	0.54
2:B:292:ILE:H	2:B:293:PRO:HD2	1.73	0.54
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.38	0.54
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.54	0.54
5:F:72:LYS:N	5:F:142:SER:HA	2.22	0.54
6:H:6:PHE:HE1	6:H:130:ARG:HE	1.53	0.54
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.67	0.54
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.71	0.54
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.42	0.54
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.89	0.54
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.88	0.54
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.23	0.54
3:C:248:ILE:HD13	9:K:101:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.88	0.54
6:H:38:LEU:CD1	6:H:125:LEU:HD13	2.38	0.54
7:I:29:CYS:O	7:I:29:CYS:SG	2.66	0.54
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.38	0.54
1:A:226:GLU:HG2	1:A:227:VAL:HG23	1.90	0.54
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.08	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.88	0.54
2:B:93:GLY:N	2:B:131:ASP:O	2.37	0.54
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.37	0.54
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.38	0.54
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.42	0.54
1:A:852:TYR:CE2	5:F:136:ARG:HG2	2.43	0.54
8:J:32:GLU:O	8:J:36:LEU:HG	2.07	0.54
1:A:1116:LEU:O	1:A:1308:THR:HB	2.07	0.54
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.10	0.54
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.42	0.54
1:A:1375:MET:HG2	1:A:1382:THR:O	2.08	0.54
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.43	0.54
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.38	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
3:C:241:ASP:O	3:C:245:VAL:HG23	2.08	0.54
5:F:114:GLU:OE1	5:F:119:ARG:HG3	2.08	0.54
5:F:118:LEU:O	5:F:122:MET:HG3	2.08	0.54
1:A:1205:LYS:O	1:A:1207:LEU:N	2.41	0.54
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.43	0.54
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.42	0.54
1:A:902:LEU:HD21	1:A:923:LEU:HD23	1.90	0.54
2:B:405:ARG:HB3	2:B:631:GLY:O	2.07	0.54
2:B:549:THR:HB	2:B:628:THR:HG23	1.89	0.54
6:H:5:LEU:CD1	6:H:135:LEU:HG	2.34	0.54
1:A:1151:GLU:CB	7:I:44:TYR:O	2.52	0.54
1:A:38:PRO:N	1:A:270:LEU:HD23	2.22	0.53
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.08	0.53
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.09	0.53
7:I:111:THR:CG2	7:I:112:SER:N	2.69	0.53
7:I:2:THR:HG22	7:I:2:THR:O	2.07	0.53
10:L:27:LEU:HD13	10:L:37:LYS:HB3	1.90	0.53
11:M:53:UNK:C	11:M:55:UNK:N	2.63	0.53
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.37	0.53
1:A:367:PRO:HB3	1:A:465:TYR:O	2.08	0.53
1:A:92:HIS:CD2	1:A:94:GLY:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ASN:ND2	2:B:486:TYR:CD1	2.76	0.53
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.38	0.53
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.43	0.53
6:H:32:THR:HG22	6:H:33:GLN:HG3	1.90	0.53
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.24	0.53
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.88	0.53
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.28	0.53
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.23	0.53
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.53
2:B:108:VAL:CG1	2:B:109:THR:H	2.18	0.53
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.90	0.53
1:A:814:PHE:CZ	2:B:514:LEU:HD11	2.43	0.53
2:B:801:LYS:O	8:J:52:THR:CG2	2.52	0.53
3:C:189:THR:HG22	3:C:190:ASP:N	2.24	0.53
4:E:78:LEU:HD21	4:E:109:ILE:HD12	1.90	0.53
1:A:225:ASN:O	1:A:227:VAL:HG23	2.09	0.53
1:A:683:ILE:HD11	1:A:764:CYS:CB	2.35	0.53
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.90	0.53
2:B:755:ILE:CG2	2:B:755:ILE:O	2.55	0.53
6:H:6:PHE:O	6:H:58:THR:HA	2.08	0.53
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.72	0.53
1:A:233:TRP:C	1:A:235:ILE:N	2.60	0.53
1:A:384:ASN:OD1	1:A:385:ILE:N	2.42	0.53
1:A:590:ARG:O	1:A:591:PHE:HB2	2.08	0.53
1:A:529:CYS:HB2	2:B:1015:HIS:CE1	2.43	0.53
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.53
2:B:916:THR:HG22	2:B:918:ILE:HG13	1.90	0.53
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.89	0.53
5:F:107:VAL:HG12	5:F:109:VAL:H	1.72	0.53
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.74	0.53
1:A:1366:ARG:O	1:A:1369:ALA:HB3	2.08	0.53
1:A:339:ASN:O	1:A:343:LYS:HG2	2.07	0.53
1:A:387:ARG:O	1:A:391:LEU:HG	2.09	0.53
1:A:399:HIS:C	1:A:401:GLY:H	2.10	0.53
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.77	0.53
2:B:287:ARG:HA	2:B:291:ILE:O	2.09	0.53
2:B:899:ILE:HD11	2:B:910:VAL:O	2.09	0.53
7:I:62:ILE:HG23	7:I:63:GLY:N	2.22	0.53
7:I:75:CYS:C	7:I:77:LYS:N	2.59	0.53
10:L:47:ARG:HG2	10:L:52:GLY:CA	2.39	0.53
10:L:51:CYS:C	10:L:53:HIS:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.74	0.53
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.24	0.53
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.39	0.53
1:A:696:GLU:OE2	1:A:702:LEU:HD23	2.08	0.53
1:A:898:ARG:HD2	1:A:899:VAL:H	1.73	0.53
2:B:234:ILE:HG21	2:B:257:LYS:HB3	1.91	0.53
2:B:90:ILE:CD1	2:B:432:MET:SD	2.97	0.53
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.41	0.53
3:C:131:HIS:O	3:C:132:PRO:C	2.43	0.53
9:K:63:VAL:HG23	9:K:63:VAL:O	2.08	0.53
1:A:817:ALA:CB	2:B:514:LEU:HD23	2.39	0.53
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.91	0.53
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.53
2:B:875:GLU:O	2:B:877:PRO:HD3	2.09	0.53
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.11	0.53
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.39	0.53
1:A:13:THR:HG23	1:A:1432:GLN:NE2	2.24	0.53
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.73	0.53
1:A:825:ILE:CG2	2:B:512:ARG:CD	2.87	0.53
5:F:77:ASP:O	5:F:78:GLN:HB2	2.09	0.53
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.24	0.53
1:A:619:LYS:O	1:A:623:GLY:N	2.38	0.53
1:A:741:ASN:ND2	1:A:741:ASN:C	2.62	0.53
2:B:235:SER:OG	2:B:236:HIS:HD2	1.91	0.53
2:B:515:HIS:H	2:B:518:HIS:HD2	1.55	0.53
2:B:552:MET:N	2:B:553:PRO:HD2	2.24	0.53
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.73	0.53
2:B:43:LEU:HD13	2:B:812:LEU:CD2	2.38	0.53
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.09	0.53
4:E:35:VAL:C	4:E:37:LEU:H	2.12	0.53
1:A:1365:TYR:O	1:A:1367:HIS:N	2.42	0.52
1:A:1436:ILE:CG2	1:A:1437:GLY:H	2.22	0.52
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.68	0.52
2:B:25:ILE:HG22	2:B:26:THR:N	2.24	0.52
2:B:806:THR:C	2:B:808:ALA:H	2.12	0.52
7:I:29:CYS:C	7:I:31:THR:H	2.13	0.52
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.24	0.52
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.91	0.52
1:A:442:VAL:O	1:A:457:ALA:HA	2.09	0.52
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.34	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:LEU:HD12	8:J:47:ARG:NH1	2.23	0.52
8:J:52:THR:O	8:J:52:THR:HG22	2.08	0.52
10:L:62:LYS:C	10:L:64:LEU:H	2.13	0.52
1:A:1220:PHE:O	1:A:1222:ASN:N	2.42	0.52
1:A:1436:ILE:CG2	1:A:1437:GLY:N	2.72	0.52
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.74	0.52
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.91	0.52
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.90	0.52
2:B:240:ILE:HG23	2:B:240:ILE:O	2.10	0.52
2:B:842:ASN:HD22	2:B:845:SER:CB	2.21	0.52
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.91	0.52
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.57	0.52
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.90	0.52
1:A:852:TYR:CZ	5:F:136:ARG:HG2	2.44	0.52
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.52
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.92	0.52
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.74	0.52
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.77	0.52
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.91	0.52
10:L:38:LEU:HG	10:L:39:SER:N	2.24	0.52
2:B:271:ALA:HB3	2:B:285:ILE:CD1	2.40	0.52
2:B:844:SER:OG	2:B:996:ARG:N	2.33	0.52
4:E:17:ARG:O	4:E:21:GLU:HG3	2.09	0.52
4:E:28:TYR:CE1	4:E:78:LEU:HD12	2.44	0.52
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.71	0.52
7:I:46:HIS:CD2	7:I:48:LEU:HD21	2.44	0.52
7:I:50:THR:HG22	7:I:52:ILE:H	1.75	0.52
1:A:219:PHE:O	1:A:222:LEU:O	2.28	0.52
1:A:261:ASP:OD2	1:A:323:LYS:HD2	2.10	0.52
1:A:61:ILE:HG22	1:A:62:ASP:N	2.16	0.52
2:B:405:ARG:CA	2:B:631:GLY:O	2.58	0.52
2:B:428:ILE:O	2:B:431:TYR:HB3	2.10	0.52
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.52
5:F:132:LEU:O	5:F:148:VAL:HG23	2.09	0.52
8:J:9:SER:CB	8:J:45:CYS:HB2	2.40	0.52
1:A:134:ARG:NH1	1:A:220:THR:O	2.42	0.52
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.92	0.52
1:A:596:THR:O	1:A:597:LEU:C	2.47	0.52
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.52
1:A:907:THR:HG22	1:A:908:LEU:N	2.25	0.52
1:A:928:LEU:O	1:A:931:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:ILE:HD13	2:B:974:PRO:HG2	1.91	0.52
2:B:98:THR:OG1	2:B:127:GLY:HA3	2.09	0.52
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.92	0.52
5:F:109:VAL:CG1	5:F:110:ASP:N	2.73	0.52
1:A:1438:THR:HG23	5:F:92:ARG:HD2	1.92	0.52
1:A:27:VAL:HG13	1:A:240:PRO:HB3	1.91	0.52
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.91	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.24	0.52
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.52
2:B:547:VAL:H	2:B:612:GLU:CD	2.12	0.52
1:A:134:ARG:HH12	1:A:220:THR:HG22	1.74	0.52
1:A:1359:ASP:C	1:A:1361:SER:H	2.13	0.52
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.91	0.52
1:A:50:ILE:HG22	1:A:51:GLY:N	2.24	0.52
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.75	0.52
1:A:91:PHE:HB2	1:A:297:GLN:OE1	2.09	0.52
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.10	0.52
2:B:234:ILE:H	2:B:234:ILE:CD1	2.16	0.52
2:B:864:LYS:HD3	2:B:871:THR:HA	1.91	0.52
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.10	0.52
1:A:1392:SER:O	1:A:1393:ASN:CB	2.58	0.52
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.52
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.50	0.52
1:A:507:VAL:N	1:A:508:PRO:CD	2.72	0.52
1:A:929:LEU:H	1:A:929:LEU:CD2	2.23	0.52
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.38	0.52
2:B:25:ILE:CG2	2:B:29:ASP:HB3	2.40	0.52
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.44	0.52
4:E:12:LEU:HD22	4:E:55:ARG:CZ	2.39	0.52
4:E:155:ARG:HD2	4:E:194:GLU:OE2	2.09	0.52
4:E:23:VAL:HG13	4:E:28:TYR:CD1	2.45	0.52
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.75	0.52
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.92	0.51
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.92	0.51
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.91	0.51
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.40	0.51
6:H:84:ALA:C	6:H:86:ASP:H	2.13	0.51
8:J:7:CYS:SG	8:J:9:SER:HB2	2.50	0.51
1:A:306:ASN:HD21	1:A:324:SER:N	2.09	0.51
1:A:41:MET:HG2	1:A:49:LYS:HG2	1.92	0.51
1:A:817:ALA:HB1	2:B:514:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.10	0.51
2:B:1163:CYS:SG	2:B:1182:CYS:SG	3.08	0.51
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.78	0.51
2:B:614:SER:OG	2:B:627:PHE:HB2	2.10	0.51
2:B:707:PRO:CG	2:B:708:GLU:H	2.21	0.51
1:A:357:PRO:HG2	2:B:833:TYR:CE1	2.45	0.51
1:A:1149:ALA:CB	7:I:46:HIS:H	2.00	0.51
9:K:46:ILE:O	9:K:50:LEU:HB2	2.09	0.51
9:K:49:GLU:OE2	9:K:97:LYS:HE3	2.10	0.51
1:A:96:ILE:O	1:A:100:LYS:HG3	2.10	0.51
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.11	0.51
2:B:130:VAL:CG1	2:B:131:ASP:N	2.74	0.51
2:B:559:SER:HA	2:B:563:MET:HB3	1.91	0.51
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.91	0.51
4:E:124:VAL:HG22	4:E:132:ILE:CG2	2.40	0.51
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.90	0.51
1:A:326:ARG:HG2	1:A:1406:VAL:CG2	2.39	0.51
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.92	0.51
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.45	0.51
2:B:248:SER:O	2:B:249:ARG:HB2	2.09	0.51
2:B:292:ILE:N	2:B:293:PRO:HD2	2.25	0.51
7:I:73:ARG:O	7:I:81:ARG:HA	2.09	0.51
10:L:62:LYS:O	10:L:64:LEU:N	2.37	0.51
1:A:341:MET:CE	1:A:1401:SER:HB2	2.41	0.51
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.45	0.51
1:A:808:LEU:O	2:B:728:ARG:NH1	2.43	0.51
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.11	0.51
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.92	0.51
2:B:463:THR:HG21	2:B:465:ASN:HD22	1.74	0.51
6:H:83:GLN:C	6:H:85:GLY:H	2.14	0.51
6:H:84:ALA:C	6:H:86:ASP:N	2.64	0.51
7:I:78:CYS:SG	7:I:106:CYS:SG	3.02	0.51
8:J:14:VAL:HG12	8:J:50:ILE:HD11	1.92	0.51
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.09	0.51
1:A:675:THR:CG2	1:A:736:ASN:HD21	2.22	0.51
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.93	0.51
2:B:247:GLY:N	2:B:418:LYS:HZ3	2.06	0.51
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.92	0.51
8:J:48:ARG:NE	8:J:49:MET:HE2	2.26	0.51
8:J:54:VAL:O	8:J:56:LEU:N	2.43	0.51
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:O	10:L:39:SER:CB	2.56	0.51
1:A:822:GLU:HA	2:B:513:GLN:HE21	1.63	0.51
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.40	0.51
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.45	0.51
1:A:1410:PHE:CE2	2:B:1212:ILE:HD11	2.45	0.51
1:A:15:LYS:CB	2:B:1220:ARG:HG2	2.33	0.51
4:E:121:MET:C	4:E:123:LEU:H	2.13	0.51
7:I:55:THR:HG21	7:I:109:ILE:HD13	1.93	0.51
1:A:1153:TYR:OH	7:I:42:LEU:HA	2.09	0.51
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.41	0.51
10:L:40:LEU:HD13	10:L:44:ASP:OD1	2.11	0.51
1:A:1150:SER:HB2	1:A:1195:LEU:HD23	1.93	0.51
1:A:115:LEU:HB2	1:A:122:MET:CE	2.41	0.51
2:B:283:VAL:HG13	2:B:297:ILE:CD1	2.41	0.51
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.93	0.51
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.41	0.51
1:A:1376:THR:HG23	4:E:212:ARG:NH2	2.26	0.51
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.26	0.51
1:A:898:ARG:HD2	1:A:899:VAL:N	2.26	0.51
2:B:283:VAL:O	2:B:286:PHE:HB2	2.11	0.51
3:C:66:ARG:NH2	8:J:2:ILE:CG2	2.74	0.51
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	2.10	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.84	0.51
1:A:233:TRP:C	1:A:235:ILE:H	2.13	0.51
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.40	0.51
2:B:405:ARG:O	2:B:406:LEU:HD23	2.11	0.51
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.25	0.51
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.93	0.51
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.51
1:A:418:SER:C	1:A:420:ARG:N	2.63	0.50
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.92	0.50
1:A:649:ILE:O	1:A:653:VAL:HG23	2.11	0.50
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.39	0.50
1:A:500:GLU:OE1	2:B:1143:ALA:HB1	2.11	0.50
2:B:185:THR:O	2:B:189:LEU:HG	2.11	0.50
2:B:737:THR:CG2	7:I:66:PRO:HB2	2.40	0.50
6:H:31:THR:O	6:H:32:THR:HB	2.11	0.50
8:J:36:LEU:HD13	8:J:47:ARG:HG2	1.92	0.50
9:K:101:LEU:HD23	9:K:101:LEU:O	2.11	0.50
1:A:100:LYS:NZ	1:A:176:LYS:HD2	2.27	0.50
1:A:1384:VAL:HG12	1:A:1384:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:HIS:HA	1:A:607:ILE:O	2.11	0.50
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.76	0.50
1:A:888:GLY:O	1:A:940:ARG:NH2	2.44	0.50
1:A:814:PHE:HZ	2:B:518:HIS:HB2	1.75	0.50
2:B:563:MET:HG3	2:B:563:MET:O	2.10	0.50
2:B:858:SER:HA	2:B:966:VAL:O	2.11	0.50
4:E:54:GLN:O	4:E:57:MET:HB3	2.11	0.50
7:I:25:LEU:HD12	7:I:26:LEU:H	1.76	0.50
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.76	0.50
1:A:332:LYS:H	1:A:337:ARG:HD2	1.76	0.50
1:A:810:PRO:O	1:A:813:PHE:HB3	2.11	0.50
1:A:771:GLU:H	1:A:822:GLU:CD	2.14	0.50
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.14	0.50
2:B:271:ALA:O	2:B:279:ASP:HA	2.11	0.50
2:B:514:LEU:HD12	2:B:515:HIS:H	1.74	0.50
8:J:7:CYS:O	8:J:8:PHE:C	2.50	0.50
1:A:706:HIS:CG	1:A:1135:ARG:CZ	2.94	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.11	0.50
1:A:167:CYS:O	1:A:169:ASN:N	2.45	0.50
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.50
2:B:271:ALA:HB3	2:B:285:ILE:HD11	1.93	0.50
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.93	0.50
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.26	0.50
6:H:128:ASN:O	6:H:131:ASN:ND2	2.45	0.50
6:H:44:VAL:O	6:H:44:VAL:HG12	2.12	0.50
1:A:994:GLN:NE2	1:A:1019:CYS:HB3	2.27	0.50
2:B:756:ILE:CG2	2:B:759:PRO:HB3	2.42	0.50
2:B:839:MET:HE2	2:B:980:PHE:CD1	2.47	0.50
4:E:157:SER:C	4:E:159:ASP:N	2.64	0.50
1:A:1362:TYR:OH	1:A:1364:ASN:HA	2.11	0.50
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.52	0.50
1:A:340:LEU:HD21	2:B:1200:ALA:CB	2.40	0.50
1:A:517:ASN:HB2	1:A:875:ALA:O	2.11	0.50
1:A:821:ARG:CG	1:A:825:ILE:HD11	2.41	0.50
1:A:329:LEU:HD22	2:B:1203:LEU:CD1	2.41	0.50
4:E:168:TYR:HB3	4:E:170:LEU:CG	2.41	0.50
7:I:99:LEU:HB2	7:I:112:SER:HB3	1.94	0.50
9:K:97:LYS:O	9:K:100:ALA:HB3	2.12	0.50
10:L:62:LYS:O	10:L:64:LEU:HG	2.11	0.50
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.94	0.50
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.50
1:A:814:PHE:HB2	2:B:519:TRP:HE3	1.75	0.50
2:B:751:VAL:HG12	2:B:752:ALA:N	2.26	0.50
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.94	0.50
1:A:573:SER:O	1:A:576:GLN:HB2	2.11	0.50
1:A:69:THR:HG22	1:A:69:THR:O	2.12	0.50
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.27	0.50
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.93	0.50
2:B:800:GLN:OE1	2:B:822:ASN:HB2	2.12	0.50
4:E:98:ILE:O	4:E:102:GLU:HG3	2.12	0.50
2:B:737:THR:CG2	7:I:66:PRO:CB	2.89	0.50
7:I:75:CYS:O	7:I:77:LYS:N	2.44	0.50
1:A:107:CYS:HB2	1:A:114:LEU:HD23	1.93	0.50
1:A:709:THR:CB	1:A:712:GLU:HG3	2.41	0.50
1:A:775:ILE:HD11	1:A:815:PHE:HB3	1.90	0.50
6:H:76:THR:HG22	6:H:76:THR:O	2.11	0.50
1:A:1326:ARG:O	1:A:1327:ILE:C	2.49	0.49
1:A:1351:GLU:O	1:A:1352:VAL:C	2.49	0.49
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.24	0.49
2:B:1106:ARG:HH12	2:B:1118:PRO:CB	2.24	0.49
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.24	0.49
2:B:1208:MET:HA	2:B:1212:ILE:O	2.12	0.49
2:B:240:ILE:O	2:B:253:THR:HG23	2.11	0.49
2:B:269:ILE:CD1	2:B:386:LEU:HD21	2.39	0.49
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.27	0.49
1:A:706:HIS:HD2	1:A:1135:ARG:NH2	2.05	0.49
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.47	0.49
1:A:834:THR:HG21	1:A:1077:THR:CA	2.43	0.49
1:A:893:PHE:CE1	1:A:940:ARG:HD2	2.46	0.49
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.51	0.49
2:B:648:HIS:NE2	2:B:650:GLU:OE1	2.43	0.49
2:B:975:GLN:O	2:B:990:ILE:HD12	2.12	0.49
8:J:57:ILE:HG12	8:J:61:LEU:HD11	1.94	0.49
11:M:17:UNK:O	11:M:18:UNK:O	2.30	0.49
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.12	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.44	0.49
1:A:819:GLY:O	1:A:820:GLY:C	2.49	0.49
1:A:810:PRO:HG2	2:B:705:MET:CG	2.42	0.49
2:B:781:PHE:O	2:B:782:LEU:HG	2.12	0.49
2:B:911:ILE:HD11	2:B:941:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.76	0.49
4:E:46:TYR:HE2	4:E:58:MET:HA	1.76	0.49
4:E:5:ASN:O	4:E:9:ILE:HG13	2.11	0.49
6:H:40:LEU:CD2	6:H:42:ILE:HD11	2.39	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.12	0.49
7:I:29:CYS:SG	7:I:31:THR:HG22	2.52	0.49
1:A:1142:THR:O	1:A:1273:LEU:HD22	2.12	0.49
1:A:1376:THR:HG23	1:A:1376:THR:O	2.12	0.49
1:A:412:ARG:O	11:M:50:UNK:C	2.60	0.49
1:A:511:ILE:HG12	1:A:521:MET:CE	2.42	0.49
2:B:25:ILE:CG2	2:B:29:ASP:CB	2.91	0.49
2:B:35:SER:O	2:B:36:ALA:C	2.50	0.49
2:B:660:LYS:O	2:B:663:ALA:HB3	2.13	0.49
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.95	0.49
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.94	0.49
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.76	0.49
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.94	0.49
8:J:16:ASP:OD1	8:J:17:LYS:HE3	2.12	0.49
1:A:418:SER:HB3	1:A:421:ALA:HB2	1.94	0.49
1:A:829:VAL:C	1:A:831:THR:H	2.15	0.49
2:B:1077:THR:HG22	2:B:1079:LYS:HB2	1.94	0.49
4:E:102:GLU:O	4:E:104:ASN:N	2.46	0.49
4:E:177:ARG:O	4:E:212:ARG:HD3	2.11	0.49
5:F:133:VAL:HG22	5:F:147:SER:HA	1.95	0.49
7:I:7:CYS:CB	7:I:14:LEU:HD21	2.32	0.49
1:A:394:ASN:OD1	1:A:398:GLU:OE1	2.30	0.49
1:A:612:ILE:O	1:A:612:ILE:HG23	2.12	0.49
1:A:751:SER:O	1:A:752:LYS:CG	2.59	0.49
3:C:33:LEU:HG	3:C:37:MET:CE	2.41	0.49
4:E:191:LYS:O	4:E:192:ARG:C	2.50	0.49
6:H:88:SER:O	6:H:89:LEU:HG	2.12	0.49
7:I:101:PHE:O	7:I:109:ILE:HA	2.12	0.49
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.93	0.49
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.42	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
5:F:82:THR:HG22	5:F:84:TYR:H	1.77	0.49
7:I:15:TYR:N	7:I:15:TYR:CD1	2.79	0.49
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.77	0.49
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.43	0.49
1:A:225:ASN:C	1:A:227:VAL:H	2.10	0.49
1:A:754:SER:O	1:A:755:PHE:C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.43	0.49
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.48	0.49
1:A:821:ARG:NE	2:B:512:ARG:O	2.44	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.75	0.49
5:F:87:LYS:HE2	5:F:88:TYR:CE1	2.48	0.49
6:H:84:ALA:HB1	6:H:87:ARG:HB2	1.94	0.49
10:L:31:CYS:SG	10:L:34:CYS:SG	3.11	0.49
1:A:1100:ARG:NH2	1:A:1330:ASN:HB2	2.28	0.49
1:A:1300:LYS:HZ2	1:A:1300:LYS:HB3	1.77	0.49
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.72	0.49
1:A:178:GLY:O	1:A:179:LEU:HD23	2.13	0.49
1:A:381:THR:O	1:A:384:ASN:N	2.41	0.49
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.95	0.49
1:A:475:THR:CG2	1:A:476:SER:N	2.76	0.49
1:A:679:ILE:HG23	1:A:729:ALA:CB	2.39	0.49
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.95	0.49
1:A:89:PRO:C	1:A:204:THR:HG21	2.33	0.49
1:A:918:GLU:O	1:A:918:GLU:HG3	2.12	0.49
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.94	0.49
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.53	0.49
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.43	0.49
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.47	0.49
2:B:365:THR:HG23	2:B:367:LEU:HG	1.93	0.49
2:B:405:ARG:CB	2:B:631:GLY:O	2.61	0.49
2:B:55:VAL:HG12	2:B:56:ASP:N	2.28	0.49
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.13	0.49
2:B:825:VAL:CG1	2:B:826:ALA:N	2.76	0.49
3:C:80:LEU:CD2	3:C:129:ILE:HD11	2.29	0.49
3:C:254:LYS:HE2	9:K:42:LEU:HD13	1.94	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
7:I:85:PHE:O	7:I:86:PHE:HB3	2.13	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.95	0.49
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.39	0.49
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.78	0.49
2:B:1043:ASP:O	2:B:1050:ILE:HD12	2.13	0.49
2:B:1053:GLU:O	2:B:1054:GLY:C	2.50	0.49
2:B:708:GLU:C	2:B:710:LEU:H	2.16	0.49
2:B:906:SER:O	2:B:907:GLY:C	2.50	0.49
6:H:36:CYS:HA	6:H:126:GLU:O	2.13	0.49
6:H:6:PHE:HE1	6:H:130:ARG:NE	2.10	0.49
1:A:538:ASP:OD1	6:H:22:LYS:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:OE1	1:A:591:PHE:HE1	1.96	0.48
1:A:61:ILE:HA	1:A:74:MET:SD	2.53	0.48
2:B:260:GLY:O	2:B:267:ARG:HD3	2.12	0.48
3:C:142:VAL:H	8:J:16:ASP:CB	2.26	0.48
4:E:100:ILE:CG2	4:E:105:PHE:HB2	2.42	0.48
4:E:78:LEU:HD21	4:E:80:VAL:HG22	1.95	0.48
6:H:125:LEU:HG	6:H:130:ARG:CZ	2.43	0.48
6:H:93:TYR:HA	6:H:145:ARG:CB	2.41	0.48
1:A:567:LYS:NZ	6:H:95:TYR:CD1	2.80	0.48
1:A:466:SER:HB3	9:K:2:ASN:ND2	2.28	0.48
1:A:1066:VAL:O	1:A:1068:ALA:N	2.46	0.48
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.13	0.48
1:A:674:PRO:O	1:A:677:ARG:HB3	2.14	0.48
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.46	0.48
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.48
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.45	0.48
6:H:33:GLN:OE1	6:H:129:TYR:CE2	2.67	0.48
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.77	0.48
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.73	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.48
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.61	0.48
1:A:226:GLU:CG	1:A:227:VAL:N	2.75	0.48
1:A:491:VAL:O	1:A:493:GLN:NE2	2.46	0.48
1:A:74:MET:O	1:A:75:ASN:HB2	2.13	0.48
2:B:1054:GLY:O	2:B:1058:LEU:HG	2.13	0.48
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.41	0.48
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.14	0.48
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.48	0.48
2:B:890:TYR:O	2:B:892:LYS:N	2.46	0.48
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.13	0.48
3:C:4:GLU:O	3:C:5:GLY:O	2.31	0.48
3:C:75:MET:HG3	3:C:246:ARG:NH2	2.28	0.48
4:E:102:GLU:C	4:E:104:ASN:N	2.67	0.48
5:F:82:THR:HG22	5:F:84:TYR:N	2.27	0.48
7:I:50:THR:HG22	7:I:51:ASN:N	2.28	0.48
9:K:43:GLY:HA2	9:K:71:PHE:CZ	2.49	0.48
9:K:55:LYS:CD	9:K:78:THR:HB	2.42	0.48
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.43	0.48
1:A:474:VAL:HG13	1:A:478:TYR:CE1	2.48	0.48
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.78	0.48
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:TYR:O	2:B:355:ILE:HG13	2.13	0.48
2:B:46:GLN:HE21	2:B:496:ARG:HG2	1.78	0.48
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.95	0.48
3:C:75:MET:HG3	3:C:246:ARG:HH22	1.77	0.48
3:C:254:LYS:O	3:C:258:ILE:HD13	2.13	0.48
5:F:81:THR:HG22	5:F:82:THR:H	1.78	0.48
1:A:1149:ALA:CA	7:I:46:HIS:HB3	2.32	0.48
1:A:1386:ARG:HE	1:A:1387:HIS:CE1	2.32	0.48
1:A:226:GLU:HG2	1:A:227:VAL:N	2.29	0.48
1:A:294:SER:HA	1:A:297:GLN:HB3	1.96	0.48
1:A:391:LEU:O	1:A:394:ASN:N	2.46	0.48
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.48
2:B:873:THR:O	2:B:914:LYS:HA	2.12	0.48
3:C:35:ARG:O	3:C:38:ILE:N	2.47	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.94	0.48
9:K:27:ALA:HB1	9:K:28:PRO:HD2	1.96	0.48
10:L:52:GLY:O	10:L:54:ARG:HG3	2.12	0.48
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.54	0.48
1:A:1406:VAL:CG1	1:A:1410:PHE:HE1	2.26	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CB	2.76	0.48
2:B:1053:GLU:O	2:B:1055:ILE:N	2.46	0.48
2:B:1104:HIS:HB2	2:B:1122:ARG:CD	2.44	0.48
2:B:570:VAL:HG11	2:B:573:GLN:OE1	2.13	0.48
2:B:864:LYS:HB3	2:B:871:THR:HA	1.96	0.48
3:C:142:VAL:H	8:J:16:ASP:HB3	1.77	0.48
6:H:39:THR:O	6:H:123:MET:HA	2.14	0.48
1:A:18:GLN:O	2:B:1215:ARG:CG	2.62	0.48
2:B:1065:GLN:HE22	2:B:1067:ARG:HG2	1.78	0.48
2:B:1106:ARG:NH2	2:B:1109:GLY:C	2.67	0.48
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.48
1:A:810:PRO:HB2	2:B:705:MET:SD	2.53	0.48
1:A:1392:SER:O	1:A:1393:ASN:CG	2.52	0.48
1:A:741:ASN:ND2	1:A:743:VAL:N	2.60	0.48
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.78	0.48
2:B:300:HIS:ND1	2:B:376:PHE:CD2	2.81	0.48
2:B:806:THR:HG22	2:B:808:ALA:H	1.79	0.48
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.68	0.48
4:E:7:ARG:C	4:E:9:ILE:H	2.17	0.48
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.95	0.48
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.49	0.48
1:A:1116:LEU:HD12	1:A:1329:THR:HG1	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.60	0.48
1:A:332:LYS:N	1:A:337:ARG:HD2	2.28	0.48
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.91	0.48
1:A:67:CYS:SG	1:A:77:CYS:SG	3.11	0.48
2:B:1106:ARG:HH21	2:B:1109:GLY:C	2.16	0.48
2:B:1182:CYS:O	2:B:1183:LYS:O	2.31	0.48
2:B:225:VAL:HG11	2:B:388:CYS:HB3	1.95	0.48
2:B:332:ASP:C	2:B:334:ILE:H	2.17	0.48
2:B:763:GLN:CG	2:B:765:PRO:HD2	2.40	0.48
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.95	0.48
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.96	0.48
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.37	0.48
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.14	0.48
2:B:230:ALA:C	2:B:232:SER:H	2.17	0.48
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.29	0.48
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.48
2:B:653:VAL:HG12	2:B:654:ARG:N	2.28	0.48
9:K:83:PRO:HA	9:K:86:ALA:HB3	1.95	0.48
1:A:116:ASP:HB2	1:A:118:HIS:CD2	2.49	0.47
1:A:1410:PHE:C	1:A:1412:ALA:N	2.67	0.47
1:A:531:ILE:CD1	1:A:617:VAL:HG11	2.44	0.47
1:A:535:THR:HG21	1:A:616:VAL:CA	2.43	0.47
1:A:954:TRP:O	1:A:956:LEU:HG	2.14	0.47
2:B:321:GLY:C	2:B:323:VAL:H	2.17	0.47
2:B:487:THR:HG22	2:B:489:SER:N	2.24	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.47
2:B:871:THR:HG22	2:B:872:GLU:O	2.14	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.47
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.14	0.47
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.79	0.47
2:B:773:MET:SD	2:B:987:LYS:HD2	2.55	0.47
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.79	0.47
2:B:800:GLN:CB	8:J:52:THR:CG2	2.89	0.47
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.96	0.47
1:A:112:LYS:HG2	1:A:113:LEU:H	1.79	0.47
1:A:20:GLY:HA2	1:A:1413:GLY:O	2.14	0.47
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.14	0.47
1:A:816:HIS:CE1	2:B:764:SER:CB	2.89	0.47
1:A:770:VAL:HG13	1:A:822:GLU:OE1	2.15	0.47
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.86	0.47
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LYS:HE2	2:B:461:LEU:O	2.14	0.47
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.96	0.47
6:H:138:GLU:O	6:H:139:ASN:C	2.53	0.47
3:C:66:ARG:CZ	8:J:2:ILE:HG21	2.44	0.47
1:A:352:VAL:HG12	1:A:353:ILE:N	2.29	0.47
1:A:89:PRO:HG3	1:A:208:LEU:CD1	2.44	0.47
2:B:100:PRO:O	2:B:180:TYR:OH	2.31	0.47
2:B:303:TYR:HH	2:B:586:TRP:HZ3	1.62	0.47
4:E:96:PHE:CE1	4:E:100:ILE:HD11	2.50	0.47
5:F:79:ARG:HG2	5:F:146:TRP:CZ2	2.49	0.47
6:H:47:PHE:CD1	6:H:95:TYR:HB2	2.49	0.47
7:I:62:ILE:CG2	7:I:63:GLY:N	2.77	0.47
9:K:59:ALA:HA	9:K:74:ARG:O	2.15	0.47
1:A:1074:GLU:C	1:A:1076:ALA:N	2.67	0.47
1:A:376:TYR:CD2	1:A:376:TYR:C	2.87	0.47
1:A:90:VAL:HG21	1:A:296:LEU:HG	1.95	0.47
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.47
2:B:956:THR:HG21	2:B:960:GLY:HA2	1.96	0.47
9:K:47:ARG:CB	9:K:47:ARG:HH11	2.23	0.47
1:A:843:LYS:HG3	1:A:1402:PHE:HD1	1.79	0.47
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.46	0.47
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.35	0.47
2:B:217:ARG:HD2	2:B:241:ARG:NH2	2.29	0.47
3:C:258:ILE:N	3:C:258:ILE:HD12	2.30	0.47
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.50	0.47
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.45	0.47
1:A:1074:GLU:C	1:A:1076:ALA:H	2.18	0.47
1:A:1134:ILE:HD11	1:A:1321:GLY:HA3	1.96	0.47
1:A:167:CYS:C	1:A:169:ASN:H	2.18	0.47
1:A:742:ASN:O	1:A:745:GLN:HB2	2.13	0.47
1:A:804:TYR:HE1	2:B:1021:MET:CE	2.27	0.47
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.15	0.47
1:A:923:LEU:O	1:A:927:VAL:HG23	2.14	0.47
2:B:1098:MET:O	2:B:1099:VAL:C	2.53	0.47
2:B:1169:MET:SD	2:B:1201:LYS:HG2	2.54	0.47
2:B:123:THR:O	2:B:125:SER:N	2.47	0.47
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.95	0.47
2:B:324:ILE:HG23	2:B:329:THR:HB	1.96	0.47
6:H:49:VAL:CG1	6:H:50:ALA:N	2.74	0.47
2:B:294:ASP:H	7:I:12:ASN:ND2	2.13	0.47
8:J:48:ARG:HH21	8:J:49:MET:CE	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.14	0.47
1:A:443:LEU:CD2	1:A:455:MET:HB3	2.42	0.47
1:A:83:HIS:CE1	1:A:238:CYS:SG	3.08	0.47
1:A:869:GLY:O	4:E:204:THR:HG21	2.14	0.47
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.62	0.47
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.50	0.47
2:B:201:GLY:H	2:B:202:TYR:HD2	1.63	0.47
2:B:65:GLU:HG3	2:B:66:ASP:N	2.27	0.47
2:B:821:GLN:HB2	2:B:851:PHE:CE2	2.49	0.47
5:F:98:ALA:O	5:F:117:PRO:HB2	2.14	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.30	0.47
1:A:12:ARG:HD3	2:B:1218:THR:HB	1.97	0.47
1:A:1392:SER:O	1:A:1393:ASN:ND2	2.48	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.46	0.47
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.45	0.47
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.50	0.47
1:A:666:ILE:HD11	2:B:1030:LEU:CD1	2.20	0.47
2:B:1060:ARG:O	2:B:1063:GLY:N	2.45	0.47
2:B:1072:MET:HE3	2:B:1085:ILE:CD1	2.44	0.47
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.49	0.47
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.79	0.47
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.80	0.47
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.30	0.47
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.98	0.47
1:A:848:ILE:CD1	1:A:1374:VAL:HG21	2.45	0.47
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.45	0.47
1:A:53:LEU:HD13	1:A:263:THR:HG23	1.97	0.47
1:A:573:SER:OG	1:A:576:GLN:HG3	2.15	0.47
1:A:829:VAL:O	1:A:831:THR:N	2.48	0.47
2:B:640:VAL:HG12	2:B:640:VAL:O	2.15	0.47
2:B:780:VAL:HG21	8:J:56:LEU:HD11	1.97	0.47
3:C:263:THR:C	3:C:265:MET:H	2.18	0.47
7:I:54:GLU:O	7:I:89:GLN:HG2	2.15	0.47
1:A:1194:ARG:HH22	1:A:1237:ILE:HD13	1.73	0.47
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.45	0.47
1:A:87:ALA:HB3	1:A:276:LEU:CD2	2.45	0.47
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.41	0.47
2:B:1198:TYR:HE1	2:B:1201:LYS:HZ2	1.63	0.47
2:B:96:TYR:CD1	2:B:96:TYR:N	2.83	0.47
2:B:298:LEU:HD23	2:B:298:LEU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.49	0.46
2:B:906:SER:CB	2:B:946:ASN:HB2	2.45	0.46
8:J:1:MET:O	8:J:2:ILE:O	2.33	0.46
1:A:1017:LEU:O	1:A:1018:PHE:C	2.53	0.46
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.15	0.46
2:B:1106:ARG:NH1	2:B:1118:PRO:CB	2.72	0.46
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.45	0.46
2:B:851:PHE:O	2:B:974:PRO:HD3	2.15	0.46
3:C:262:LEU:O	3:C:265:MET:HB3	2.15	0.46
3:C:43:THR:HG22	3:C:44:LEU:N	2.29	0.46
5:F:101:ILE:HD11	5:F:124:GLU:OE1	2.15	0.46
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.45	0.46
1:A:329:LEU:HA	1:A:335:ARG:HB2	1.98	0.46
1:A:813:PHE:HE2	2:B:524:PRO:CG	2.15	0.46
2:B:1182:CYS:O	2:B:1183:LYS:HD2	2.15	0.46
2:B:167:ILE:HG22	2:B:167:ILE:O	2.14	0.46
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.80	0.46
2:B:864:LYS:H	2:B:872:GLU:CG	2.28	0.46
2:B:890:TYR:C	2:B:892:LYS:H	2.19	0.46
3:C:180:TYR:O	3:C:181:ASP:HB3	2.15	0.46
10:L:30:ILE:CD1	10:L:59:ALA:HA	2.44	0.46
11:M:76:UNK:O	11:M:77:UNK:O	2.33	0.46
1:A:1209:MET:CG	1:A:1236:LEU:HD22	2.45	0.46
1:A:418:SER:O	1:A:421:ALA:N	2.49	0.46
1:A:50:ILE:HG22	1:A:51:GLY:H	1.81	0.46
1:A:658:LEU:HD13	2:B:831:SER:HA	1.98	0.46
1:A:890:ASP:N	1:A:1296:GLY:HA3	2.30	0.46
1:A:964:ILE:HD13	1:A:1035:TYR:CZ	2.50	0.46
2:B:332:ASP:C	2:B:334:ILE:N	2.68	0.46
2:B:574:SER:HB3	2:B:577:ALA:HB2	1.98	0.46
2:B:805:THR:HA	2:B:809:MET:HE1	1.98	0.46
9:K:83:PRO:O	9:K:87:LEU:N	2.46	0.46
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.15	0.46
1:A:1394:THR:CG2	1:A:1395:GLY:N	2.78	0.46
1:A:530:GLY:O	1:A:531:ILE:C	2.54	0.46
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.98	0.46
1:A:893:PHE:CD1	1:A:940:ARG:HD2	2.51	0.46
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.98	0.46
2:B:1117:GLN:HG3	2:B:1156:ASP:OD1	2.16	0.46
2:B:322:PHE:CG	2:B:322:PHE:O	2.69	0.46
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.97	0.46
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.78	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.29	0.46
1:A:1405:THR:O	1:A:1406:VAL:C	2.54	0.46
1:A:666:ILE:O	1:A:667:GLY:C	2.53	0.46
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.98	0.46
2:B:300:HIS:ND1	2:B:376:PHE:CE2	2.83	0.46
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.97	0.46
2:B:758:PHE:C	2:B:760:ASP:N	2.68	0.46
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.49	0.46
3:C:5:GLY:O	3:C:6:PRO:C	2.54	0.46
4:E:56:LYS:HG3	4:E:84:ASP:CB	2.42	0.46
7:I:100:PHE:HZ	7:I:118:ARG:HH12	1.62	0.46
1:A:849:MET:HB2	1:A:1063:MET:SD	2.55	0.46
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.46
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.81	0.46
1:A:418:SER:HA	11:M:46:UNK:C	2.45	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CH2	2.48	0.46
2:B:1177:HIS:C	2:B:1179:GLN:N	2.68	0.46
2:B:230:ALA:N	2:B:231:PRO:HD2	2.31	0.46
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.50	0.46
2:B:515:HIS:O	2:B:516:ASN:C	2.54	0.46
2:B:680:THR:O	2:B:683:SER:OG	2.34	0.46
3:C:236:GLY:C	3:C:238:ILE:N	2.69	0.46
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.19	0.46
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.16	0.46
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.96	0.46
1:A:1394:THR:HG23	1:A:1398:MET:CE	2.46	0.46
1:A:517:ASN:OD1	1:A:517:ASN:O	2.34	0.46
1:A:592:ASP:N	1:A:595:THR:OG1	2.48	0.46
2:B:1051:THR:HG21	2:B:1053:GLU:HB2	1.97	0.46
2:B:914:LYS:H	2:B:938:SER:HB3	1.81	0.46
5:F:117:PRO:O	5:F:120:ILE:HB	2.16	0.46
6:H:40:LEU:HG	6:H:42:ILE:HG13	1.98	0.46
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.37	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.46
1:A:573:SER:H	1:A:576:GLN:HG3	1.81	0.46
1:A:645:LEU:O	1:A:649:ILE:HG13	2.15	0.46
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.78	0.46
2:B:282:ILE:HG13	2:B:283:VAL:N	2.31	0.46
2:B:893:LEU:HD22	2:B:897:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.16	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
3:C:252:GLN:CG	9:K:95:ILE:HG23	2.46	0.46
3:C:62:PHE:CD2	3:C:62:PHE:C	2.89	0.46
4:E:10:SER:O	4:E:14:ARG:HG3	2.16	0.46
4:E:58:MET:O	4:E:59:SER:C	2.53	0.46
9:K:91:CYS:O	9:K:94:ILE:HB	2.16	0.46
1:A:1153:TYR:CD2	7:I:41:PRO:HB2	2.51	0.46
1:A:47:ARG:O	1:A:48:ALA:HB2	2.16	0.46
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.51	0.46
1:A:709:THR:C	1:A:711:ARG:N	2.67	0.46
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.31	0.46
2:B:50:SER:O	2:B:53:GLN:HB3	2.16	0.46
2:B:704:ALA:HB2	2:B:738:PHE:CE1	2.51	0.46
3:C:173:ALA:O	3:C:174:ALA:CB	2.64	0.46
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.97	0.46
9:K:113:THR:O	9:K:114:LEU:CB	2.47	0.46
9:K:73:LEU:CD2	9:K:75:ILE:HD11	2.46	0.46
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.97	0.45
1:A:112:LYS:HG2	1:A:113:LEU:N	2.31	0.45
1:A:420:ARG:O	1:A:424:ILE:HG13	2.16	0.45
1:A:814:PHE:CE1	2:B:519:TRP:N	2.83	0.45
2:B:1158:PHE:HE2	2:B:1201:LYS:HE3	1.80	0.45
2:B:361:LEU:N	2:B:362:PRO:HD2	2.31	0.45
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.97	0.45
6:H:101:ALA:HB2	6:H:116:TYR:CD2	2.51	0.45
7:I:75:CYS:O	7:I:76:PRO:C	2.52	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.45
1:A:542:GLU:C	1:A:546:VAL:HG23	2.36	0.45
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.44	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
2:B:345:LYS:O	2:B:347:LYS:N	2.49	0.45
2:B:25:ILE:HD11	2:B:653:VAL:CB	2.46	0.45
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.98	0.45
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.78	0.45
4:E:190:LEU:HD11	4:E:196:VAL:HG11	1.98	0.45
4:E:94:LYS:O	4:E:98:ILE:HG13	2.16	0.45
6:H:98:TYR:O	6:H:118:PHE:HD2	1.99	0.45
8:J:5:VAL:O	8:J:6:ARG:HB2	2.15	0.45
2:B:887:HIS:CD2	11:M:37:UNK:O	2.39	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.98	0.45
1:A:50:ILE:C	1:A:52:GLY:N	2.69	0.45
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.99	0.45
1:A:666:ILE:HG13	1:A:666:ILE:H	1.33	0.45
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.15	0.45
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.36	0.45
2:B:1154:ALA:O	2:B:1155:SER:CB	2.63	0.45
2:B:260:GLY:HA3	2:B:267:ARG:HG2	1.98	0.45
2:B:589:VAL:HG12	2:B:590:HIS:H	1.81	0.45
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.46	0.45
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.47	0.45
3:C:120:ILE:HD11	3:C:130:GLY:O	2.17	0.45
6:H:116:TYR:HE2	6:H:140:ALA:CB	2.30	0.45
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.46	0.45
7:I:29:CYS:O	7:I:31:THR:N	2.49	0.45
1:A:1147:THR:HB	7:I:48:LEU:HD11	1.98	0.45
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	1.98	0.45
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.31	0.45
1:A:337:ARG:CD	1:A:839:ARG:HH22	2.29	0.45
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.31	0.45
2:B:100:PRO:HA	2:B:125:SER:O	2.17	0.45
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.82	0.45
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.45
7:I:34:TYR:O	7:I:35:VAL:CG2	2.65	0.45
9:K:12:LEU:CD1	9:K:12:LEU:H	2.23	0.45
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.49	0.45
1:A:388:LEU:O	1:A:392:VAL:HG23	2.17	0.45
1:A:545:GLN:O	1:A:546:VAL:C	2.55	0.45
1:A:337:ARG:CZ	1:A:839:ARG:HH12	2.26	0.45
1:A:994:GLN:HE21	1:A:1019:CYS:CB	2.26	0.45
2:B:977:GLY:C	2:B:1099:VAL:HG23	2.37	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:CG1	2.46	0.45
2:B:370:PHE:N	2:B:371:GLU:OE1	2.50	0.45
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.99	0.45
2:B:542:MET:HG3	2:B:747:MET:CE	2.39	0.45
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.81	0.45
1:A:738:LYS:NZ	3:C:194:GLU:CA	2.79	0.45
4:E:179:GLN:OE1	4:E:179:GLN:HA	2.16	0.45
7:I:99:LEU:HB2	7:I:112:SER:CB	2.46	0.45
1:A:701:LEU:HA	7:I:115:LYS:HE3	1.98	0.45
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.32	0.45
1:A:1336:MET:SD	1:A:1381:LEU:HG	2.56	0.45
1:A:210:ILE:O	1:A:214:ILE:HG13	2.17	0.45
1:A:223:GLY:HA3	1:A:1415:SER:HB3	1.98	0.45
1:A:540:PHE:C	1:A:541:ILE:HD12	2.35	0.45
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.98	0.45
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.45	0.45
2:B:295:GLY:O	2:B:299:GLU:HG3	2.16	0.45
2:B:276:ILE:HD13	2:B:334:ILE:CG2	2.47	0.45
2:B:405:ARG:HD2	2:B:631:GLY:O	2.17	0.45
2:B:745:PRO:C	2:B:747:MET:N	2.70	0.45
11:M:40:UNK:C	11:M:41:UNK:O	2.45	0.45
1:A:960:ILE:HD12	1:A:1021:LEU:HD21	1.99	0.45
1:A:1114:PRO:O	1:A:1330:ASN:OD1	2.35	0.45
1:A:336:ILE:CD1	1:A:1405:THR:HG21	2.44	0.45
1:A:233:TRP:O	1:A:235:ILE:N	2.50	0.45
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.98	0.45
2:B:316:PRO:HA	2:B:319:GLU:HG2	1.98	0.45
2:B:276:ILE:HD13	2:B:334:ILE:HG23	1.99	0.45
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.64	0.45
3:C:18:VAL:O	3:C:18:VAL:HG12	2.15	0.45
6:H:111:LEU:HA	6:H:127:GLY:O	2.17	0.45
9:K:61:TYR:CD1	9:K:61:TYR:C	2.89	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.17	0.45
2:B:1149:GLU:HG3	2:B:1153:GLU:OE1	2.17	0.45
2:B:653:VAL:C	2:B:654:ARG:HG2	2.36	0.45
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.45
4:E:112:TYR:CE2	4:E:134:THR:HB	2.51	0.45
4:E:147:HIS:CD2	4:E:149:LEU:H	2.35	0.45
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.45
7:I:34:TYR:O	7:I:35:VAL:HG23	2.16	0.45
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.45
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.99	0.45
2:B:1200:ALA:O	2:B:1201:LYS:C	2.54	0.45
2:B:168:GLY:H	2:B:450:ALA:HB1	1.82	0.45
2:B:332:ASP:O	2:B:334:ILE:N	2.50	0.45
2:B:957:ASN:O	2:B:958:GLN:C	2.55	0.45
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.16	0.45
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.99	0.45
3:C:8:VAL:CG1	3:C:9:LYS:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.98	0.45
1:A:1144:LYS:O	7:I:48:LEU:HD13	2.17	0.45
1:A:1153:TYR:CZ	7:I:42:LEU:HD12	2.51	0.45
1:A:541:ILE:HG12	1:A:549:MET:HE3	1.99	0.45
1:A:55:ASP:HB3	1:A:56:PRO:HD3	1.98	0.45
1:A:84:ILE:HG23	1:A:84:ILE:O	2.17	0.45
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.98	0.45
2:B:1060:ARG:C	2:B:1062:HIS:N	2.69	0.45
2:B:130:VAL:CG1	2:B:131:ASP:H	2.29	0.45
2:B:365:THR:CG2	2:B:367:LEU:H	2.30	0.45
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.47	0.45
3:C:148:ARG:HD3	3:C:149:LYS:H	1.83	0.45
4:E:102:GLU:C	4:E:104:ASN:H	2.20	0.45
4:E:205:SER:O	4:E:206:GLY:C	2.54	0.45
6:H:114:VAL:O	6:H:124:ARG:HA	2.16	0.45
1:A:1049:ILE:O	1:A:1050:GLU:C	2.56	0.44
1:A:1410:PHE:C	1:A:1412:ALA:H	2.19	0.44
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.98	0.44
1:A:821:ARG:HG2	2:B:512:ARG:O	2.17	0.44
1:A:845:LEU:O	1:A:848:ILE:HG13	2.17	0.44
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.44
2:B:1038:SER:HB3	2:B:1062:HIS:NE2	2.33	0.44
2:B:1169:MET:HE3	2:B:1205:GLN:HG2	1.98	0.44
2:B:185:THR:H	2:B:188:ASP:HB2	1.81	0.44
2:B:519:TRP:HE1	2:B:635:ARG:HH22	1.64	0.44
6:H:5:LEU:O	6:H:133:ASN:HB3	2.17	0.44
7:I:8:ARG:HG3	7:I:9:ASP:CG	2.37	0.44
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.47	0.44
1:A:829:VAL:C	1:A:831:THR:N	2.70	0.44
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	3.00	0.44
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.17	0.44
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.35	0.44
2:B:101:MET:HE2	2:B:169:ARG:HH12	1.83	0.44
2:B:247:GLY:O	2:B:248:SER:HB3	2.17	0.44
2:B:288:ALA:HA	2:B:331:LEU:HD13	1.99	0.44
2:B:371:GLU:N	2:B:371:GLU:OE1	2.49	0.44
2:B:781:PHE:CE2	2:B:795:ILE:HD11	2.53	0.44
2:B:915:THR:HG21	2:B:934:LYS:HG2	2.00	0.44
3:C:166:GLU:CG	9:K:10:PHE:CZ	2.96	0.44
4:E:137:GLU:O	4:E:140:LEU:N	2.43	0.44
6:H:49:VAL:CG1	6:H:50:ALA:H	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.98	0.44
7:I:10:CYS:SG	7:I:29:CYS:SG	3.12	0.44
9:K:10:PHE:CE1	9:K:11:LEU:HD13	2.49	0.44
10:L:61:THR:HG22	10:L:62:LYS:N	2.33	0.44
11:M:79:UNK:O	11:M:84:UNK:CA	2.65	0.44
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.17	0.44
1:A:1409:LEU:HA	1:A:1409:LEU:HD23	1.84	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.52	0.44
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.46	0.44
1:A:815:PHE:O	1:A:818:MET:N	2.50	0.44
1:A:885:THR:HG23	1:A:893:PHE:CE1	2.36	0.44
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.53	0.44
1:A:778:GLY:HA3	2:B:516:ASN:CB	2.46	0.44
2:B:549:THR:H	2:B:628:THR:HG22	1.81	0.44
2:B:690:VAL:HG12	2:B:691:GLU:N	2.32	0.44
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.38	0.44
2:B:864:LYS:HD3	2:B:871:THR:CB	2.47	0.44
7:I:106:CYS:O	7:I:107:SER:HB2	2.18	0.44
10:L:43:THR:HG22	10:L:43:THR:O	2.18	0.44
1:A:1046:LEU:O	1:A:1047:SER:C	2.55	0.44
1:A:1347:ALA:O	1:A:1348:LEU:C	2.55	0.44
1:A:1415:SER:O	1:A:1416:ALA:C	2.55	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	2.00	0.44
1:A:78:PRO:O	1:A:79:GLY:C	2.56	0.44
1:A:825:ILE:C	1:A:827:THR:N	2.70	0.44
2:B:566:LEU:CD1	2:B:588:GLY:HA2	2.43	0.44
2:B:707:PRO:O	2:B:708:GLU:O	2.35	0.44
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.30	0.44
2:B:847:ASP:O	3:C:65:HIS:HE1	2.01	0.44
4:E:138:ALA:C	4:E:140:LEU:H	2.21	0.44
4:E:185:ALA:CB	4:E:190:LEU:HD12	2.47	0.44
7:I:92:ARG:CG	7:I:93:LYS:H	2.30	0.44
8:J:32:GLU:CD	8:J:32:GLU:H	2.19	0.44
1:A:850:VAL:O	1:A:1060:PRO:HA	2.18	0.44
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.32	0.44
1:A:69:THR:O	2:B:1174:LYS:HG2	2.17	0.44
1:A:340:LEU:CD2	2:B:1200:ALA:HB2	2.46	0.44
2:B:361:LEU:O	2:B:363:HIS:O	2.35	0.44
2:B:377:PHE:C	2:B:379:GLY:N	2.68	0.44
2:B:664:THR:HG1	2:B:678:GLU:N	2.14	0.44
4:E:133:GLU:HB3	4:E:135:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:C	5:F:113:GLY:N	2.71	0.44
6:H:84:ALA:CA	6:H:87:ARG:HB2	2.48	0.44
7:I:74:GLU:OE1	7:I:79:HIS:ND1	2.47	0.44
1:A:401:GLY:H	1:A:435:HIS:HD2	1.66	0.44
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.39	0.44
1:A:54:ASN:O	1:A:55:ASP:HB2	2.18	0.44
1:A:742:ASN:C	1:A:745:GLN:HB2	2.38	0.44
1:A:881:GLN:NE2	1:A:958:VAL:O	2.46	0.44
1:A:373:THR:HG21	2:B:1105:ALA:O	2.18	0.44
2:B:216:GLU:OE1	2:B:537:LYS:CE	2.66	0.44
2:B:230:ALA:O	2:B:232:SER:N	2.47	0.44
2:B:446:LEU:HD23	2:B:446:LEU:N	2.33	0.44
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.53	0.44
1:A:525:GLN:HB2	2:B:835:GLN:HG2	2.00	0.44
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.63	0.44
3:C:62:PHE:C	3:C:62:PHE:HD2	2.20	0.44
1:A:1121:GLU:O	1:A:1122:PRO:C	2.56	0.44
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.44
1:A:644:LYS:O	1:A:645:LEU:C	2.55	0.44
1:A:901:LEU:HD13	1:A:919:ILE:CG2	2.48	0.44
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.70	0.44
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.31	0.44
2:B:315:LYS:O	2:B:318:VAL:N	2.46	0.44
2:B:642:ASP:O	2:B:643:ASP:C	2.56	0.44
6:H:57:VAL:HG12	6:H:58:THR:N	2.32	0.44
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.17	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:OE1	2.17	0.44
1:A:412:ARG:CZ	2:B:1108:ARG:NH2	2.81	0.44
2:B:1106:ARG:HG2	2:B:1107:ALA:N	2.31	0.44
2:B:1171:VAL:HG13	2:B:1191:ILE:HD13	1.99	0.44
2:B:562:GLY:O	2:B:563:MET:C	2.56	0.44
4:E:9:ILE:C	4:E:11:ARG:N	2.71	0.44
9:K:24:ASP:HB3	9:K:30:ALA:CB	2.47	0.44
1:A:968:GLN:NE2	1:A:1035:TYR:HB2	2.32	0.44
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.99	0.44
1:A:148:CYS:HB3	1:A:167:CYS:O	2.18	0.44
1:A:494:SER:HB2	1:A:497:THR:OG1	2.18	0.44
1:A:595:THR:HG22	1:A:596:THR:N	2.33	0.44
1:A:825:ILE:HD11	2:B:512:ARG:C	2.36	0.44
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1103:ILE:O	2:B:1104:HIS:C	2.56	0.44
2:B:1159:ARG:NE	2:B:1193:GLN:NE2	2.33	0.44
2:B:1175:LEU:O	2:B:1176:ASN:CG	2.56	0.44
2:B:194:GLU:HA	2:B:194:GLU:OE1	2.18	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.32	0.44
1:A:810:PRO:C	2:B:519:TRP:HZ3	2.21	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG12	2.00	0.44
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.48	0.44
2:B:864:LYS:HD3	2:B:871:THR:CA	2.47	0.44
2:B:904:ARG:CZ	2:B:948:ILE:HD11	2.48	0.44
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.44
3:C:135:GLN:C	3:C:136:ASP:O	2.56	0.44
4:E:82:PHE:N	4:E:82:PHE:CD1	2.85	0.44
1:A:709:THR:HG23	7:I:94:ASP:HA	2.00	0.44
9:K:78:THR:O	9:K:79:GLU:C	2.56	0.44
1:A:834:THR:HG21	1:A:1077:THR:HA	2.00	0.43
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.18	0.43
1:A:306:ASN:OD1	1:A:313:GLN:NE2	2.51	0.43
1:A:458:HIS:ND1	1:A:507:VAL:HG21	2.32	0.43
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.00	0.43
2:B:274:PRO:O	2:B:276:ILE:N	2.51	0.43
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.52	0.43
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.77	0.43
3:C:9:LYS:HB2	3:C:21:ILE:HB	1.99	0.43
4:E:7:ARG:C	4:E:9:ILE:N	2.71	0.43
7:I:50:THR:HG22	7:I:52:ILE:N	2.33	0.43
10:L:38:LEU:HG	10:L:39:SER:H	1.82	0.43
1:A:1068:ALA:O	1:A:1069:ALA:C	2.55	0.43
1:A:852:TYR:CE2	5:F:136:ARG:NE	2.86	0.43
2:B:1002:THR:CG2	2:B:1004:GLU:HB2	2.47	0.43
2:B:200:GLY:HA2	2:B:202:TYR:CD2	2.50	0.43
2:B:426:LYS:O	2:B:430:ARG:HG3	2.17	0.43
2:B:912:ILE:O	2:B:938:SER:CB	2.59	0.43
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.43
3:C:39:ALA:HA	3:C:164:ALA:CB	2.46	0.43
3:C:59:ALA:O	3:C:63:ILE:HG13	2.19	0.43
4:E:138:ALA:O	4:E:140:LEU:N	2.50	0.43
5:F:89:GLU:HB3	5:F:134:ILE:HD13	2.01	0.43
9:K:24:ASP:OD1	9:K:26:LYS:N	2.51	0.43
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.47	0.43
1:A:13:THR:HG23	1:A:1432:GLN:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.43
1:A:614:PHE:C	1:A:614:PHE:CD1	2.92	0.43
1:A:679:ILE:O	1:A:682:THR:HB	2.18	0.43
2:B:1118:PRO:HD3	2:B:1155:SER:HA	2.00	0.43
2:B:205:ILE:HG12	2:B:461:LEU:HB3	1.99	0.43
2:B:995:ARG:HH11	2:B:995:ARG:HB2	1.81	0.43
3:C:8:VAL:HA	3:C:21:ILE:O	2.18	0.43
3:C:249:ASP:OD1	3:C:253:LYS:HE3	2.19	0.43
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.47	0.43
3:C:76:ASP:OD2	3:C:128:ASN:N	2.47	0.43
6:H:5:LEU:O	6:H:6:PHE:HB2	2.19	0.43
9:K:55:LYS:HD3	9:K:78:THR:OG1	2.18	0.43
10:L:45:ALA:O	10:L:46:VAL:CG2	2.64	0.43
1:A:1066:VAL:O	1:A:1067:LEU:C	2.56	0.43
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.39	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.43
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.48	0.43
1:A:633:VAL:HG11	1:A:645:LEU:HD22	2.00	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.71	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
2:B:202:TYR:CD2	2:B:202:TYR:N	2.87	0.43
2:B:329:THR:O	2:B:332:ASP:HB3	2.18	0.43
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.53	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.43
7:I:75:CYS:C	7:I:77:LYS:H	2.20	0.43
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.51	0.43
1:A:113:LEU:HG	1:A:218:ASP:OD1	2.19	0.43
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.52	0.43
2:B:1152:MET:SD	2:B:1197:PRO:HD3	2.59	0.43
2:B:214:ALA:HB2	2:B:408:LEU:CD1	2.48	0.43
2:B:686:ASN:C	2:B:688:GLY:N	2.70	0.43
2:B:708:GLU:C	2:B:710:LEU:N	2.72	0.43
2:B:800:GLN:CB	8:J:52:THR:HG22	2.47	0.43
3:C:251:LEU:HG	9:K:98:LEU:HD11	2.01	0.43
3:C:73:GLN:HE21	3:C:75:MET:N	1.97	0.43
4:E:168:TYR:CB	4:E:170:LEU:HG	2.49	0.43
7:I:84:VAL:CG1	7:I:84:VAL:O	2.65	0.43
1:A:1384:VAL:O	1:A:1389:PHE:HE2	2.01	0.43
1:A:535:THR:HG22	1:A:616:VAL:HA	1.98	0.43
1:A:534:LEU:HD13	1:A:656:TRP:CD1	2.54	0.43
2:B:287:ARG:HG2	2:B:292:ILE:CA	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:GLU:HG2	2:B:654:ARG:NH1	2.33	0.43
4:E:114:ASN:O	4:E:115:ASN:HB3	2.18	0.43
4:E:28:TYR:CE2	4:E:64:PRO:HG3	2.53	0.43
6:H:24:CYS:CB	6:H:44:VAL:HG21	2.47	0.43
7:I:91:ARG:HD3	7:I:91:ARG:HA	1.75	0.43
8:J:53:HIS:CE1	8:J:55:ASP:HA	2.54	0.43
9:K:92:ASN:O	9:K:93:SER:C	2.56	0.43
1:A:86:LEU:HB3	1:A:296:LEU:HD21	2.00	0.43
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.99	0.43
1:A:35:ILE:HD13	1:A:53:LEU:HD23	2.01	0.43
1:A:565:ILE:HD13	1:A:567:LYS:HE2	2.01	0.43
1:A:741:ASN:HD22	1:A:743:VAL:N	2.16	0.43
1:A:845:LEU:O	1:A:846:GLU:C	2.57	0.43
2:B:1204:PHE:O	2:B:1207:LEU:HB2	2.19	0.43
2:B:366:GLN:O	2:B:367:LEU:O	2.36	0.43
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.71	0.43
2:B:487:THR:O	2:B:488:TYR:C	2.56	0.43
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.53	0.43
2:B:784:ASN:HD21	2:B:788:ARG:HD2	1.84	0.43
2:B:806:THR:C	2:B:808:ALA:N	2.71	0.43
2:B:955:THR:HA	10:L:54:ARG:O	2.19	0.43
3:C:135:GLN:O	3:C:136:ASP:O	2.37	0.43
6:H:143:LEU:HD12	6:H:143:LEU:N	2.34	0.43
7:I:55:THR:HG21	7:I:109:ILE:CD1	2.48	0.43
1:A:1155:ASP:O	1:A:1190:PRO:O	2.37	0.43
1:A:131:SER:OG	1:A:132:LYS:N	2.51	0.43
1:A:446:ARG:HG2	1:A:446:ARG:NH1	2.28	0.43
1:A:42:ASP:OD1	1:A:45:GLN:O	2.36	0.43
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.43
2:B:1108:ARG:O	2:B:1108:ARG:CG	2.67	0.43
2:B:345:LYS:N	2:B:348:ARG:HE	2.15	0.43
2:B:55:VAL:O	2:B:59:LEU:HB3	2.19	0.43
2:B:834:ASN:HB2	2:B:838:SER:O	2.19	0.43
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.43
3:C:77:ILE:CG2	3:C:161:LYS:HE3	2.48	0.43
7:I:46:HIS:O	7:I:47:GLU:HB2	2.18	0.43
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.13	0.43
1:A:166:GLY:O	1:A:167:CYS:CB	2.67	0.43
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.00	0.43
1:A:562:THR:HA	1:A:563:PRO:HD3	1.92	0.43
1:A:639:PRO:HG2	1:A:640:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLY:N	1:A:674:PRO:HD2	2.34	0.43
1:A:760:GLN:HB2	2:B:1021:MET:HE1	2.00	0.43
1:A:774:ARG:O	1:A:775:ILE:C	2.57	0.43
2:B:101:MET:HE3	2:B:169:ARG:NH2	2.34	0.43
2:B:666:TYR:C	2:B:668:ASP:N	2.72	0.43
2:B:794:ASN:O	2:B:795:ILE:HD12	2.19	0.43
2:B:850:LEU:CD2	2:B:1009:ASP:HB3	2.48	0.43
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.83	0.43
4:E:69:ILE:O	4:E:73:PRO:HG3	2.19	0.43
4:E:79:TRP:HD1	4:E:96:PHE:HE1	1.67	0.43
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.83	0.43
7:I:98:VAL:CG1	7:I:99:LEU:N	2.81	0.43
8:J:9:SER:HB2	8:J:45:CYS:HB2	2.01	0.43
9:K:95:ILE:O	9:K:98:LEU:HB2	2.19	0.43
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.43
1:A:1193:LEU:CD2	1:A:1267:MET:HE2	2.48	0.43
1:A:326:ARG:HE	1:A:1406:VAL:HG11	1.82	0.43
2:B:877:PRO:O	2:B:878:GLN:HG2	2.19	0.43
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.31	0.43
3:C:148:ARG:H	3:C:151:GLN:HG3	1.84	0.43
3:C:5:GLY:O	3:C:6:PRO:O	2.37	0.43
11:M:65:UNK:CA	11:M:78:UNK:O	2.67	0.43
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.83	0.42
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.45	0.42
1:A:48:ALA:O	1:A:49:LYS:CG	2.65	0.42
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.01	0.42
1:A:711:ARG:HA	7:I:97:MET:HE1	2.01	0.42
1:A:760:GLN:CB	2:B:1021:MET:HE1	2.49	0.42
1:A:901:LEU:HG	1:A:926:GLN:NE2	2.30	0.42
1:A:984:LYS:O	1:A:988:LEU:HB2	2.19	0.42
1:A:99:ILE:O	1:A:102:VAL:HB	2.19	0.42
2:B:295:GLY:H	2:B:298:LEU:HG	1.84	0.42
2:B:358:LYS:O	2:B:359:GLU:OE1	2.36	0.42
2:B:546:SER:OG	2:B:631:GLY:N	2.52	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.67	0.42
6:H:38:LEU:HD13	6:H:125:LEU:CD1	2.46	0.42
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.31	0.42
2:B:955:THR:CG2	10:L:54:ARG:O	2.65	0.42
1:A:1348:LEU:CD2	1:A:1372:VAL:HG13	2.39	0.42
1:A:151:ASP:OD1	1:A:163:SER:HA	2.19	0.42
1:A:337:ARG:NE	1:A:839:ARG:NH2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:HB2	1:A:454:SER:OG	2.19	0.42
1:A:466:SER:HB3	9:K:2:ASN:HD22	1.82	0.42
1:A:672:ASP:O	1:A:675:THR:HB	2.19	0.42
1:A:814:PHE:HB2	2:B:519:TRP:CE3	2.52	0.42
2:B:1177:HIS:O	2:B:1179:GLN:HG3	2.19	0.42
2:B:705:MET:N	2:B:710:LEU:HD12	2.34	0.42
2:B:709:ASP:C	2:B:710:LEU:HD23	2.38	0.42
4:E:113:GLN:HG2	4:E:137:GLU:OE1	2.18	0.42
4:E:137:GLU:O	4:E:138:ALA:C	2.57	0.42
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.53	0.42
6:H:84:ALA:CB	6:H:87:ARG:HB2	2.49	0.42
1:A:134:ARG:O	1:A:137:ALA:N	2.52	0.42
1:A:30:ILE:O	1:A:31:SER:O	2.37	0.42
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.42
1:A:68:GLN:O	1:A:70:CYS:N	2.52	0.42
1:A:751:SER:O	1:A:752:LYS:CB	2.67	0.42
1:A:853:ASP:OD1	1:A:855:THR:CB	2.64	0.42
2:B:1177:HIS:C	2:B:1179:GLN:H	2.22	0.42
2:B:1177:HIS:O	2:B:1179:GLN:N	2.52	0.42
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.00	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.18	0.42
2:B:484:ASN:CG	2:B:486:TYR:HE1	2.23	0.42
2:B:702:LEU:HD22	2:B:737:THR:CG2	2.49	0.42
2:B:749:LEU:HD22	2:B:753:ALA:CB	2.49	0.42
2:B:806:THR:O	2:B:808:ALA:N	2.53	0.42
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.54	0.42
7:I:59:VAL:HG12	7:I:60:GLN:N	2.34	0.42
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.18	0.42
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.16	0.42
1:A:457:ALA:O	1:A:507:VAL:HG23	2.19	0.42
1:A:813:PHE:CE2	2:B:524:PRO:CG	2.97	0.42
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.49	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.42
2:B:705:MET:H	2:B:710:LEU:CD1	2.32	0.42
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.55	0.42
3:C:101:LEU:HD12	3:C:101:LEU:HA	1.89	0.42
4:E:117:THR:C	4:E:119:SER:N	2.73	0.42
4:E:178:ILE:CG2	4:E:214:CYS:HA	2.48	0.42
5:F:140:ASP:OD1	5:F:141:GLY:N	2.52	0.42
6:H:111:LEU:HD23	6:H:127:GLY:O	2.18	0.42
11:M:63:UNK:N	11:M:64:UNK:N	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:C	1:A:401:GLY:N	2.71	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.54	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:N	2.44	0.42
2:B:105:SER:O	2:B:106:ASP:HB2	2.20	0.42
2:B:368:GLU:O	2:B:371:GLU:OE1	2.37	0.42
2:B:34:ILE:HG12	2:B:542:MET:CE	2.49	0.42
2:B:601:ARG:O	2:B:605:ARG:HG3	2.19	0.42
2:B:640:VAL:HG22	2:B:651:LEU:HD23	2.01	0.42
2:B:955:THR:HG1	10:L:55:ILE:HA	1.83	0.42
6:H:83:GLN:C	6:H:85:GLY:N	2.73	0.42
7:I:103:CYS:HG	7:I:106:CYS:HG	1.67	0.42
1:A:474:VAL:O	1:A:474:VAL:HG13	2.19	0.42
1:A:541:ILE:N	1:A:541:ILE:HD12	2.34	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.52	0.42
1:A:89:PRO:HG3	1:A:208:LEU:HD12	2.00	0.42
1:A:982:THR:HB	1:A:985:ASP:CG	2.40	0.42
2:B:1106:ARG:HH12	2:B:1118:PRO:CA	2.33	0.42
2:B:1106:ARG:HH12	2:B:1118:PRO:HA	1.85	0.42
1:A:810:PRO:HG3	2:B:745:PRO:HB2	2.01	0.42
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.83	0.42
2:B:864:LYS:CG	2:B:865:LYS:N	2.80	0.42
2:B:969:ARG:HG2	2:B:970:THR:N	2.33	0.42
9:K:98:LEU:O	9:K:99:GLY:C	2.58	0.42
10:L:27:LEU:HD13	10:L:37:LYS:CB	2.48	0.42
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.42
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.17	0.42
1:A:591:PHE:HD2	1:A:595:THR:HB	1.83	0.42
1:A:709:THR:O	1:A:712:GLU:N	2.52	0.42
1:A:960:ILE:O	1:A:961:ARG:C	2.57	0.42
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.85	0.42
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.19	0.42
4:E:59:SER:HA	4:E:80:VAL:O	2.19	0.42
6:H:12:VAL:HG13	6:H:26:ILE:HG23	2.01	0.42
6:H:96:VAL:HG13	6:H:143:LEU:HG	2.02	0.42
6:H:4:THR:O	6:H:5:LEU:HD23	2.19	0.42
7:I:101:PHE:HD1	7:I:110:PHE:O	2.02	0.42
9:K:82:ASP:O	9:K:85:ASP:HB2	2.20	0.42
1:A:1126:ALA:O	1:A:1128:GLN:N	2.53	0.42
1:A:1152:ILE:C	7:I:43:VAL:HB	2.39	0.42
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	2.20	0.42
1:A:568:PRO:CB	3:C:221:TYR:CZ	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:C	1:A:70:CYS:N	2.73	0.42
1:A:725:ALA:HA	1:A:728:LYS:HE2	2.02	0.42
1:A:866:PHE:C	1:A:867:ILE:HG13	2.40	0.42
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.55	0.42
2:B:995:ARG:CB	2:B:995:ARG:HH11	2.33	0.42
8:J:21:TYR:CA	8:J:39:LEU:HD11	2.49	0.42
8:J:53:HIS:CD2	8:J:54:VAL:N	2.88	0.42
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.49	0.42
1:A:1187:GLN:HA	1:A:1243:VAL:HG23	2.02	0.42
1:A:1192:LEU:HD11	1:A:1239:ARG:CB	2.37	0.42
1:A:366:VAL:HA	1:A:367:PRO:HD2	1.81	0.42
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.49	0.42
1:A:481:ASP:C	1:A:481:ASP:OD1	2.58	0.42
1:A:530:GLY:O	1:A:532:ARG:N	2.53	0.42
1:A:533:LYS:C	1:A:535:THR:H	2.23	0.42
1:A:751:SER:OG	2:B:1015:HIS:HE1	2.03	0.42
1:A:810:PRO:CB	2:B:705:MET:SD	3.08	0.42
2:B:542:MET:HE2	2:B:747:MET:HE2	2.01	0.42
2:B:54:PHE:HA	2:B:58:THR:CB	2.47	0.42
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.84	0.42
2:B:887:HIS:HD2	11:M:37:UNK:O	1.47	0.42
3:C:214:ASN:CB	3:C:217:ASP:OD2	2.68	0.42
4:E:131:THR:HG21	4:E:191:LYS:HE2	2.02	0.42
4:E:168:TYR:O	4:E:170:LEU:HD23	2.19	0.42
4:E:19:VAL:O	4:E:19:VAL:HG12	2.20	0.42
9:K:103:THR:O	9:K:106:GLU:N	2.53	0.42
9:K:93:SER:O	9:K:97:LYS:HG3	2.20	0.42
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.18	0.42
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42
1:A:1317:MET:CA	1:A:1322:ILE:HD11	2.46	0.42
1:A:114:LEU:HD12	1:A:142:CYS:O	2.18	0.42
1:A:401:GLY:N	1:A:435:HIS:HD2	2.18	0.42
1:A:76:GLU:O	1:A:78:PRO:CD	2.68	0.42
1:A:80:HIS:N	1:A:243:PRO:HB3	2.34	0.42
2:B:276:ILE:HD11	2:B:355:ILE:CD1	2.50	0.42
2:B:346:GLU:O	2:B:347:LYS:C	2.58	0.42
2:B:499:ASN:OD1	2:B:500:THR:N	2.53	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.95	0.42
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.55	0.42
2:B:879:ARG:O	2:B:880:THR:HB	2.20	0.42
3:C:27:LEU:HD12	3:C:27:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	3:C:75:MET:H	1.97	0.42
1:A:782:ARG:NH2	7:I:67:THR:HG22	2.34	0.42
9:K:71:PHE:CD1	9:K:71:PHE:C	2.93	0.42
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.18	0.41
1:A:1349:TYR:O	1:A:1350:LYS:C	2.56	0.41
1:A:843:LYS:HA	1:A:843:LYS:HD3	1.90	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.34	0.41
4:E:28:TYR:CE1	4:E:78:LEU:CD1	3.03	0.41
6:H:57:VAL:CG1	6:H:58:THR:N	2.83	0.41
7:I:63:GLY:O	7:I:70:ARG:NH2	2.53	0.41
3:C:14:SER:HA	9:K:114:LEU:HD22	2.02	0.41
1:A:108:MET:O	1:A:109:HIS:CB	2.66	0.41
1:A:115:LEU:HB2	1:A:122:MET:HE1	2.02	0.41
1:A:1366:ARG:HH11	1:A:1366:ARG:HG2	1.84	0.41
1:A:14:VAL:O	1:A:15:LYS:HD3	2.20	0.41
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.41
1:A:335:ARG:HA	1:A:335:ARG:HD3	1.87	0.41
1:A:474:VAL:HG13	1:A:478:TYR:HE1	1.86	0.41
1:A:533:LYS:C	1:A:535:THR:N	2.72	0.41
1:A:598:LEU:HD22	6:H:25:ARG:CZ	2.50	0.41
1:A:629:LEU:CD1	1:A:645:LEU:HD21	2.48	0.41
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.34	0.41
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.01	0.41
2:B:269:ILE:HB	2:B:317:CYS:SG	2.60	0.41
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.34	0.41
2:B:737:THR:HG23	7:I:66:PRO:HB3	2.01	0.41
2:B:843:GLN:HB2	2:B:993:THR:OG1	2.20	0.41
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.85	0.41
3:C:242:GLN:O	3:C:246:ARG:N	2.52	0.41
8:J:34:THR:O	8:J:35:ALA:C	2.58	0.41
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.34	0.41
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.19	0.41
1:A:1438:THR:CG2	5:F:92:ARG:HD2	2.50	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.55	0.41
1:A:530:GLY:O	1:A:533:LYS:N	2.53	0.41
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.84	0.41
1:A:960:ILE:HD12	1:A:1021:LEU:CD2	2.50	0.41
2:B:850:LEU:HD22	2:B:1009:ASP:HB3	2.01	0.41
2:B:913:GLY:HA2	2:B:938:SER:HB2	2.02	0.41
3:C:252:GLN:NE2	9:K:99:GLY:N	2.68	0.41
8:J:3:VAL:CG2	8:J:18:TRP:CG	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:35:PHE:O	9:K:70:ARG:HB2	2.21	0.41
10:L:41:SER:O	10:L:44:ASP:HB2	2.21	0.41
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.60	0.41
1:A:683:ILE:O	1:A:686:ALA:N	2.53	0.41
1:A:84:ILE:HG21	1:A:239:LEU:HD23	2.01	0.41
2:B:199:MET:N	2:B:199:MET:SD	2.87	0.41
2:B:315:LYS:O	2:B:317:CYS:N	2.53	0.41
2:B:435:THR:O	2:B:435:THR:HG22	2.20	0.41
2:B:53:GLN:HG2	2:B:547:VAL:HG13	2.02	0.41
2:B:880:THR:O	2:B:881:ASN:HB2	2.19	0.41
4:E:71:LYS:C	4:E:73:PRO:HD3	2.40	0.41
5:F:138:LEU:HD23	5:F:138:LEU:HA	1.82	0.41
6:H:84:ALA:HA	6:H:87:ARG:CB	2.50	0.41
7:I:84:VAL:HG13	7:I:84:VAL:O	2.19	0.41
7:I:98:VAL:HG12	7:I:99:LEU:N	2.35	0.41
8:J:52:THR:CG2	8:J:52:THR:O	2.68	0.41
2:B:120:ARG:HH12	10:L:54:ARG:NH1	2.18	0.41
1:A:419:LYS:HG2	11:M:46:UNK:O	2.19	0.41
1:A:101:LYS:HG2	1:A:139:TRP:CZ2	2.55	0.41
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.19	0.41
1:A:1322:ILE:HD12	1:A:1327:ILE:HD12	2.03	0.41
1:A:134:ARG:O	1:A:136:ALA:N	2.53	0.41
1:A:908:LEU:O	1:A:909:ASP:C	2.58	0.41
1:A:913:LEU:CD1	1:A:981:LEU:O	2.69	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:CB	2.51	0.41
2:B:171:PRO:HD2	2:B:457:LEU:HD12	2.03	0.41
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.44	0.41
1:A:825:ILE:HG21	2:B:512:ARG:HG3	2.01	0.41
3:C:146:LYS:O	3:C:147:LEU:HD23	2.20	0.41
6:H:139:ASN:O	6:H:140:ALA:CB	2.68	0.41
10:L:28:LYS:O	10:L:29:TYR:CG	2.74	0.41
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.20	0.41
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.41
1:A:1150:SER:HB2	1:A:1195:LEU:CD2	2.49	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.20	0.41
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.34	0.41
1:A:574:GLY:O	1:A:577:ILE:HG12	2.21	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.59	0.41
1:A:756:ILE:CG2	1:A:757:ASN:N	2.80	0.41
1:A:760:GLN:OE1	2:B:1021:MET:HE2	2.20	0.41
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:LEU:CD2	2:B:735:ALA:HB1	2.51	0.41
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.64	0.41
1:A:738:LYS:HZ1	3:C:194:GLU:CA	2.33	0.41
3:C:29:MET:O	3:C:30:ALA:C	2.58	0.41
4:E:100:ILE:O	4:E:101:GLN:C	2.58	0.41
1:A:567:LYS:CD	6:H:95:TYR:CD1	3.00	0.41
7:I:25:LEU:HD12	7:I:26:LEU:N	2.35	0.41
10:L:34:CYS:HG	10:L:51:CYS:HG	1.57	0.41
1:A:1098:VAL:O	1:A:1099:PRO:C	2.59	0.41
1:A:1149:ALA:CB	7:I:47:GLU:N	2.75	0.41
1:A:1293:SER:OG	1:A:1294:PRO:CD	2.68	0.41
1:A:344:ARG:O	2:B:1118:PRO:HD2	2.20	0.41
1:A:441:PRO:HG2	1:A:441:PRO:O	2.20	0.41
1:A:810:PRO:HG3	2:B:745:PRO:CB	2.51	0.41
1:A:928:LEU:O	1:A:929:LEU:C	2.59	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.57	0.41
2:B:1115:THR:CG2	2:B:1199:ALA:HB2	2.50	0.41
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.60	0.41
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.41
5:F:138:LEU:HB3	5:F:139:PRO:CD	2.51	0.41
7:I:16:PRO:HA	7:I:26:LEU:O	2.20	0.41
7:I:7:CYS:HB2	7:I:14:LEU:CD2	2.34	0.41
9:K:46:ILE:CG2	9:K:50:LEU:HD12	2.51	0.41
10:L:55:ILE:H	10:L:55:ILE:HG12	1.53	0.41
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.03	0.41
1:A:223:GLY:O	1:A:1415:SER:CA	2.64	0.41
1:A:302:THR:O	1:A:313:GLN:NE2	2.54	0.41
1:A:403:LYS:O	1:A:404:TYR:O	2.39	0.41
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.51	0.41
1:A:765:VAL:HG12	1:A:766:GLY:N	2.35	0.41
1:A:783:THR:HG21	1:A:815:PHE:HZ	1.19	0.41
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.56	0.41
2:B:1152:MET:O	2:B:1156:ASP:O	2.39	0.41
2:B:175:ARG:HH11	2:B:175:ARG:CG	2.34	0.41
1:A:825:ILE:CD1	2:B:512:ARG:C	2.89	0.41
2:B:911:ILE:HD11	2:B:941:LEU:CB	2.50	0.41
3:C:31:ASN:O	3:C:32:SER:C	2.56	0.41
4:E:13:TRP:O	4:E:16:PHE:HB3	2.21	0.41
4:E:3:GLN:HG3	4:E:5:ASN:H	1.85	0.41
9:K:106:GLU:O	9:K:110:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:SER:HG	7:I:44:TYR:HE2	1.45	0.41
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	3.03	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.66	0.41
1:A:458:HIS:CE1	1:A:507:VAL:CG2	3.00	0.41
1:A:367:PRO:CB	1:A:466:SER:HA	2.47	0.41
1:A:542:GLU:OE1	1:A:569:LYS:HE2	2.20	0.41
1:A:79:GLY:C	1:A:243:PRO:HG3	2.41	0.41
1:A:894:GLU:C	1:A:896:ARG:N	2.74	0.41
2:B:205:ILE:CD1	2:B:205:ILE:N	2.84	0.41
2:B:418:LYS:O	2:B:420:LEU:N	2.54	0.41
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.24	0.41
2:B:872:GLU:HA	2:B:915:THR:O	2.21	0.41
2:B:941:LEU:HD21	2:B:946:ASN:HA	2.02	0.41
2:B:911:ILE:HG21	2:B:966:VAL:HG11	2.01	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.56	0.41
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	2.01	0.41
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.21	0.41
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.89	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.56	0.41
1:A:535:THR:O	1:A:536:LEU:C	2.59	0.41
1:A:598:LEU:HD22	6:H:25:ARG:HH12	1.83	0.41
2:B:1020:ARG:O	2:B:1021:MET:C	2.58	0.41
2:B:778:MET:HE3	2:B:1094:ARG:HD3	2.00	0.41
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.85	0.41
2:B:240:ILE:C	2:B:253:THR:HG23	2.41	0.41
2:B:380:TYR:O	2:B:384:ARG:HG2	2.21	0.41
2:B:578:THR:HG23	2:B:622:LYS:C	2.41	0.41
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.51	0.41
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.51	0.41
4:E:116:ILE:CG2	4:E:117:THR:N	2.84	0.41
6:H:138:GLU:HG2	6:H:139:ASN:N	2.35	0.41
7:I:50:THR:HG22	7:I:52:ILE:HG23	1.99	0.41
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.34	0.41
1:A:379:VAL:HG22	1:A:431:LYS:HG2	2.03	0.41
1:A:443:LEU:HD22	1:A:455:MET:CE	2.48	0.41
1:A:568:PRO:HB3	3:C:221:TYR:OH	2.21	0.41
2:B:205:ILE:HG21	2:B:462:ALA:HB2	2.03	0.41
2:B:901:PRO:O	2:B:949:VAL:O	2.38	0.41
2:B:121:ASN:HD21	2:B:965:LYS:HE3	1.86	0.41
7:I:6:PHE:HD2	7:I:13:MET:HA	1.86	0.41
9:K:47:ARG:HH11	9:K:48:ALA:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:O	2:B:1215:ARG:HG3	2.21	0.40
1:A:225:ASN:C	1:A:227:VAL:N	2.71	0.40
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.36	0.40
1:A:432:VAL:O	1:A:434:ARG:N	2.54	0.40
1:A:909:ASP:OD1	1:A:910:PRO:HD2	2.21	0.40
1:A:980:ASP:OD2	1:A:1039:LYS:HB3	2.21	0.40
2:B:185:THR:N	2:B:188:ASP:HB2	2.36	0.40
2:B:350:GLN:O	2:B:351:TYR:C	2.59	0.40
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.36	0.40
2:B:627:PHE:O	2:B:632:ARG:NH1	2.54	0.40
1:A:810:PRO:CG	2:B:705:MET:SD	3.06	0.40
2:B:707:PRO:O	2:B:708:GLU:C	2.59	0.40
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.62	0.40
3:C:66:ARG:NH2	8:J:3:VAL:O	2.54	0.40
1:A:871:ASP:CB	4:E:204:THR:CG2	2.99	0.40
1:A:1149:ALA:CA	7:I:47:GLU:H	2.33	0.40
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.86	0.40
2:B:818:PRO:HG3	8:J:54:VAL:HG21	2.03	0.40
9:K:21:ILE:HG12	9:K:33:ILE:HG12	2.03	0.40
10:L:60:ARG:CG	10:L:61:THR:N	2.62	0.40
1:A:1107:VAL:CG2	1:A:1383:SER:HA	2.51	0.40
1:A:14:VAL:HB	1:A:1430:LEU:HD13	2.02	0.40
1:A:203:SER:O	1:A:207:ILE:HG12	2.21	0.40
1:A:331:GLY:O	1:A:332:LYS:O	2.39	0.40
1:A:784:LEU:HD12	1:A:811:GLN:HB3	2.03	0.40
1:A:921:GLY:O	1:A:922:ASP:C	2.59	0.40
2:B:244:LEU:HB2	2:B:249:ARG:HA	2.03	0.40
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.47	0.40
2:B:284:ILE:HG12	2:B:324:ILE:HD12	2.03	0.40
2:B:51:PHE:O	2:B:54:PHE:N	2.54	0.40
3:C:153:LEU:HD12	3:C:153:LEU:HA	1.91	0.40
4:E:7:ARG:HG3	4:E:8:ASN:N	2.36	0.40
4:E:90:VAL:HA	4:E:120:ALA:HB2	2.04	0.40
6:H:126:GLU:N	6:H:130:ARG:HH12	2.19	0.40
2:B:120:ARG:HH22	10:L:54:ARG:HD2	1.86	0.40
1:A:1107:VAL:HG23	1:A:1383:SER:HA	2.03	0.40
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	2.04	0.40
1:A:244:PRO:O	1:A:245:PRO:C	2.59	0.40
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.94	0.40
1:A:719:VAL:HG22	1:A:774:ARG:HD2	2.03	0.40
1:A:808:LEU:HD12	1:A:808:LEU:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.57	0.40
1:A:1436:ILE:CG2	2:B:1142:GLY:HA2	2.51	0.40
1:A:19:PHE:HA	2:B:1213:THR:O	2.22	0.40
2:B:167:ILE:O	2:B:168:GLY:O	2.38	0.40
2:B:283:VAL:HG13	2:B:297:ILE:HD12	2.03	0.40
2:B:363:HIS:O	2:B:364:ILE:CG1	2.70	0.40
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.85	0.40
2:B:549:THR:HG22	2:B:550:ASP:N	2.36	0.40
2:B:704:ALA:HB2	2:B:738:PHE:CD1	2.56	0.40
6:H:117:SER:HA	6:H:122:LEU:HD23	2.02	0.40
1:A:1006:ILE:HG22	1:A:1007:ILE:N	2.36	0.40
1:A:113:LEU:C	1:A:115:LEU:H	2.23	0.40
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.20	0.40
1:A:650:GLN:O	1:A:651:LYS:C	2.58	0.40
1:A:88:LYS:HD2	1:A:293:GLU:OE1	2.20	0.40
2:B:1117:GLN:NE2	2:B:1156:ASP:OD2	2.54	0.40
2:B:484:ASN:ND2	2:B:486:TYR:HD1	2.19	0.40
2:B:495:LEU:HA	2:B:495:LEU:HD23	1.86	0.40
2:B:583:ASN:HD21	2:B:628:THR:CB	2.28	0.40
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.51	0.40
4:E:116:ILE:HG22	4:E:117:THR:N	2.36	0.40
4:E:136:ASN:C	4:E:136:ASN:OD1	2.60	0.40
5:F:109:VAL:HG12	5:F:110:ASP:H	1.82	0.40
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.39	0.40
7:I:34:TYR:C	7:I:35:VAL:HG23	2.41	0.40
1:A:1158:PRO:HB3	1:A:1241:ARG:HH12	1.84	0.40
1:A:1116:LEU:CD2	1:A:1316:VAL:HG21	2.51	0.40
1:A:1378:GLN:O	1:A:1380:GLY:N	2.55	0.40
1:A:1394:THR:CG2	1:A:1398:MET:CE	3.00	0.40
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.96	0.40
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.50	0.40
1:A:477:PRO:CG	1:A:521:MET:HG2	2.52	0.40
1:A:531:ILE:CG2	1:A:532:ARG:N	2.84	0.40
1:A:848:ILE:HG23	1:A:864:ILE:HD12	2.03	0.40
2:B:737:THR:O	2:B:738:PHE:C	2.60	0.40
2:B:801:LYS:HE2	8:J:51:LEU:O	2.22	0.40
2:B:992:ILE:CD1	2:B:994:TYR:CE2	3.04	0.40
1:A:569:LYS:NZ	3:C:221:TYR:O	2.40	0.40
4:E:72:PHE:CD1	4:E:72:PHE:N	2.89	0.40
6:H:82:PRO:HB2	6:H:83:GLN:H	1.78	0.40
7:I:99:LEU:HB2	7:I:112:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:99:LEU:O	7:I:111:THR:HG23	2.21	0.40
3:C:66:ARG:HB3	8:J:5:VAL:HG21	2.04	0.40
9:K:92:ASN:C	9:K:94:ILE:N	2.75	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:OD1	7:I:33:SER:OG[7_554]	1.06	1.14
2:B:1223:ASP:O	2:B:1223:ASP:CB[2_565]	1.71	0.49
1:A:903:ASN:OD1	7:I:33:SER:CB[7_554]	2.14	0.06
1:A:163:SER:OG	4:E:74:ASP:OD1[2_565]	2.19	0.01

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	1362/1733 (79%)	1020 (75%)	252 (18%)	90 (7%)	1	18
2	B	1077/1224 (88%)	836 (78%)	172 (16%)	69 (6%)	1	19
3	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	1	19
4	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	25
5	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	3	28
6	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	6
7	I	114/122 (93%)	90 (79%)	15 (13%)	9 (8%)	1	14
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	19
9	K	112/120 (93%)	96 (86%)	16 (14%)	0	100	100
10	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3459/4173 (83%)	2647 (76%)	587 (17%)	225 (6%)	1	18

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	74	MET
1	A	75	ASN
1	A	167	CYS
1	A	322	VAL
1	A	404	TYR
1	A	418	SER
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	598	LEU
1	A	628	GLY
1	A	752	LYS
1	A	846	GLU
1	A	998	LEU
1	A	1036	ARG
1	A	1127	ASP
1	A	1206	ASP
1	A	1221	LYS
1	A	1223	ASP
1	A	1392	SER
1	A	1393	ASN
1	A	1403	GLU
1	A	1406	VAL
1	A	1416	ALA
2	B	65	GLU
2	B	124	TYR
2	B	174	LEU
2	B	175	ARG
2	B	200	GLY
2	B	229	ALA
2	B	364	ILE
2	B	367	LEU
2	B	531	GLN
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	751	VAL
2	B	958	GLN

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Mol	Chain	Res	Type
2	B	959	ASP
2	B	1046	PRO
2	B	1103	ILE
2	B	1167	GLY
2	B	1176	ASN
2	B	1183	LYS
3	C	4	GLU
3	C	5	GLY
3	C	6	PRO
3	C	110	THR
3	C	142	VAL
3	C	215	GLU
5	F	73	ALA
6	H	32	THR
6	H	81	PRO
6	H	140	ALA
7	I	8	ARG
8	J	2	ILE
8	J	55	ASP
10	L	27	LEU
10	L	38	LEU
10	L	64	LEU
1	A	35	ILE
1	A	54	ASN
1	A	62	ASP
1	A	87	ALA
1	A	109	HIS
1	A	135	PHE
1	A	168	GLY
1	A	332	LYS
1	A	385	ILE
1	A	419	LYS
1	A	534	LEU
1	A	568	PRO
1	A	790	ASP
1	A	986	ILE
1	A	1114	PRO
1	A	1365	TYR
1	A	1366	ARG
1	A	1379	GLY
2	B	55	VAL
2	B	168	GLY

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Mol	Chain	Res	Type
2	B	275	TYR
2	B	346	GLU
2	B	410	GLY
2	B	480	SER
2	B	641	GLU
2	B	643	ASP
2	B	792	MET
2	B	864	LYS
2	B	866	TYR
2	B	884	ARG
2	B	891	ASP
2	B	992	ILE
2	B	1066	SER
2	B	1155	SER
3	C	136	ASP
5	F	142	SER
6	H	61	SER
6	H	77	ARG
6	H	88	SER
6	H	128	ASN
7	I	30	ARG
7	I	79	HIS
10	L	39	SER
10	L	52	GLY
1	A	6	TYR
1	A	45	GLN
1	A	59	GLY
1	A	67	CYS
1	A	69	THR
1	A	335	ARG
1	A	433	GLU
1	A	596	THR
1	A	737	LEU
1	A	775	ILE
1	A	830	LYS
1	A	920	LEU
2	B	28	GLU
2	B	249	ARG
2	B	277	LYS
2	B	447	ALA
2	B	629	ASP
2	B	735	ALA

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Mol	Chain	Res	Type
2	B	807	ARG
2	B	880	THR
2	B	1017	ILE
2	B	1099	VAL
2	B	1104	HIS
3	C	48	SER
3	C	212	PRO
3	C	227	THR
4	E	31	THR
4	E	102	GLU
4	E	103	LYS
4	E	122	LYS
4	E	139	ALA
4	E	206	GLY
5	F	128	LYS
6	H	8	ASP
6	H	17	PRO
6	H	82	PRO
6	H	135	LEU
6	H	139	ASN
7	I	9	ASP
7	I	33	SER
7	I	86	PHE
8	J	9	SER
10	L	63	ARG
1	A	101	LYS
1	A	134	ARG
1	A	139	TRP
1	A	424	ILE
1	A	599	SER
1	A	1067	LEU
1	A	1097	GLY
1	A	1115	SER
1	A	1122	PRO
1	A	1405	THR
2	B	304	ASP
2	B	436	VAL
2	B	501	PRO
2	B	667	GLN
2	B	791	THR
2	B	1097	HIS
2	B	1178	ASN

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Mol	Chain	Res	Type
3	C	18	VAL
3	C	149	LYS
3	C	174	ALA
4	E	59	SER
8	J	6	ARG
10	L	50	ASP
10	L	56	LEU
1	A	58	LEU
1	A	223	GLY
1	A	400	PRO
1	A	958	VAL
1	A	972	HIS
1	A	1098	VAL
1	A	1130	GLN
1	A	1282	VAL
1	A	1378	GLN
2	B	248	SER
2	B	419	THR
2	B	619	ILE
2	B	648	HIS
2	B	687	GLU
2	B	707	PRO
2	B	712	PRO
2	B	764	SER
2	B	907	GLY
2	B	982	SER
2	B	1054	GLY
2	B	1108	ARG
4	E	36	GLU
6	H	62	SER
6	H	89	LEU
7	I	47	GLU
7	I	88	SER
1	A	226	GLU
1	A	368	LYS
1	A	399	HIS
1	A	531	ILE
1	A	1014	ALA
1	A	1314	SER
1	A	1351	GLU
1	A	1352	VAL
2	B	27	ALA

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Mol	Chain	Res	Type
4	E	167	ARG
6	H	138	GLU
7	I	98	VAL
10	L	59	ALA
2	B	247	GLY
1	A	336	ILE
1	A	1104	ILE
10	L	55	ILE
1	A	1242	VAL
3	C	172	PRO
3	C	216	GLY
1	A	78	PRO
1	A	1075	PRO
2	B	511	PRO
3	C	218	PRO

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	1205/1520 (79%)	1128 (94%)	77 (6%)	17	44
2	B	952/1061 (90%)	886 (93%)	66 (7%)	15	42
3	C	234/274 (85%)	222 (95%)	12 (5%)	24	50
4	E	196/197 (100%)	189 (96%)	7 (4%)	35	60
5	F	74/137 (54%)	68 (92%)	6 (8%)	11	37
6	H	117/128 (91%)	112 (96%)	5 (4%)	29	55
7	I	113/116 (97%)	104 (92%)	9 (8%)	12	38
8	J	60/65 (92%)	56 (93%)	4 (7%)	16	43
9	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	21
All	All	3090/3657 (84%)	2890 (94%)	200 (6%)	17	44

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	31	SER
1	A	56	PRO
1	A	70	CYS
1	A	93	VAL
1	A	122	MET
1	A	247	ARG
1	A	269	ILE
1	A	302	THR
1	A	322	VAL
1	A	326	ARG
1	A	351	THR
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	397	ASN
1	A	412	ARG
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	503	GLN
1	A	524	VAL
1	A	538	ASP
1	A	590	ARG
1	A	596	THR
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	682	THR
1	A	740	LEU
1	A	741	ASN
1	A	745	GLN
1	A	756	ILE
1	A	768	GLN

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Mol	Chain	Res	Type
1	A	774	ARG
1	A	821	ARG
1	A	845	LEU
1	A	849	MET
1	A	855	THR
1	A	858	ASN
1	A	920	LEU
1	A	929	LEU
1	A	948	VAL
1	A	949	ASP
1	A	979	SER
1	A	1029	ARG
1	A	1035	TYR
1	A	1043	ASP
1	A	1057	VAL
1	A	1077	THR
1	A	1128	GLN
1	A	1222	ASN
1	A	1232	ASN
1	A	1258	HIS
1	A	1264	GLU
1	A	1295	THR
1	A	1308	THR
1	A	1318	THR
1	A	1332	PHE
1	A	1335	ILE
1	A	1351	GLU
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1375	MET
1	A	1376	THR
1	A	1425	SER
1	A	1442	ASP
2	B	20	ASP
2	B	43	LEU
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	98	THR
2	B	109	THR
2	B	121	ASN

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Mol	Chain	Res	Type
2	B	175	ARG
2	B	194	GLU
2	B	232	SER
2	B	234	ILE
2	B	261	ARG
2	B	268	THR
2	B	278	GLN
2	B	309	GLN
2	B	313	MET
2	B	317	CYS
2	B	320	ASP
2	B	331	LEU
2	B	376	PHE
2	B	387	LEU
2	B	396	ASP
2	B	408	LEU
2	B	466	TRP
2	B	485	ARG
2	B	513	GLN
2	B	514	LEU
2	B	538	ASN
2	B	547	VAL
2	B	570	VAL
2	B	576	ASP
2	B	624	LEU
2	B	629	ASP
2	B	644	GLU
2	B	680	THR
2	B	723	VAL
2	B	732	SER
2	B	762	ASN
2	B	764	SER
2	B	780	VAL
2	B	791	THR
2	B	835	GLN
2	B	901	PRO
2	B	909	ASP
2	B	915	THR
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	976	ILE

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Mol	Chain	Res	Type
2	B	986	GLN
2	B	987	LYS
2	B	996	ARG
2	B	999	MET
2	B	1007	VAL
2	B	1021	MET
2	B	1049	ASP
2	B	1103	ILE
2	B	1111	MET
2	B	1118	PRO
2	B	1132	GLU
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1183	LYS
2	B	1185	CYS
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	62	PHE
3	C	69	LEU
3	C	77	ILE
3	C	133	ILE
3	C	148	ARG
3	C	229	TYR
3	C	233	GLU
3	C	240	VAL
3	C	264	GLN
4	E	40	GLU
4	E	60	PHE
4	E	74	ASP
4	E	84	ASP
4	E	92	THR
4	E	104	ASN
4	E	183	PRO
5	F	79	ARG
5	F	90	ARG
5	F	103	MET
5	F	111	LEU
5	F	115	THR
5	F	133	VAL
6	H	21	ASN

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Mol	Chain	Res	Type
6	H	27	GLU
6	H	109	LYS
6	H	110	ASP
6	H	134	ASN
7	I	7	CYS
7	I	12	ASN
7	I	29	CYS
7	I	31	THR
7	I	52	ILE
7	I	75	CYS
7	I	76	PRO
7	I	87	GLN
7	I	103	CYS
8	J	2	ILE
8	J	7	CYS
8	J	47	ARG
8	J	48	ARG
9	K	20	LYS
9	K	25	THR
9	K	31	VAL
9	K	47	ARG
9	K	50	LEU
9	K	61	TYR
9	K	77	THR
9	K	81	TYR
9	K	114	LEU
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
10	L	68	GLU
10	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	169	ASN
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	445	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	587	HIS
1	A	631	HIS
1	A	706	HIS
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	968	GLN
1	A	969	GLN
1	A	994	GLN
1	A	1364	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	862	GLN
2	B	957	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	5	ASN
4	E	32	GLN
4	E	101	GLN
4	E	104	ASN
4	E	114	ASN
4	E	147	HIS
6	H	33	GLN
7	I	12	ASN
8	J	53	HIS
9	K	52	ASN
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	M	12
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	88:UNK	C	106:UNK	N	28.95
1	A	1274:ARG	C	1275:GLY	N	1.70
1	M	75:UNK	C	76:UNK	N	1.17
1	M	84:UNK	C	85:UNK	N	1.16
1	M	72:UNK	C	73:UNK	N	1.13
1	M	87:UNK	C	88:UNK	N	1.12
1	M	61:UNK	C	62:UNK	N	1.10
1	M	111:UNK	C	112:UNK	N	1.09
1	M	77:UNK	C	78:UNK	N	1.08
1	M	80:UNK	C	81:UNK	N	1.06
1	M	54:UNK	C	55:UNK	N	1.03
1	B	217:ARG	C	218:SER	N	1.01
1	M	70:UNK	C	71:UNK	N	0.98
1	M	108:UNK	C	109:UNK	N	0.98

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	1380/1733 (79%)	0.02	36 (2%) 56 46	47, 179, 269, 300	0
2	B	1097/1224 (89%)	0.09	43 (3%) 39 31	26, 192, 280, 300	0
3	C	266/318 (83%)	-0.07	2 (0%) 86 79	45, 168, 245, 293	0
4	E	214/215 (99%)	0.12	12 (5%) 24 21	76, 206, 284, 300	0
5	F	84/155 (54%)	0.02	1 (1%) 79 70	61, 160, 231, 277	0
6	H	133/146 (91%)	0.36	5 (3%) 40 32	119, 207, 300, 300	0
7	I	118/122 (96%)	0.86	20 (16%) 1 2	133, 246, 300, 300	0
8	J	65/70 (92%)	-0.07	0 100 100	76, 169, 231, 270	0
9	K	114/120 (95%)	-0.14	0 100 100	72, 155, 241, 274	0
10	L	46/70 (65%)	0.68	7 (15%) 2 3	129, 222, 288, 300	0
11	M	0/86	-	-	-	-
All	All	3517/4259 (82%)	0.08	126 (3%) 42 35	26, 186, 278, 300	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	919	SER	8.5
10	L	26	THR	8.0
2	B	881	ASN	6.8
10	L	25	ALA	6.8
7	I	41	PRO	6.3
7	I	74	GLU	5.1
1	A	170	THR	4.9
2	B	882	THR	4.9
1	A	1125	ALA	4.9
1	A	1176	LEU	4.8
1	A	1175	SER	4.6
1	A	422	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	366	GLN	4.4
1	A	60	SER	4.1
2	B	729	ILE	4.1
6	H	83	GLN	4.1
2	B	866	TYR	4.0
10	L	50	ASP	4.0
1	A	153	PRO	4.0
2	B	133	LYS	3.9
4	E	51	GLY	3.8
1	A	44	THR	3.7
4	E	52	ARG	3.7
7	I	8	ARG	3.6
1	A	1232	ASN	3.6
1	A	313	GLN	3.6
7	I	118	ARG	3.6
2	B	877	PRO	3.6
6	H	146	ARG	3.5
2	B	868	MET	3.5
7	I	40	SER	3.4
2	B	880	THR	3.4
7	I	116	ASN	3.4
2	B	164	LYS	3.3
2	B	869	SER	3.3
2	B	733	HIS	3.3
4	E	93	MET	3.3
7	I	102	VAL	3.3
2	B	345	LYS	3.3
2	B	734	HIS	3.2
2	B	715	ALA	3.2
2	B	730	ARG	3.2
1	A	1126	ALA	3.2
2	B	359	GLU	3.1
4	E	53	PRO	3.1
2	B	432	MET	3.0
1	A	424	ILE	3.0
1	A	88	LYS	3.0
2	B	722	ASP	2.9
2	B	918	ILE	2.9
4	E	2	ASP	2.9
4	E	97	VAL	2.9
2	B	1173	ALA	2.9
2	B	437	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
7	I	76	PRO	2.9
7	I	42	LEU	2.9
2	B	134	LYS	2.8
7	I	110	PHE	2.8
7	I	119	THR	2.8
2	B	132	VAL	2.8
1	A	1231	ASP	2.8
2	B	732	SER	2.7
7	I	73	ARG	2.7
1	A	152	VAL	2.7
1	A	419	LYS	2.7
3	C	267	GLN	2.7
2	B	865	LYS	2.7
2	B	723	VAL	2.7
2	B	435	THR	2.6
7	I	84	VAL	2.6
2	B	428	ILE	2.6
7	I	2	THR	2.6
6	H	35	GLN	2.6
10	L	37	LYS	2.6
1	A	1172	LEU	2.5
4	E	50	MET	2.5
1	A	821	ARG	2.5
1	A	49	LYS	2.5
7	I	43	VAL	2.5
2	B	90	ILE	2.5
2	B	714	GLU	2.4
1	A	171	GLN	2.4
7	I	81	ARG	2.4
1	A	428	TYR	2.4
1	A	144	THR	2.4
1	A	141	LEU	2.4
2	B	569	TYR	2.4
2	B	678	GLU	2.4
7	I	57	GLY	2.4
1	A	421	ALA	2.4
4	E	118	PRO	2.3
2	B	358	LYS	2.3
4	E	88	VAL	2.3
5	F	104	ASN	2.3
2	B	870	ILE	2.3
10	L	27	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	512	ARG	2.3
2	B	477	ALA	2.3
1	A	420	ARG	2.2
4	E	116	ILE	2.2
7	I	83	ASN	2.2
4	E	121	MET	2.2
1	A	199	LEU	2.2
7	I	34	TYR	2.2
2	B	893	LEU	2.2
2	B	467	GLY	2.2
6	H	110	ASP	2.2
1	A	50	ILE	2.2
1	A	223	GLY	2.1
1	A	280	GLU	2.1
4	E	29	PHE	2.1
1	A	1236	LEU	2.1
1	A	1188	GLN	2.1
1	A	53	LEU	2.1
6	H	85	GLY	2.1
2	B	466	TRP	2.1
1	A	1233	ASP	2.1
7	I	120	GLN	2.1
10	L	38	LEU	2.1
3	C	268	ASP	2.1
2	B	725	PRO	2.0
10	L	45	ALA	2.0
2	B	724	ASP	2.0
1	A	69	THR	2.0
1	A	1169	ILE	2.0
1	A	115	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
12	ZN	M	209	1/1	0.36	0.27	156,156,156,156	0
12	ZN	I	203	1/1	0.44	0.64	166,166,166,166	0
12	ZN	I	204	1/1	0.84	0.10	166,166,166,166	0
13	MG	A	1736	1/1	0.88	0.40	47,47,47,47	0
12	ZN	A	1735	1/1	0.89	0.11	166,166,166,166	0
12	ZN	A	1734	1/1	0.92	0.12	166,166,166,166	0
12	ZN	B	1307	1/1	0.93	0.14	166,166,166,166	0
12	ZN	L	105	1/1	0.95	0.11	175,175,175,175	0
12	ZN	C	319	1/1	0.97	0.15	166,166,166,166	0
12	ZN	J	101	1/1	0.99	0.13	166,166,166,166	0

6.5 Other polymers [i](#)

There are no such residues in this entry.