



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:19 PM UTC

PDB ID : 2JA5 / pdb_00002ja5
Title : CPD lesion containing RNA Polymerase II elongation complex A
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

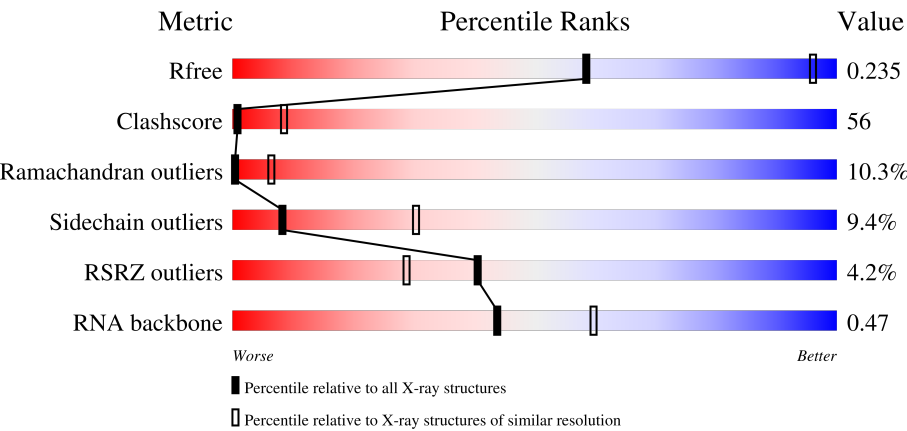
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 23%45%13%•18%
2	B	1224	5% 24%52%14%•9%
3	C	318	% 23%47%11%•16%
4	D	221	4% 22%40%15%•20%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	P	11	
14	T	25	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 31660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

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

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

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

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			

- Molecule 14 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*

TP*TTP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	11	Total	Br	C	N	O	P	0	0	0
			219	1	106	34	68	10			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

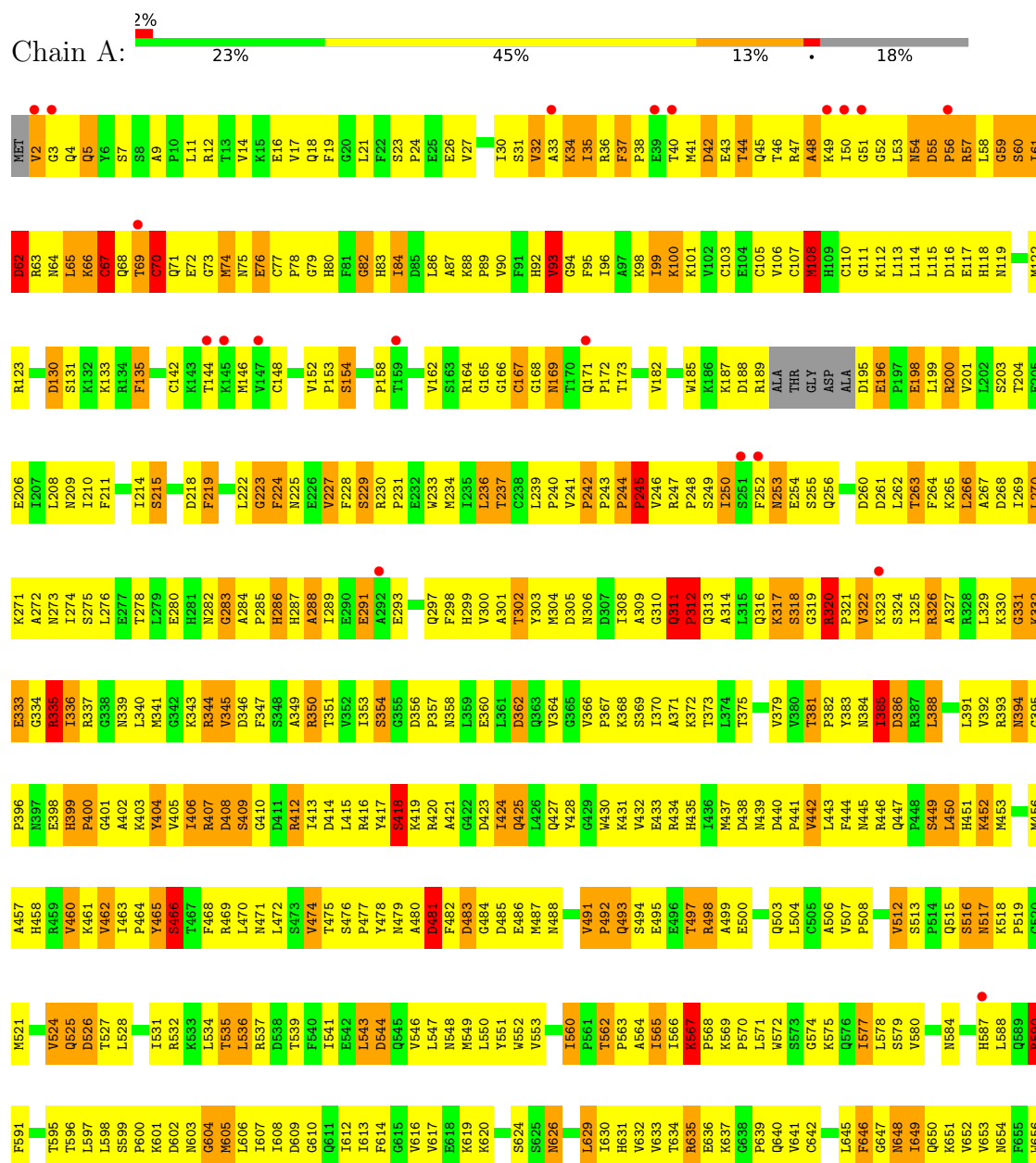
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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

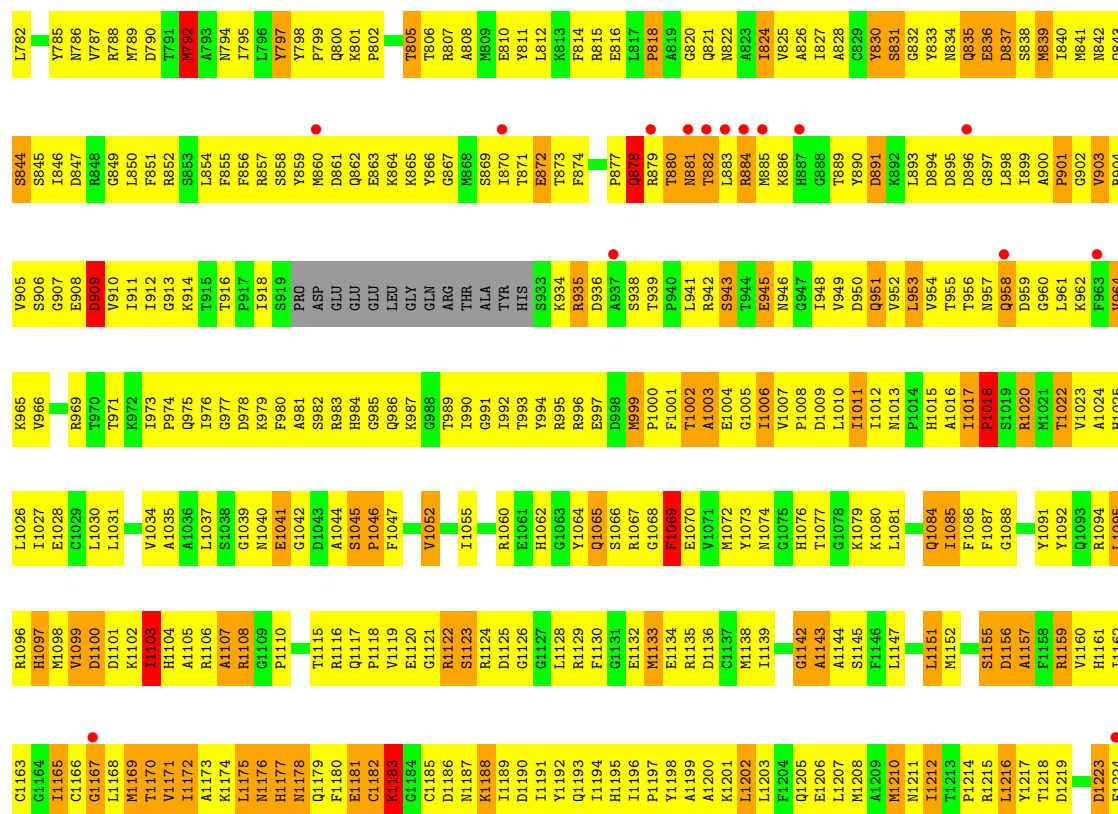
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1



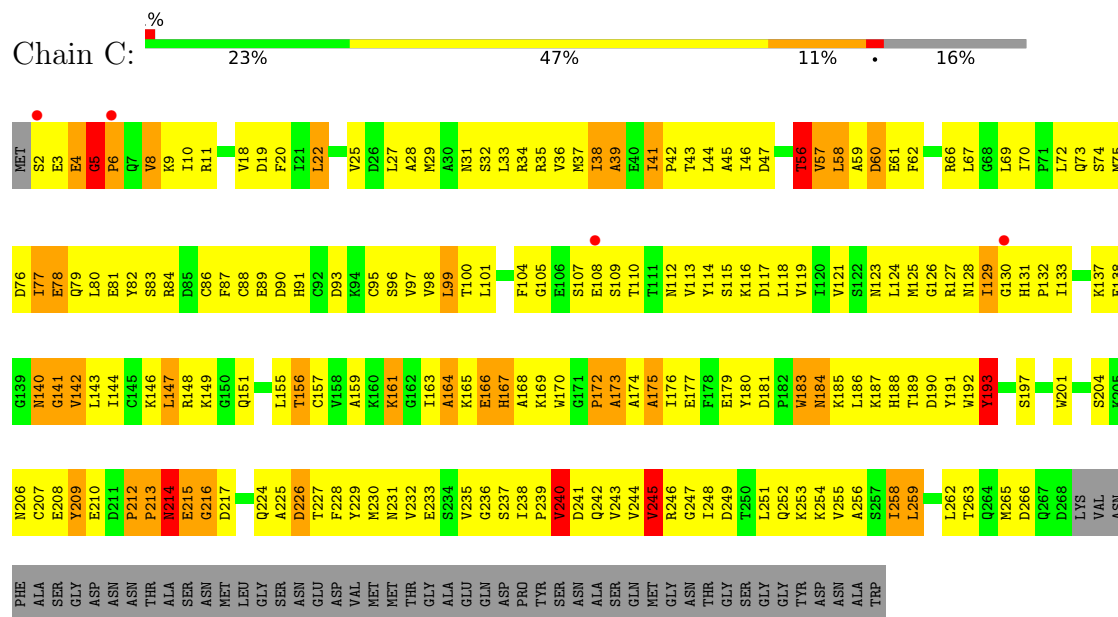


Chain B: 5% 24% 52% 14% 9%

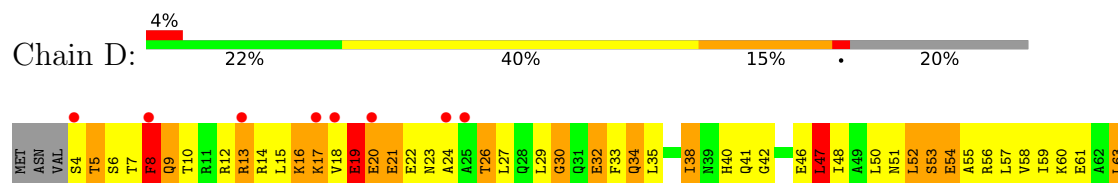


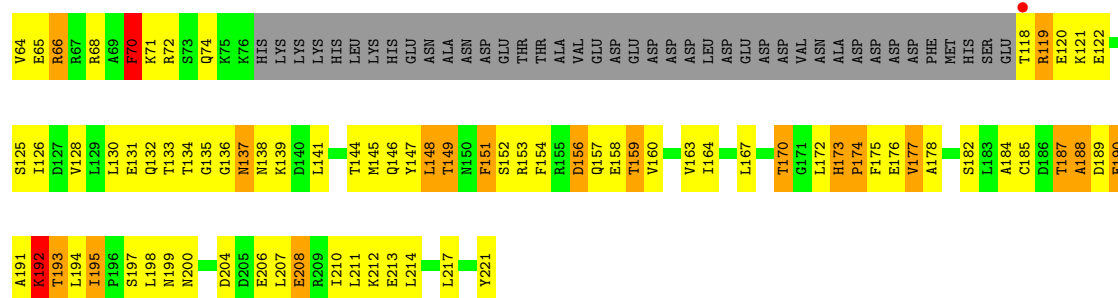


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

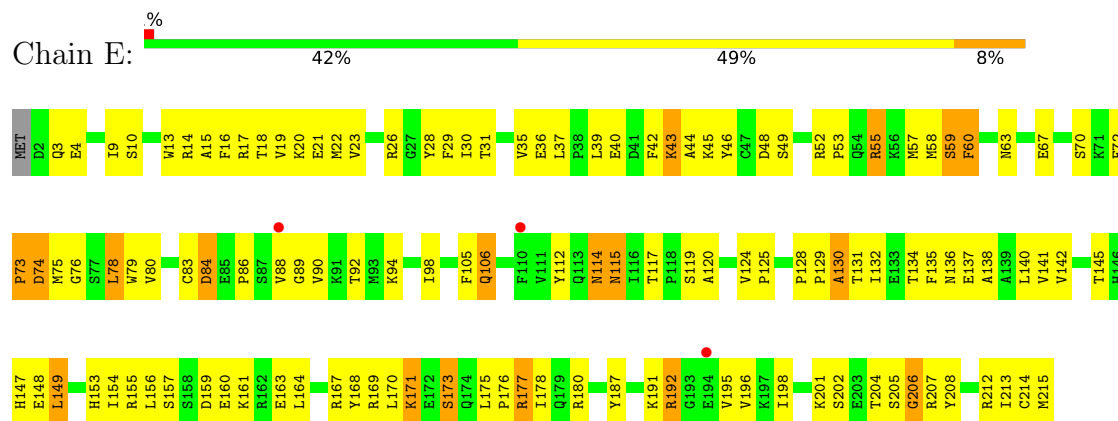


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

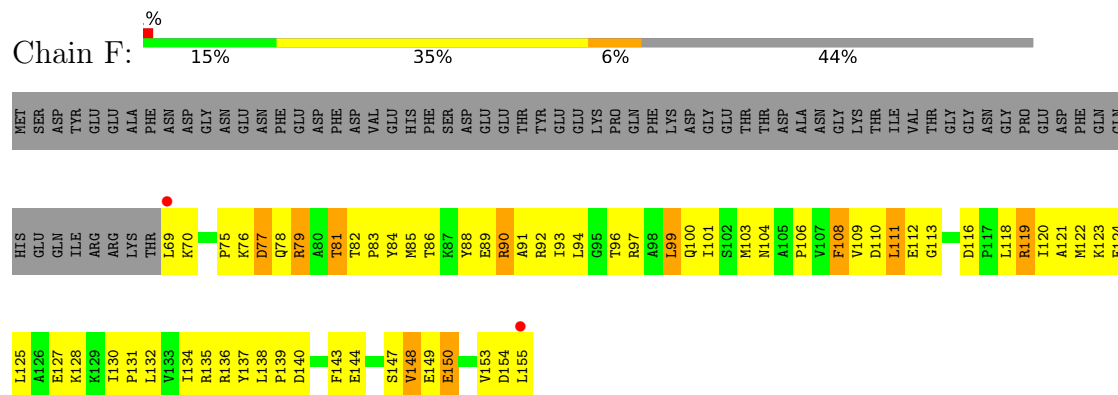




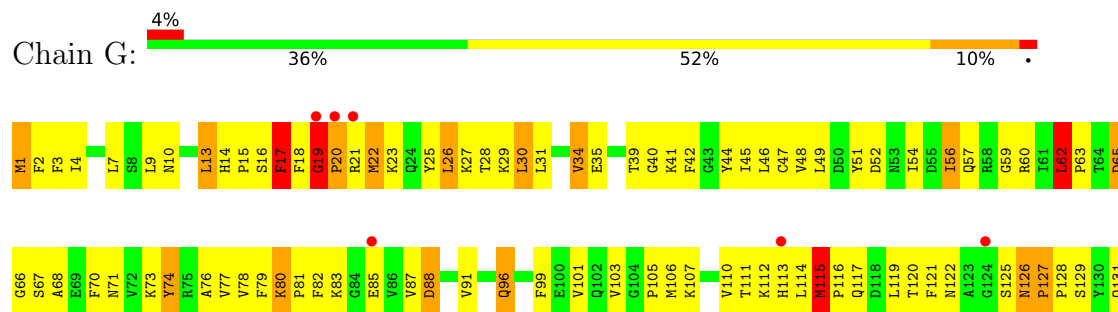
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

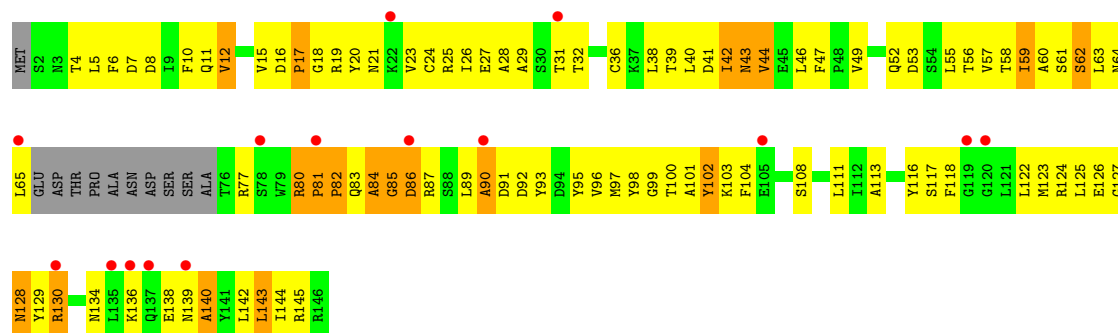


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7





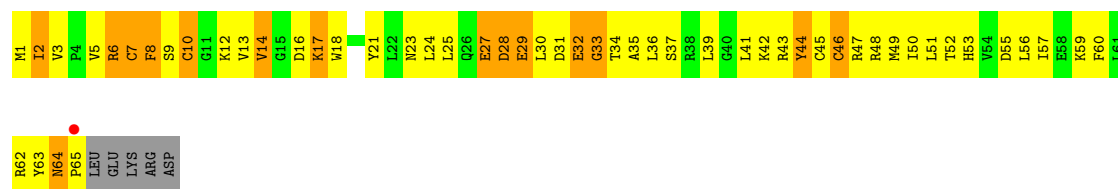
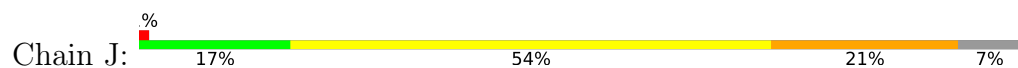
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



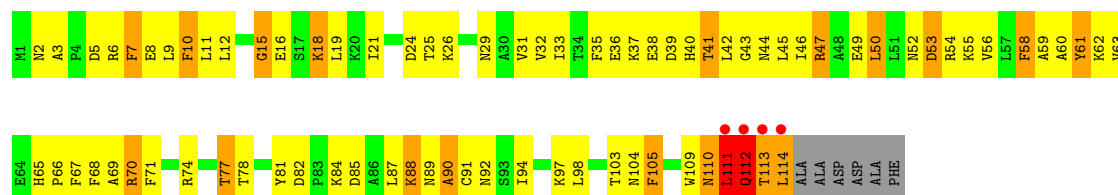
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



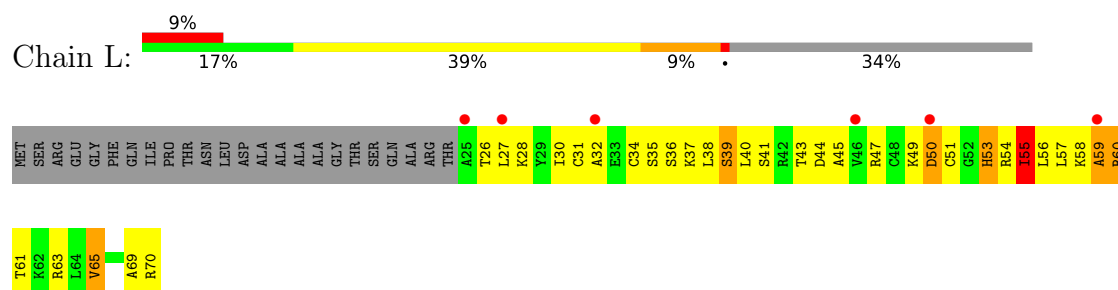
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



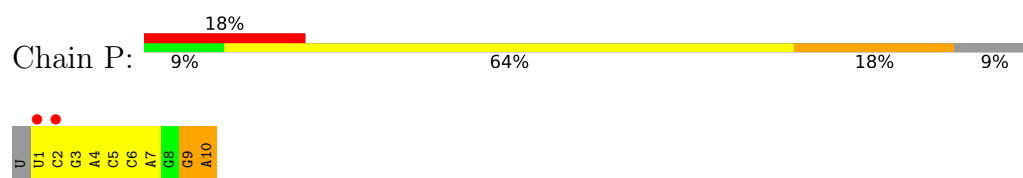
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



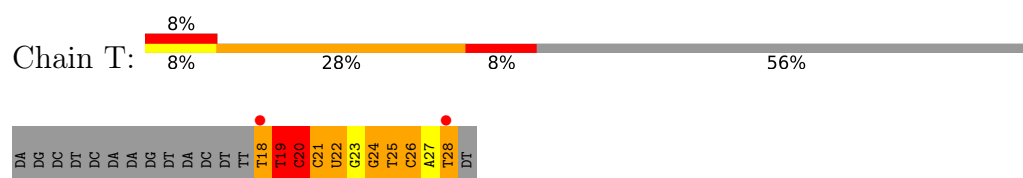
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.21Å 392.21Å 284.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 97.4 (50.00-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.280 0.215 , 0.235	Depositor DCC
R_{free} test set	4681 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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, BRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/11385	1.11	79/15393 (0.5%)
2	B	0.56	1/9037 (0.0%)	1.08	62/12181 (0.5%)
3	C	0.59	0/2138	1.10	14/2896 (0.5%)
4	D	0.47	0/1437	1.11	17/1925 (0.9%)
5	E	0.51	0/1788	0.98	11/2406 (0.5%)
6	F	0.65	0/716	1.14	3/964 (0.3%)
7	G	0.54	0/1368	1.13	13/1844 (0.7%)
8	H	0.48	0/1102	1.04	6/1492 (0.4%)
9	I	0.47	0/962	1.08	6/1295 (0.5%)
10	J	0.56	0/541	1.01	1/727 (0.1%)
11	K	1.27	9/937 (1.0%)	1.43	16/1265 (1.3%)
12	L	0.55	0/366	0.94	0/485
13	P	0.80	0/237	1.28	4/368 (1.1%)
14	T	0.61	0/220	1.62	8/335 (2.4%)
All	All	0.60	10/32234 (0.0%)	1.10	240/43576 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
14	T	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	112	GLN	CA-C	19.29	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	CA-C	13.26	1.69	1.53
11	K	113	THR	N-CA	12.98	1.64	1.46
11	K	112	GLN	N-CA	12.71	1.62	1.46
11	K	112	GLN	CB-CG	8.18	1.76	1.52
11	K	112	GLN	C-N	7.48	1.42	1.33
11	K	111	LEU	CA-C	6.58	1.62	1.53
11	K	111	LEU	C-N	5.91	1.42	1.33
11	K	112	GLN	CG-CD	5.64	1.66	1.52
2	B	792	MET	SD-CE	5.12	1.92	1.79

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	21.59	136.74	108.24
4	D	26	THR	N-CA-C	-13.01	96.72	112.59
2	B	1185	CYS	N-CA-C	-12.95	97.49	113.28
2	B	473	MET	N-CA-C	-11.50	98.90	113.16
11	K	112	GLN	N-CA-C	11.01	134.26	110.80
2	B	427	ASP	N-CA-C	-10.96	99.63	113.43
1	A	452	LYS	N-CA-C	-10.59	99.73	111.07
1	A	242	PRO	CA-C-N	10.49	131.18	120.38
1	A	242	PRO	C-N-CA	10.49	131.18	120.38
4	D	72	ARG	N-CA-C	-10.39	100.04	111.36
7	G	22	MET	N-CA-C	-9.81	99.64	112.68
14	T	19	DT	C2'-C3'-O3'	-9.51	97.23	111.50
7	G	52	ASP	N-CA-C	9.48	121.37	111.14
13	P	1	U	N1-C1'-C2'	9.45	126.18	112.00
1	A	288	ALA	N-CA-C	-9.24	100.96	112.88
4	D	54	GLU	N-CA-C	-9.13	102.27	113.41
11	K	114	LEU	CA-C-O	-8.96	105.57	120.80
8	H	80	ARG	CA-C-N	8.75	129.39	120.38
8	H	80	ARG	C-N-CA	8.75	129.39	120.38
11	K	111	LEU	N-CA-C	8.73	126.60	108.53
1	A	982	THR	N-CA-C	-8.54	99.02	110.55
1	A	266	LEU	N-CA-C	-8.25	102.23	111.14
1	A	466	SER	N-CA-C	8.24	123.93	112.72
3	C	41	ILE	CA-C-N	8.15	128.15	119.76
3	C	41	ILE	C-N-CA	8.15	128.15	119.76
2	B	66	ASP	N-CA-C	-8.04	102.50	112.88
2	B	1009	ASP	N-CA-C	-7.96	104.09	113.88
1	A	60	SER	N-CA-C	7.95	119.04	108.07
2	B	1177	HIS	N-CA-C	-7.92	104.57	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	62	LEU	CA-C-N	-7.90	109.96	119.84
7	G	62	LEU	C-N-CA	-7.90	109.96	119.84
1	A	567	LYS	CA-C-N	-7.87	110.00	119.84
1	A	567	LYS	C-N-CA	-7.87	110.00	119.84
2	B	296	GLU	N-CA-C	-7.79	103.23	112.89
7	G	2	PHE	N-CA-C	-7.79	98.95	110.48
1	A	1275	GLY	N-CA-C	7.76	121.63	111.70
2	B	111	ALA	N-CA-C	-7.67	96.06	108.41
11	K	114	LEU	N-CA-C	7.65	132.41	111.00
3	C	38	ILE	N-CA-C	7.61	117.68	110.30
1	A	1243	VAL	N-CA-C	7.57	121.08	108.81
1	A	293	GLU	N-CA-C	-7.51	104.26	113.50
11	K	113	THR	CB-CA-C	-7.48	96.48	112.78
1	A	698	GLN	N-CA-C	-7.39	104.65	112.93
2	B	882	THR	N-CA-C	7.35	119.99	111.02
4	D	38	ILE	N-CA-C	7.29	118.38	108.17
1	A	539	THR	N-CA-C	7.29	120.14	108.41
2	B	99	LYS	CA-C-N	7.26	128.92	119.84
2	B	99	LYS	C-N-CA	7.26	128.92	119.84
1	A	291	GLU	N-CA-C	-7.24	104.31	113.72
1	A	344	ARG	N-CA-C	-7.24	99.80	110.52
1	A	1422	ARG	N-CA-C	-7.20	103.95	114.39
1	A	67	CYS	N-CA-C	-7.18	98.69	109.83
2	B	363	HIS	N-CA-C	-7.12	101.34	110.53
1	A	938	LYS	N-CA-C	-7.00	103.64	111.28
8	H	85	GLY	N-CA-C	-7.00	104.07	113.24
1	A	560	ILE	CA-C-N	6.95	127.34	119.83
1	A	560	ILE	C-N-CA	6.95	127.34	119.83
1	A	1262	LYS	N-CA-C	-6.94	104.29	112.89
1	A	998	LEU	N-CA-C	6.92	119.76	109.59
8	H	129	TYR	N-CA-C	6.87	120.55	112.72
1	A	1138	ILE	CB-CA-C	-6.87	105.87	111.71
2	B	294	ASP	N-CA-C	-6.83	101.72	110.19
1	A	440	ASP	N-CA-C	-6.83	97.74	109.15
5	E	149	LEU	N-CA-C	6.78	118.75	111.36
3	C	39	ALA	N-CA-C	6.78	122.65	113.97
1	A	227	VAL	N-CA-C	6.78	117.39	111.90
2	B	805	THR	N-CA-C	6.75	118.38	108.86
14	T	18	DT	C2'-C3'-O3'	-6.75	101.37	111.50
14	T	21	DC	C2'-C3'-O3'	-6.72	101.42	111.50
14	T	24	DG	C2'-C3'-O3'	-6.71	101.44	111.50
1	A	320	ARG	CA-C-N	6.70	128.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	C-N-CA	6.70	128.22	119.84
6	F	127	GLU	N-CA-C	-6.70	104.68	112.92
13	P	9	G	C4'-C3'-O3'	-6.68	102.97	113.00
1	A	1261	LYS	N-CA-C	-6.68	106.08	114.56
2	B	555	ILE	N-CA-C	-6.59	105.32	111.45
1	A	82	GLY	N-CA-C	-6.57	101.16	112.06
14	T	20	DC	C2'-C3'-O3'	-6.53	101.71	111.50
5	E	171	LYS	N-CA-C	-6.52	99.58	109.95
6	F	77	ASP	N-CA-C	-6.47	100.40	110.17
1	A	590	ARG	N-CA-C	6.46	119.14	108.48
1	A	513	SER	CA-C-N	6.42	126.05	119.56
1	A	513	SER	C-N-CA	6.42	126.05	119.56
3	C	173	ALA	N-CA-C	6.40	118.83	111.02
3	C	5	GLY	CA-C-N	6.40	127.84	119.84
3	C	5	GLY	C-N-CA	6.40	127.84	119.84
1	A	861	GLY	N-CA-C	-6.38	106.33	115.64
2	B	292	ILE	N-CA-C	6.37	120.63	112.67
2	B	1052	VAL	N-CA-C	-6.35	104.30	110.72
1	A	398	GLU	N-CA-C	-6.33	102.62	110.41
8	H	12	VAL	N-CA-C	6.33	116.60	108.12
2	B	361	LEU	CA-C-N	6.31	127.72	119.84
2	B	361	LEU	C-N-CA	6.31	127.72	119.84
2	B	112	LEU	N-CA-C	6.30	120.34	110.32
2	B	213	ILE	N-CA-C	6.30	117.66	108.53
2	B	681	TRP	N-CA-C	-6.24	103.05	112.04
9	I	85	PHE	N-CA-C	6.24	119.70	110.46
1	A	425	GLN	N-CA-C	-6.21	99.06	109.07
11	K	111	LEU	CA-C-O	-6.20	110.20	122.23
1	A	729	ALA	N-CA-C	-6.19	104.46	111.14
9	I	31	THR	N-CA-C	-6.16	104.84	112.72
7	G	129	SER	N-CA-C	6.14	117.51	108.86
2	B	837	ASP	N-CA-C	6.13	120.33	111.56
3	C	258	ILE	N-CA-C	-6.13	104.87	110.82
1	A	1344	GLY	N-CA-C	-6.13	105.39	112.50
2	B	292	ILE	CB-CA-C	-6.12	107.89	113.70
14	T	28	DT	C2'-C3'-O3'	-6.08	102.38	111.50
1	A	474	VAL	N-CA-C	-6.08	106.50	111.91
5	E	63	ASN	CA-C-N	6.05	125.99	119.76
5	E	63	ASN	C-N-CA	6.05	125.99	119.76
1	A	481	ASP	N-CA-C	-6.04	100.98	109.69
2	B	1142	GLY	N-CA-C	-6.04	106.99	115.32
1	A	928	LEU	N-CA-C	-6.03	104.63	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	VAL	N-CA-C	6.02	119.48	111.17
7	G	65	ASP	N-CA-C	-6.00	98.87	109.06
1	A	173	THR	N-CA-C	-6.00	102.62	110.53
2	B	748	ILE	N-CA-C	-5.99	105.21	113.00
2	B	1020	ARG	N-CA-C	-5.99	104.88	111.82
2	B	616	ILE	N-CA-C	5.97	116.47	107.75
1	A	710	LEU	N-CA-C	-5.97	104.84	111.71
7	G	19	GLY	CA-C-N	5.96	127.29	119.84
7	G	19	GLY	C-N-CA	5.96	127.29	119.84
2	B	836	GLU	N-CA-C	5.95	119.55	111.17
2	B	628	THR	N-CA-C	-5.93	105.88	114.12
14	T	25	DT	C2'-C3'-O3'	-5.92	102.62	111.50
1	A	1113	THR	CA-C-N	-5.87	112.50	119.84
1	A	1113	THR	C-N-CA	-5.87	112.50	119.84
1	A	950	GLY	N-CA-C	-5.84	108.12	115.08
11	K	18	LYS	N-CA-C	-5.83	104.92	111.28
11	K	113	THR	CA-C-N	5.83	132.19	121.70
11	K	113	THR	C-N-CA	5.83	132.19	121.70
9	I	65	ASP	CA-C-N	5.82	125.51	119.05
9	I	65	ASP	C-N-CA	5.82	125.51	119.05
2	B	1045	SER	CA-C-N	5.81	127.10	119.84
2	B	1045	SER	C-N-CA	5.81	127.10	119.84
10	J	42	LYS	N-CA-C	5.80	118.72	111.24
1	A	237	THR	N-CA-C	-5.78	106.26	113.55
9	I	68	LEU	CA-C-N	5.78	126.96	120.66
9	I	68	LEU	C-N-CA	5.78	126.96	120.66
1	A	1403	GLU	N-CA-C	5.74	123.03	110.80
2	B	1129	ARG	N-CA-C	5.73	117.74	108.34
2	B	165	VAL	N-CA-C	5.73	116.73	108.48
5	E	173	SER	N-CA-C	5.72	117.52	111.28
1	A	227	VAL	CB-CA-C	-5.69	105.83	111.30
4	D	8	PHE	N-CA-C	5.69	122.92	110.80
2	B	392	ARG	N-CA-C	-5.69	106.99	114.04
3	C	193	TYR	N-CA-C	5.68	116.88	108.86
1	A	682	THR	N-CA-C	-5.67	105.86	112.89
1	A	1311	VAL	N-CA-C	5.67	116.99	107.18
4	D	16	LYS	N-CA-C	5.67	118.40	109.39
1	A	158	PRO	N-CA-C	-5.66	106.62	114.27
2	B	1223	ASP	CB-CA-C	-5.65	109.06	115.79
1	A	311	GLN	N-CA-C	5.65	122.30	109.81
2	B	1173	ALA	N-CA-C	5.64	117.27	109.15
1	A	776	ALA	N-CA-C	5.63	118.58	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	896	ASP	N-CA-C	-5.62	106.27	113.01
11	K	77	THR	N-CA-C	5.61	116.77	108.86
2	B	964	VAL	N-CA-C	5.61	116.20	108.12
1	A	983	ILE	N-CA-C	-5.61	104.08	111.09
14	T	26	DC	C2'-C3'-O3'	-5.59	103.11	111.50
7	G	56	ILE	CB-CA-C	-5.59	106.14	111.06
1	A	491	VAL	N-CA-C	5.59	114.10	107.73
1	A	424	ILE	N-CA-C	5.58	120.94	109.34
2	B	424	LEU	N-CA-C	-5.57	104.83	111.69
2	B	543	SER	N-CA-C	5.57	117.93	110.35
5	E	4	GLU	N-CA-C	5.57	117.04	110.97
1	A	1291	VAL	CA-C-N	5.54	126.76	119.84
1	A	1291	VAL	C-N-CA	5.54	126.76	119.84
2	B	606	LYS	N-CA-C	-5.54	106.57	113.55
2	B	468	GLU	CB-CA-C	-5.53	108.59	116.34
1	A	1010	ALA	N-CA-C	-5.53	104.89	111.69
13	P	1	U	C4'-C3'-O3'	-5.52	104.71	113.00
7	G	30	LEU	N-CA-C	-5.52	104.49	111.11
7	G	127	PRO	CA-C-N	5.49	125.81	119.93
7	G	127	PRO	C-N-CA	5.49	125.81	119.93
2	B	1107	ALA	N-CA-C	-5.49	98.06	107.23
3	C	96	SER	N-CA-C	5.48	117.40	109.07
2	B	1104	HIS	N-CA-C	5.47	117.29	108.32
1	A	1444	MET	N-CA-C	5.47	117.71	109.23
13	P	9	G	C1'-C2'-O2'	5.47	116.60	108.40
4	D	34	GLN	N-CA-C	-5.46	103.49	110.53
1	A	236	LEU	N-CA-C	5.45	117.59	109.25
1	A	360	GLU	N-CA-C	-5.45	103.19	110.55
2	B	732	SER	N-CA-C	5.44	115.46	108.34
11	K	105	PHE	N-CA-C	-5.43	105.45	112.68
1	A	564	ALA	N-CA-C	-5.42	106.17	112.89
2	B	472	ALA	N-CA-C	5.42	117.33	108.55
2	B	1210	MET	N-CA-C	-5.39	106.89	112.93
5	E	84	ASP	N-CA-C	-5.39	106.74	113.15
2	B	1172	ILE	N-CA-C	5.38	111.97	106.21
2	B	395	GLN	N-CA-C	-5.35	103.47	110.53
11	K	112	GLN	N-CA-CB	-5.34	101.47	110.49
11	K	112	GLN	O-C-N	-5.33	115.51	122.59
5	E	52	ARG	CA-C-N	5.32	125.08	119.76
5	E	52	ARG	C-N-CA	5.32	125.08	119.76
1	A	1155	ASP	CA-C-N	5.30	124.99	119.64
1	A	1155	ASP	C-N-CA	5.30	124.99	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	188	ALA	N-CA-C	-5.29	105.57	112.23
4	D	15	LEU	N-CA-C	5.28	122.04	110.80
6	F	108	PHE	N-CA-C	5.26	118.82	112.93
5	E	177	ARG	N-CA-C	5.25	118.15	109.85
11	K	84	LYS	N-CA-C	-5.25	104.98	111.33
3	C	226	ASP	N-CA-C	-5.24	101.62	109.95
1	A	199	LEU	N-CA-C	5.23	116.83	108.41
1	A	224	PHE	N-CA-C	5.23	116.24	108.86
1	A	1445	ILE	CB-CA-C	-5.23	104.61	111.25
2	B	872	GLU	N-CA-C	-5.22	103.79	110.53
2	B	660	LYS	N-CA-C	-5.22	106.92	113.28
2	B	563	MET	N-CA-C	5.20	116.64	109.15
1	A	646	PHE	N-CA-C	-5.20	104.68	111.02
4	D	173	HIS	CA-C-N	5.18	126.32	119.84
4	D	173	HIS	C-N-CA	5.18	126.32	119.84
1	A	56	PRO	N-CA-C	-5.16	101.84	112.47
2	B	99	LYS	N-CA-C	-5.16	102.53	110.01
4	D	195	ILE	CA-C-N	5.16	126.29	119.84
4	D	195	ILE	C-N-CA	5.16	126.29	119.84
3	C	245	VAL	CB-CA-C	-5.15	105.23	111.87
2	B	771	SER	N-CA-C	-5.12	106.24	113.20
8	H	16	ASP	N-CA-C	5.12	118.40	107.91
2	B	413	LEU	N-CA-C	-5.11	105.83	111.71
2	B	195	CYS	CA-C-N	5.11	124.90	119.28
2	B	195	CYS	C-N-CA	5.11	124.90	119.28
4	D	157	GLN	N-CA-C	-5.11	107.11	113.19
2	B	943	SER	N-CA-C	5.10	121.66	110.80
2	B	1151	LEU	N-CA-C	5.10	116.92	111.36
4	D	66	ARG	N-CA-C	-5.09	104.71	112.04
1	A	1072	ILE	CB-CA-C	-5.09	105.25	111.92
1	A	778	GLY	N-CA-C	-5.08	106.56	113.37
5	E	55	ARG	N-CA-C	5.08	116.63	111.14
4	D	190	GLU	N-CA-C	-5.07	105.20	111.33
2	B	903	VAL	N-CA-C	5.05	119.84	109.34
3	C	183	TRP	N-CA-C	-5.05	98.36	107.75
2	B	277	LYS	N-CA-C	5.04	117.43	111.33
1	A	553	VAL	CA-C-N	5.04	126.14	119.84
1	A	553	VAL	C-N-CA	5.04	126.14	119.84
4	D	70	PHE	N-CA-C	-5.04	106.82	113.17
1	A	229	SER	N-CA-C	5.03	116.08	107.28
11	K	58	PHE	N-CA-C	5.03	116.05	108.46
1	A	831	THR	N-CA-C	-5.02	107.71	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	225	ALA	N-CA-C	5.01	118.16	107.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
2	B	486	TYR	Sidechain
14	T	19	DT	Sidechain
14	T	20	DC	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11186	0	11266	1395	0
2	B	8866	0	8898	1083	0
3	C	2101	0	2055	285	0
4	D	1427	0	1451	151	0
5	E	1752	0	1776	140	0
6	F	705	0	730	89	0
7	G	1340	0	1357	172	0
8	H	1084	0	1057	130	0
9	I	944	0	899	110	0
10	J	532	0	542	104	0
11	K	919	0	929	120	0
12	L	364	0	386	44	0
13	P	212	0	109	20	0
14	T	219	0	125	31	0
15	A	1	0	0	0	0
16	A	8	0	0	0	0
All	All	31660	0	31580	3568	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (3568) 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)
11:K:112:GLN:CB	11:K:112:GLN:CG	1.77	1.62
11:K:112:GLN:C	11:K:112:GLN:CA	1.78	1.56
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.18	1.17
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.26	1.17
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.12	1.15
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.28	1.13
1:A:53:LEU:HD23	1:A:54:ASN:N	1.64	1.11
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.33	1.06
1:A:855:THR:HG21	1:A:857:ARG:HE	1.15	1.05
2:B:214:ALA:HB3	2:B:498:THR:HA	1.32	1.05
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.35	1.04
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.21	1.04
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.39	1.04
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.72	1.03
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.70	1.03
1:A:225:ASN:HD22	1:A:228:PHE:H	1.05	1.02
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.38	1.02
7:G:138:THR:HG22	7:G:139:ILE:H	1.23	1.02
2:B:502:ILE:H	2:B:502:ILE:HD12	1.21	1.02
14:T:26:DC:H2''	14:T:27:DA:O5'	1.60	1.02
1:A:53:LEU:CD2	1:A:54:ASN:H	1.72	1.01
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.25	1.00
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.39	1.00
3:C:43:THR:HG22	3:C:44:LEU:H	1.27	0.99
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.43	0.99
1:A:34:LYS:HD3	1:A:57:ARG:HH22	0.86	0.99
2:B:589:VAL:HG12	2:B:590:HIS:H	1.25	0.99
1:A:567:LYS:HB3	8:H:96:VAL:H	1.28	0.99
1:A:524:VAL:HG12	1:A:525:GLN:H	1.25	0.98
14:T:26:DC:H2''	14:T:27:DA:C5'	1.93	0.98
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.63	0.98
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.44	0.97
2:B:65:GLU:HG3	2:B:66:ASP:H	1.29	0.97
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.95	0.96
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.46	0.96
11:K:65:HIS:HD2	11:K:67:PHE:H	1.11	0.96
1:A:53:LEU:HD23	1:A:54:ASN:H	0.81	0.95
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.96	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.46	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.31	0.95
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.29	0.95
1:A:40:THR:HG22	1:A:41:MET:HG3	1.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.31	0.94
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.49	0.94
2:B:516:ASN:HD22	2:B:516:ASN:N	1.63	0.94
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.50	0.94
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.31	0.94
10:J:1:MET:H1	10:J:57:ILE:N	1.64	0.94
4:D:144:THR:O	4:D:148:LEU:HB2	1.66	0.93
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.46	0.93
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.93
1:A:754:SER:H	1:A:757:ASN:HD22	1.14	0.93
2:B:806:THR:HG22	2:B:808:ALA:H	1.31	0.93
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.50	0.93
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.03	0.93
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.98	0.92
3:C:6:PRO:HB3	3:C:25:VAL:CG1	1.99	0.92
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.70	0.92
1:A:709:THR:HG22	1:A:711:ARG:H	1.33	0.91
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.91
2:B:168:GLY:H	2:B:450:ALA:HB1	1.35	0.91
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.51	0.91
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.51	0.91
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.71	0.91
6:F:111:LEU:HD12	6:F:111:LEU:H	1.35	0.91
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.36	0.91
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.52	0.90
9:I:85:PHE:H	9:I:85:PHE:HD2	1.18	0.90
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.51	0.90
11:K:65:HIS:CD2	11:K:67:PHE:H	1.89	0.90
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.51	0.90
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.50	0.90
10:J:1:MET:N	10:J:57:ILE:H	1.68	0.89
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.37	0.89
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.55	0.89
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.53	0.89
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.33	0.89
7:G:81:PRO:HG3	7:G:106:MET:SD	2.12	0.89
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.55	0.89
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.39	0.88
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.02	0.88
2:B:98:THR:O	2:B:126:SER:HB2	1.72	0.88
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.36	0.88
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.56	0.88
2:B:516:ASN:HD22	2:B:516:ASN:H	1.22	0.88
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.81	0.88
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.03	0.88
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.54	0.88
1:A:913:LEU:HD12	1:A:914:GLU:H	1.38	0.88
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.55	0.88
2:B:549:THR:HG22	2:B:550:ASP:H	1.38	0.87
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.56	0.87
8:H:36:CYS:HA	8:H:126:GLU:O	1.72	0.87
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.56	0.87
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.39	0.87
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.57	0.87
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.40	0.87
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.55	0.86
1:A:866:PHE:C	1:A:867:ILE:HD12	1.99	0.86
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.57	0.86
1:A:58:LEU:CD1	1:A:59:GLY:H	1.88	0.86
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.56	0.86
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.53	0.86
10:J:1:MET:H1	10:J:57:ILE:H	0.88	0.86
5:E:19:VAL:O	5:E:23:VAL:HG23	1.75	0.86
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.57	0.86
1:A:1094:VAL:HG12	1:A:1095:THR:N	1.91	0.86
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.11	0.85
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.56	0.85
2:B:515:HIS:H	2:B:518:HIS:HD2	1.24	0.85
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.58	0.85
2:B:654:ARG:H	2:B:657:HIS:HD2	1.19	0.85
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.57	0.85
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.40	0.85
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.11	0.85
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.55	0.85
1:A:67:CYS:O	1:A:70:CYS:HB3	1.77	0.85
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.41	0.85
1:A:709:THR:HG23	9:I:94:ASP:HA	1.58	0.84
7:G:80:LYS:HD3	7:G:80:LYS:N	1.92	0.84
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.18	0.84
2:B:46:GLN:HG3	2:B:47:GLN:H	1.39	0.84
2:B:842:ASN:ND2	2:B:845:SER:H	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:THR:HG21	9:I:66:PRO:HA	1.60	0.84
2:B:332:ASP:O	2:B:336:ARG:HG3	1.78	0.84
8:H:4:THR:HA	8:H:60:ALA:HB2	1.58	0.84
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.59	0.84
1:A:308:ILE:HG22	1:A:309:ALA:H	1.42	0.83
1:A:858:ASN:C	1:A:858:ASN:HD22	1.84	0.83
1:A:1329:THR:HG22	1:A:1331:SER:H	1.43	0.83
3:C:32:SER:O	3:C:36:VAL:HG23	1.77	0.83
1:A:58:LEU:HD12	1:A:59:GLY:H	1.44	0.83
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.08	0.83
3:C:33:LEU:HG	3:C:37:MET:HE2	1.60	0.83
6:F:82:THR:HG22	6:F:84:TYR:H	1.42	0.83
1:A:885:THR:O	1:A:940:ARG:HD2	1.78	0.83
2:B:465:ASN:HD22	2:B:465:ASN:N	1.77	0.83
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.91	0.83
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.43	0.83
8:H:100:THR:HG23	8:H:138:GLU:HA	1.57	0.83
1:A:741:ASN:HD22	1:A:744:LYS:H	1.27	0.83
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.79	0.83
1:A:855:THR:HG21	1:A:857:ARG:NE	1.93	0.83
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.25	0.83
4:D:40:HIS:CB	7:G:73:LYS:HZ3	1.91	0.83
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.94	0.83
2:B:336:ARG:NH2	2:B:345:LYS:HG2	1.94	0.83
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.83
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.60	0.83
1:A:34:LYS:H	1:A:57:ARG:NH2	1.77	0.82
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.13	0.82
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.59	0.82
2:B:365:THR:HG23	2:B:367:LEU:H	1.42	0.82
2:B:955:THR:HG22	2:B:956:THR:H	1.44	0.82
14:T:21:DC:H2''	14:T:22:BRU:H5''	1.62	0.82
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.94	0.82
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.60	0.82
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.08	0.82
7:G:14:HIS:ND1	7:G:15:PRO:HD2	1.95	0.82
13:P:3:G:H2'	13:P:4:A:C8	2.15	0.82
1:A:901:LEU:H	1:A:926:GLN:NE2	1.78	0.82
2:B:615:MET:C	2:B:616:ILE:HD12	2.05	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.61	0.81
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.16	0.81
1:A:903:ASN:ND2	1:A:905:ASP:H	1.78	0.81
2:B:467:GLY:N	2:B:475:SER:HB3	1.95	0.81
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.10	0.81
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.62	0.81
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.81	0.81
2:B:343:ILE:HG21	2:B:348:ARG:N	1.95	0.81
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.62	0.81
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.61	0.81
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.81	0.81
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.10	0.81
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.45	0.81
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.44	0.81
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.14	0.81
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.60	0.81
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.63	0.81
8:H:59:ILE:HG22	8:H:60:ALA:N	1.94	0.81
1:A:321:PRO:O	1:A:322:VAL:HB	1.79	0.80
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.61	0.80
1:A:535:THR:HG21	1:A:616:VAL:HA	1.63	0.80
1:A:70:CYS:O	1:A:72:GLU:HG2	1.81	0.80
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.45	0.80
14:T:26:DC:H2''	14:T:27:DA:H5'	1.62	0.80
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.47	0.80
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.17	0.80
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.64	0.80
3:C:47:ASP:HA	12:L:69:ALA:CB	2.12	0.80
3:C:167:HIS:HD2	3:C:168:ALA:H	1.30	0.80
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.65	0.79
1:A:886:ILE:HG22	1:A:887:GLY:N	1.96	0.79
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.64	0.79
9:I:105:SER:O	9:I:106:CYS:HB3	1.80	0.79
1:A:903:ASN:HD22	1:A:904:THR:N	1.79	0.79
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.62	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.83	0.79
4:D:47:LEU:HD13	4:D:48:ILE:H	1.47	0.79
14:T:25:DT:H2''	14:T:26:DC:O5'	1.82	0.79
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.18	0.79
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.18	0.79
1:A:450:LEU:H	1:A:450:LEU:HD12	1.48	0.79
7:G:80:LYS:HD3	7:G:80:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.65	0.79
3:C:35:ARG:NH1	11:K:41:THR:H	1.80	0.78
3:C:73:GLN:HE21	3:C:75:MET:N	1.81	0.78
11:K:112:GLN:C	11:K:112:GLN:HA	2.02	0.78
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.65	0.78
1:A:903:ASN:HD22	1:A:903:ASN:C	1.89	0.78
2:B:336:ARG:HD3	2:B:348:ARG:NH1	1.98	0.78
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.84	0.78
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.65	0.78
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.98	0.78
2:B:975:GLN:O	2:B:990:ILE:HD12	1.83	0.78
1:A:472:LEU:O	1:A:475:THR:HB	1.83	0.78
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.10	0.78
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.64	0.78
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.64	0.78
1:A:385:ILE:HG22	1:A:386:ASP:N	1.97	0.78
2:B:336:ARG:CD	2:B:348:ARG:HH11	1.96	0.78
2:B:708:GLU:O	2:B:710:LEU:N	2.17	0.78
1:A:341:MET:HE2	1:A:843:LYS:NZ	1.98	0.78
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.65	0.78
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.65	0.78
1:A:768:GLN:CG	1:A:816:HIS:HA	2.13	0.78
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.48	0.78
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.49	0.78
9:I:111:THR:HG22	9:I:112:SER:H	1.49	0.78
14:T:18:DT:H2''	14:T:19:DT:H5'	1.66	0.78
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.99	0.77
3:C:244:VAL:O	3:C:248:ILE:HG13	1.84	0.77
6:F:85:MET:HE2	6:F:93:ILE:HD12	1.66	0.77
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.64	0.77
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.49	0.77
11:K:47:ARG:HB3	11:K:47:ARG:NH1	1.99	0.77
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.25	0.77
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.49	0.77
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.64	0.77
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.65	0.77
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.67	0.77
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.99	0.77
6:F:69:LEU:HA	6:F:70:LYS:N	1.98	0.77
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.65	0.77
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.67	0.77
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.20	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.99	0.77
2:B:359:GLU:O	2:B:362:PRO:HD3	1.84	0.77
8:H:56:THR:HB	8:H:145:ARG:HG2	1.65	0.77
1:A:567:LYS:HB3	8:H:96:VAL:N	1.99	0.76
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.00	0.76
3:C:43:THR:HG22	3:C:44:LEU:N	1.98	0.76
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.67	0.76
1:A:341:MET:HE1	2:B:1135:ARG:NH1	1.99	0.76
9:I:34:TYR:CD2	9:I:35:VAL:N	2.53	0.76
11:K:12:LEU:H	11:K:12:LEU:HD12	1.49	0.76
1:A:63:ARG:HA	1:A:74:MET:SD	2.25	0.76
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.51	0.76
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.19	0.76
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.50	0.76
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.03	0.76
1:A:58:LEU:CG	1:A:59:GLY:H	1.97	0.76
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.68	0.76
1:A:858:ASN:ND2	1:A:860:LEU:H	1.83	0.76
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.84	0.76
3:C:167:HIS:HD2	3:C:168:ALA:N	1.83	0.76
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.67	0.76
2:B:128:LEU:HB2	2:B:168:GLY:O	1.85	0.76
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.21	0.76
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.49	0.76
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.00	0.76
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.50	0.76
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.65	0.76
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.00	0.76
3:C:2:SER:N	3:C:3:GLU:N	2.33	0.76
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.68	0.76
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.12	0.76
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.86	0.76
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.16	0.76
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.26	0.76
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.67	0.76
8:H:130:ARG:H	8:H:130:ARG:HD2	1.48	0.76
1:A:230:ARG:H	1:A:233:TRP:HE3	1.31	0.75
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.85	0.75
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:SD	1:A:577:ILE:HD11	2.26	0.75
2:B:189:LEU:O	2:B:192:LEU:N	2.15	0.75
2:B:467:GLY:H	2:B:475:SER:HB3	1.51	0.75
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.68	0.75
1:A:646:PHE:O	1:A:650:GLN:HG3	1.87	0.75
2:B:112:LEU:HD12	2:B:113:TYR:H	1.51	0.75
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.20	0.75
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.67	0.75
6:F:103:MET:HE2	7:G:66:GLY:H	1.49	0.75
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.67	0.75
1:A:35:ILE:HG22	1:A:35:ILE:O	1.86	0.75
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.49	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.21	0.75
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.50	0.75
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.86	0.75
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.21	0.75
1:A:1325:THR:O	5:E:148:GLU:HB2	1.86	0.75
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.16	0.75
3:C:73:GLN:HE21	3:C:75:MET:H	1.33	0.75
3:C:164:ALA:HA	3:C:167:HIS:O	1.86	0.75
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.67	0.74
8:H:61:SER:O	8:H:62:SER:HB3	1.85	0.74
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.23	0.74
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.00	0.74
2:B:65:GLU:HG3	2:B:66:ASP:N	2.01	0.74
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.69	0.74
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.17	0.74
3:C:142:VAL:H	10:J:16:ASP:HB3	1.52	0.74
7:G:128:PRO:O	7:G:138:THR:HG23	1.87	0.74
1:A:714:PHE:O	1:A:718:VAL:HG23	1.87	0.74
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.74
1:A:512:VAL:HA	1:A:519:PRO:HA	1.68	0.74
1:A:534:LEU:O	1:A:574:GLY:HA3	1.85	0.74
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.69	0.74
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.28	0.74
2:B:35:SER:HA	2:B:811:TYR:HE2	1.52	0.74
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.88	0.74
4:D:22:GLU:H	4:D:22:GLU:CD	1.96	0.74
4:D:176:GLU:C	4:D:178:ALA:H	1.96	0.74
7:G:111:THR:HG22	7:G:113:HIS:H	1.51	0.74
11:K:111:LEU:C	11:K:112:GLN:HG2	2.13	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.23	0.74
1:A:58:LEU:HD13	1:A:80:HIS:O	1.87	0.74
2:B:830:TYR:O	2:B:832:GLY:N	2.21	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.02	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.70	0.74
1:A:1436:ILE:O	1:A:1437:GLY:C	2.31	0.74
3:C:213:PRO:O	3:C:214:ASN:HB2	1.87	0.74
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.68	0.74
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.17	0.74
8:H:59:ILE:HG22	8:H:60:ALA:H	1.53	0.74
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.68	0.74
2:B:336:ARG:HH22	2:B:345:LYS:CE	1.99	0.74
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.03	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.36	0.74
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.69	0.74
4:D:7:THR:HG21	4:D:32:GLU:CD	2.13	0.74
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.70	0.74
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.14	0.73
2:B:516:ASN:N	2:B:516:ASN:ND2	2.36	0.73
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.18	0.73
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.52	0.73
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.03	0.73
6:F:125:LEU:HG	6:F:125:LEU:O	1.88	0.73
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.53	0.73
1:A:225:ASN:ND2	1:A:228:PHE:H	1.84	0.73
1:A:518:LYS:HE2	1:A:624:SER:O	1.88	0.73
2:B:378:LEU:O	2:B:382:ILE:HG13	1.88	0.73
2:B:863:GLU:OE2	2:B:873:THR:HA	1.88	0.73
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.23	0.73
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.03	0.73
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.54	0.73
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.69	0.73
13:P:5:C:H2'	13:P:6:C:C6	2.23	0.73
13:P:5:C:H2'	13:P:6:C:H6	1.53	0.73
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.69	0.73
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.24	0.73
2:B:434:ARG:O	2:B:437:GLU:HB2	1.87	0.73
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.20	0.73
12:L:38:LEU:O	12:L:39:SER:HB3	1.89	0.73
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.70	0.73
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:HB	1:A:985:ASP:H	1.53	0.73
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.19	0.73
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.70	0.73
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.71	0.73
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.01	0.73
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.18	0.73
2:B:502:ILE:HD12	2:B:502:ILE:N	2.01	0.73
1:A:68:GLN:C	1:A:70:CYS:H	1.94	0.72
3:C:253:LYS:O	3:C:256:ALA:HB3	1.88	0.72
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.71	0.72
2:B:864:LYS:N	2:B:872:GLU:OE1	2.22	0.72
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.72
1:A:347:PHE:H	2:B:1107:ALA:HA	1.54	0.72
4:D:53:SER:HB3	4:D:152:SER:HB2	1.71	0.72
1:A:384:ASN:O	1:A:385:ILE:C	2.32	0.72
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.52	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.24	0.72
1:A:92:HIS:O	1:A:94:GLY:N	2.21	0.72
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.72
1:A:106:VAL:HG13	1:A:112:LYS:O	1.88	0.72
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.70	0.72
1:A:960:ILE:O	1:A:963:ILE:HG22	1.89	0.72
2:B:616:ILE:HD12	2:B:616:ILE:N	2.04	0.72
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.25	0.72
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.24	0.72
7:G:79:PHE:HZ	7:G:106:MET:HE2	1.54	0.72
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.52	0.72
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.05	0.72
4:D:34:GLN:O	4:D:47:LEU:HD23	1.89	0.72
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.90	0.71
5:E:22:MET:CE	5:E:26:ARG:HH21	2.02	0.71
7:G:47:CYS:O	7:G:76:ALA:HB1	1.90	0.71
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.53	0.71
11:K:31:VAL:HG12	11:K:32:VAL:N	2.04	0.71
1:A:58:LEU:HG	1:A:59:GLY:N	2.04	0.71
1:A:1329:THR:HG22	1:A:1331:SER:N	2.05	0.71
2:B:882:THR:HG22	2:B:884:ARG:N	2.04	0.71
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.73	0.71
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.71
11:K:65:HIS:HD2	11:K:67:PHE:N	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.25	0.71
2:B:37:PHE:HE2	2:B:542:MET:HA	1.55	0.71
1:A:567:LYS:CB	8:H:95:TYR:HA	2.20	0.71
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.72	0.71
2:B:842:ASN:O	2:B:846:ILE:HG13	1.90	0.71
14:T:20:DC:H2''	14:T:21:DC:H5'	1.71	0.71
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.71	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.71
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.71	0.71
2:B:589:VAL:HG12	2:B:590:HIS:N	2.04	0.71
1:A:754:SER:H	1:A:757:ASN:ND2	1.89	0.71
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.71
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.73	0.71
1:A:832:ALA:HB2	14:T:18:DT:H71	1.72	0.71
2:B:63:ILE:O	2:B:67:SER:HB3	1.90	0.71
3:C:133:ILE:HD11	3:C:237:SER:HA	1.73	0.71
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.73	0.71
4:D:7:THR:HB	7:G:42:PHE:CE2	2.26	0.71
14:T:24:DG:H2''	14:T:25:DT:H5'	1.72	0.71
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.06	0.70
1:A:741:ASN:ND2	1:A:744:LYS:H	1.87	0.70
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.06	0.70
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.07	0.70
2:B:247:GLY:C	2:B:249:ARG:H	1.96	0.70
3:C:98:VAL:C	3:C:99:LEU:HD23	2.16	0.70
4:D:53:SER:HB3	4:D:152:SER:CB	2.21	0.70
2:B:95:ILE:HG13	2:B:129:PHE:O	1.90	0.70
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.72	0.70
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.06	0.70
6:F:111:LEU:HD12	6:F:111:LEU:N	2.06	0.70
1:A:58:LEU:HG	1:A:59:GLY:H	1.56	0.70
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.56	0.70
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.26	0.70
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.73	0.70
4:D:130:LEU:C	4:D:132:GLN:H	1.99	0.70
11:K:6:ARG:O	11:K:9:LEU:HG	1.91	0.70
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.02	0.70
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.74	0.70
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.73	0.70
1:A:254:GLU:O	1:A:256:GLN:N	2.24	0.70
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:O	1:A:531:ILE:HG22	1.91	0.70
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.72	0.70
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.39	0.70
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.22	0.70
7:G:18:PHE:HA	7:G:22:MET:HE3	1.74	0.70
2:B:232:SER:CB	2:B:261:ARG:HH21	2.03	0.70
2:B:278:GLN:HG2	2:B:279:ASP:H	1.55	0.70
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.55	0.70
3:C:56:THR:HG22	3:C:57:VAL:H	1.55	0.70
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.73	0.70
2:B:942:ARG:NH2	14:T:24:DG:OP2	2.21	0.70
1:A:50:ILE:C	1:A:52:GLY:H	2.00	0.70
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.27	0.70
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.74	0.70
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.55	0.70
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.21	0.70
14:T:18:DT:H2''	14:T:19:DT:C5'	2.21	0.70
2:B:557:PHE:C	2:B:557:PHE:CD2	2.70	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.92	0.70
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.57	0.69
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.22	0.69
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.22	0.69
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.73	0.69
1:A:1005:GLU:O	1:A:1009:ASN:HB2	1.92	0.69
1:A:663:SER:OG	1:A:664:THR:N	2.25	0.69
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.57	0.69
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.72	0.69
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.74	0.69
2:B:180:TYR:HD1	2:B:180:TYR:H	1.40	0.69
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.56	0.69
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.74	0.69
2:B:860:MET:HG2	2:B:861:ASP:H	1.57	0.69
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.22	0.69
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.74	0.69
2:B:295:GLY:H	2:B:298:LEU:HD23	1.56	0.69
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.73	0.69
2:B:745:PRO:O	2:B:748:ILE:HG12	1.92	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.72	0.69
1:A:913:LEU:HD12	1:A:914:GLU:N	2.07	0.69
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:O	1:A:598:LEU:N	2.26	0.69
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.22	0.69
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.73	0.69
6:F:103:MET:O	6:F:104:ASN:HB2	1.91	0.69
1:A:23:SER:HA	1:A:233:TRP:CD1	2.28	0.69
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.23	0.69
2:B:953:LEU:HD23	2:B:953:LEU:O	1.92	0.69
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.69
3:C:35:ARG:NH1	11:K:41:THR:N	2.40	0.69
4:D:134:THR:HG22	4:D:135:GLY:N	2.08	0.69
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.08	0.69
7:G:138:THR:HG22	7:G:139:ILE:N	2.04	0.69
14:T:21:DC:H2''	14:T:22:BRU:C5'	2.23	0.69
1:A:58:LEU:CG	1:A:59:GLY:N	2.55	0.69
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.21	0.69
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.75	0.69
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.75	0.69
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.75	0.69
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.93	0.68
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.28	0.68
2:B:860:MET:HG2	2:B:861:ASP:N	2.08	0.68
3:C:167:HIS:CD2	3:C:168:ALA:N	2.61	0.68
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.56	0.68
12:L:30:ILE:O	12:L:56:LEU:HA	1.93	0.68
1:A:55:ASP:N	1:A:56:PRO:HD3	2.09	0.68
1:A:388:LEU:O	1:A:392:VAL:HG23	1.93	0.68
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.57	0.68
1:A:881:GLN:NE2	1:A:958:VAL:O	2.26	0.68
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.23	0.68
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.74	0.68
2:B:339:THR:O	2:B:339:THR:HG22	1.93	0.68
10:J:23:ASN:C	10:J:25:LEU:H	2.00	0.68
11:K:67:PHE:C	11:K:68:PHE:HD2	2.00	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.94	0.68
2:B:705:MET:H	2:B:710:LEU:HD12	1.58	0.68
1:A:35:ILE:HA	1:A:52:GLY:O	1.94	0.68
1:A:694:THR:O	1:A:698:GLN:HG3	1.94	0.68
2:B:411:PRO:O	2:B:414:ALA:HB3	1.94	0.68
2:B:841:MET:HE1	2:B:980:PHE:CE1	2.28	0.68
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.41	0.68
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.75	0.68
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.94	0.68
3:C:90:ASP:O	3:C:91:HIS:HB3	1.93	0.68
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.09	0.68
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.09	0.68
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.58	0.68
2:B:114:PRO:HG2	2:B:115:GLN:H	1.56	0.68
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.58	0.68
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.75	0.68
1:A:979:SER:OG	1:A:980:ASP:N	2.25	0.68
2:B:315:LYS:N	2:B:316:PRO:HD2	2.08	0.68
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.09	0.68
1:A:57:ARG:O	1:A:68:GLN:HG3	1.94	0.68
1:A:69:THR:C	1:A:71:GLN:H	2.01	0.68
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.76	0.68
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.24	0.68
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.23	0.68
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.92	0.68
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.28	0.68
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.23	0.68
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.33	0.68
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.59	0.67
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.10	0.67
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.29	0.67
1:A:524:VAL:HG12	1:A:525:GLN:N	2.03	0.67
1:A:657:LEU:O	1:A:657:LEU:HD12	1.95	0.67
2:B:549:THR:H	2:B:628:THR:HG23	1.59	0.67
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.76	0.67
3:C:73:GLN:NE2	3:C:74:SER:H	1.92	0.67
11:K:61:TYR:C	11:K:61:TYR:CD2	2.72	0.67
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.60	0.67
1:A:675:THR:O	1:A:679:ILE:HG13	1.93	0.67
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.95	0.67
4:D:189:ASP:O	4:D:193:THR:HB	1.93	0.67
1:A:401:GLY:C	1:A:435:HIS:HD2	2.02	0.67
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.75	0.67
2:B:516:ASN:H	2:B:516:ASN:ND2	1.85	0.67
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.74	0.67
3:C:147:LEU:N	3:C:147:LEU:HD23	2.09	0.67
4:D:63:LEU:HD13	4:D:133:THR:OG1	1.94	0.67
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:O	1:A:253:ASN:HB2	1.95	0.67
7:G:39:THR:HG22	7:G:41:LYS:H	1.60	0.67
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.95	0.67
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.76	0.67
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.59	0.67
5:E:157:SER:C	5:E:159:ASP:H	2.03	0.67
1:A:33:ALA:HA	1:A:57:ARG:NH2	2.09	0.67
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.29	0.67
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.75	0.67
2:B:601:ARG:O	2:B:605:ARG:HG3	1.94	0.67
4:D:60:LYS:O	4:D:64:VAL:HG23	1.95	0.67
5:E:157:SER:OG	5:E:160:GLU:HG3	1.94	0.67
6:F:81:THR:HG23	6:F:144:GLU:OE2	1.95	0.67
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.95	0.67
1:A:265:LYS:N	1:A:265:LYS:HD2	2.09	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
2:B:794:ASN:O	2:B:795:ILE:HD12	1.94	0.67
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.10	0.67
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.75	0.67
9:I:34:TYR:HD2	9:I:35:VAL:N	1.92	0.67
3:C:35:ARG:HH12	11:K:41:THR:H	1.40	0.67
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.67
8:H:4:THR:HA	8:H:60:ALA:CB	2.25	0.67
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.29	0.66
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.76	0.66
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.59	0.66
3:C:147:LEU:HD12	3:C:151:GLN:O	1.95	0.66
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.75	0.66
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.77	0.66
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.26	0.66
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.24	0.66
8:H:143:LEU:HD12	8:H:143:LEU:N	2.10	0.66
1:A:69:THR:C	1:A:71:GLN:N	2.53	0.66
1:A:164:ARG:HG3	1:A:165:GLY:N	2.09	0.66
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.60	0.66
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	1.94	0.66
1:A:1445:ILE:HD12	1:A:1445:ILE:N	1.96	0.66
4:D:52:LEU:C	4:D:54:GLU:H	2.04	0.66
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.77	0.66
2:B:857:ARG:NH2	14:T:24:DG:OP1	2.29	0.66
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:VAL:O	10:J:14:VAL:HG12	1.95	0.66
1:A:856:THR:HB	1:A:865:GLN:HB2	1.77	0.66
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.78	0.66
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.20	0.66
1:A:986:ILE:HG22	1:A:987:VAL:N	2.09	0.66
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.77	0.66
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.62	0.66
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.94	0.66
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.42	0.66
1:A:844:ALA:C	1:A:845:LEU:HD23	2.21	0.66
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.77	0.66
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.61	0.66
6:F:97:ARG:O	6:F:101:ILE:HG13	1.96	0.66
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.76	0.66
4:D:128:VAL:O	4:D:132:GLN:HG3	1.96	0.66
5:E:117:THR:HG22	5:E:119:SER:H	1.60	0.66
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.78	0.66
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.78	0.66
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.08	0.66
1:A:438:ASP:OD1	1:A:462:VAL:HG23	1.96	0.66
2:B:642:ASP:O	2:B:644:GLU:N	2.28	0.66
2:B:882:THR:HB	2:B:934:LYS:O	1.96	0.66
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.95	0.66
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.77	0.66
1:A:546:VAL:O	1:A:550:LEU:HG	1.95	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.96	0.65
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.79	0.65
1:A:58:LEU:HD12	1:A:59:GLY:N	2.11	0.65
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.26	0.65
1:A:699:ALA:CB	1:A:701:LEU:HG	2.27	0.65
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.78	0.65
1:A:1035:TYR:O	1:A:1037:LEU:N	2.29	0.65
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	1.95	0.65
9:I:82:GLU:O	9:I:104:LEU:HG	1.96	0.65
10:J:1:MET:N	10:J:56:LEU:N	2.44	0.65
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.78	0.65
3:C:66:ARG:NH1	3:C:144:ILE:O	2.28	0.65
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.77	0.65
8:H:81:PRO:CB	8:H:82:PRO:CD	2.74	0.65
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.77	0.65
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.12	0.65
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.97	0.65
2:B:756:ILE:O	2:B:759:PRO:HD3	1.96	0.65
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.32	0.65
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.27	0.65
6:F:111:LEU:C	6:F:113:GLY:H	2.05	0.65
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.25	0.65
1:A:265:LYS:HD2	1:A:265:LYS:H	1.62	0.65
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.75	0.65
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.65
2:B:18:PHE:N	2:B:19:GLU:N	2.44	0.65
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.60	0.65
4:D:7:THR:HB	7:G:42:PHE:HE2	1.62	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.78	0.65
2:B:563:MET:HE3	2:B:580:VAL:HB	1.79	0.65
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.44	0.65
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.11	0.65
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.62	0.65
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.65
1:A:450:LEU:HB3	1:A:838:GLN:NE2	2.12	0.65
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.62	0.65
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.27	0.65
7:G:49:LEU:HG	7:G:76:ALA:HA	1.78	0.65
9:I:75:CYS:SG	9:I:79:HIS:N	2.69	0.65
1:A:311:GLN:O	1:A:312:PRO:C	2.40	0.65
1:A:588:LEU:O	1:A:606:LEU:HA	1.96	0.65
1:A:901:LEU:O	1:A:921:GLY:N	2.25	0.65
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.78	0.65
2:B:57:TYR:N	2:B:57:TYR:HD1	1.95	0.65
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.79	0.65
2:B:850:LEU:HD12	2:B:851:PHE:N	2.11	0.65
1:A:450:LEU:HD12	1:A:450:LEU:N	2.12	0.64
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.26	0.64
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.79	0.64
2:B:906:SER:O	2:B:941:LEU:HD23	1.97	0.64
8:H:44:VAL:O	8:H:44:VAL:HG12	1.97	0.64
11:K:47:ARG:O	11:K:47:ARG:HD2	1.96	0.64
1:A:42:ASP:HB3	1:A:45:GLN:H	1.63	0.64
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.61	0.64
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.33	0.64
2:B:1172:ILE:HG22	2:B:1172:ILE:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:26:DC:C2'	14:T:27:DA:O5'	2.41	0.64
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.62	0.64
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.13	0.64
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.32	0.64
2:B:999:MET:HA	2:B:999:MET:HE3	1.79	0.64
1:A:108:MET:N	1:A:108:MET:SD	2.70	0.64
1:A:626:ASN:O	1:A:631:HIS:CD2	2.50	0.64
2:B:57:TYR:N	2:B:57:TYR:CD1	2.66	0.64
2:B:336:ARG:NH2	2:B:345:LYS:HE2	2.06	0.64
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.64
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.78	0.64
5:E:114:ASN:O	5:E:115:ASN:HB3	1.96	0.64
13:P:3:G:H2'	13:P:4:A:H8	1.58	0.64
1:A:23:SER:HA	1:A:233:TRP:NE1	2.13	0.64
1:A:244:PRO:O	1:A:246:VAL:N	2.30	0.64
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.30	0.64
2:B:433:GLN:O	2:B:437:GLU:HG3	1.96	0.64
2:B:542:MET:HE2	2:B:743:ILE:HG13	1.78	0.64
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.62	0.64
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.10	0.64
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.45	0.64
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.78	0.64
1:A:69:THR:O	1:A:71:GLN:N	2.30	0.64
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.80	0.64
2:B:654:ARG:H	2:B:657:HIS:CD2	2.10	0.64
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.63	0.64
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.26	0.64
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.28	0.64
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.62	0.64
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.64
6:F:85:MET:HE2	6:F:93:ILE:CD1	2.27	0.64
7:G:111:THR:HB	7:G:114:LEU:HB2	1.80	0.64
7:G:119:LEU:HD12	7:G:131:GLN:O	1.97	0.64
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.64
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.98	0.64
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.33	0.64
1:A:984:LYS:O	1:A:988:LEU:HB2	1.98	0.64
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.26	0.64
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.13	0.64
4:D:51:ASN:O	4:D:54:GLU:HB3	1.97	0.64
1:A:58:LEU:CD2	1:A:244:PRO:HD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD12	1:A:667:GLY:H	1.63	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.28	0.64
7:G:145:VAL:HG12	7:G:146:LYS:N	2.12	0.64
10:J:48:ARG:HE	10:J:49:MET:CE	2.11	0.64
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.28	0.64
1:A:485:ASP:OD1	13:P:10:A:O2'	2.15	0.64
1:A:590:ARG:HB3	1:A:605:MET:N	2.12	0.64
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.64
2:B:842:ASN:HB3	2:B:845:SER:OG	1.98	0.64
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.32	0.64
6:F:79:ARG:HG3	6:F:144:GLU:OE1	1.98	0.64
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.98	0.64
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	0.64
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.13	0.63
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.63
1:A:728:LYS:O	1:A:732:LEU:HG	1.98	0.63
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.61	0.63
6:F:85:MET:CE	6:F:93:ILE:HD12	2.29	0.63
7:G:143:ILE:HG22	7:G:144:ARG:N	2.13	0.63
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.63
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.32	0.63
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.28	0.63
1:A:19:PHE:O	1:A:1416:ALA:HA	1.98	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.27	0.63
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.29	0.63
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.63	0.63
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.63	0.63
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.64	0.63
2:B:806:THR:HG22	2:B:808:ALA:N	2.07	0.63
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.12	0.63
3:C:22:LEU:HD13	3:C:230:MET:CE	2.29	0.63
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.23	0.63
1:A:105:CYS:O	1:A:114:LEU:HG	1.98	0.63
1:A:401:GLY:C	1:A:435:HIS:CD2	2.76	0.63
1:A:743:VAL:O	1:A:747:VAL:HG23	1.99	0.63
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.99	0.63
2:B:589:VAL:CG1	2:B:590:HIS:H	2.08	0.63
3:C:167:HIS:CD2	3:C:168:ALA:H	2.16	0.63
3:C:214:ASN:HB3	3:C:217:ASP:OD2	1.98	0.63
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.32	0.63
7:G:51:TYR:C	7:G:51:TYR:CD2	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:CG	1:A:55:ASP:O	2.39	0.63
1:A:58:LEU:CD1	1:A:80:HIS:H	2.12	0.63
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.63	0.63
3:C:189:THR:HG22	3:C:190:ASP:N	2.14	0.63
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.33	0.63
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.80	0.63
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.63	0.63
2:B:825:VAL:CG1	2:B:826:ALA:N	2.62	0.63
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.81	0.63
7:G:39:THR:HG22	7:G:40:GLY:N	2.13	0.63
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.80	0.63
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.28	0.63
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.14	0.63
2:B:235:SER:HA	2:B:261:ARG:NH1	2.13	0.63
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.81	0.63
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.98	0.63
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.81	0.63
3:C:100:THR:OG1	3:C:121:VAL:HG21	1.99	0.63
4:D:51:ASN:O	4:D:52:LEU:O	2.17	0.63
1:A:475:THR:HG23	1:A:476:SER:N	2.13	0.62
1:A:648:ASN:O	1:A:649:ILE:C	2.42	0.62
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.34	0.62
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.62
2:B:654:ARG:C	2:B:656:GLY:H	2.05	0.62
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.81	0.62
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.99	0.62
14:T:20:DC:H2''	14:T:21:DC:C5'	2.29	0.62
1:A:34:LYS:CE	1:A:57:ARG:HH12	2.12	0.62
1:A:1187:GLN:O	1:A:1243:VAL:HG13	1.99	0.62
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.99	0.62
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.28	0.62
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.34	0.62
2:B:880:THR:O	2:B:881:ASN:HB2	1.98	0.62
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.97	0.62
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.97	0.62
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.81	0.62
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.79	0.62
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.30	0.62
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.33	0.62
3:C:124:LEU:O	3:C:127:ARG:HG2	1.99	0.62
8:H:89:LEU:C	8:H:91:ASP:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:THR:HG22	9:I:52:ILE:H	1.64	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.32	0.62
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.14	0.62
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.62
3:C:69:LEU:N	3:C:69:LEU:HD12	2.15	0.62
9:I:2:THR:O	9:I:3:THR:C	2.41	0.62
2:B:515:HIS:H	2:B:518:HIS:CD2	2.10	0.62
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.15	0.62
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.81	0.62
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.80	0.62
6:F:77:ASP:C	6:F:79:ARG:H	2.07	0.62
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.81	0.62
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.29	0.62
6:F:69:LEU:CA	6:F:70:LYS:N	2.62	0.62
6:F:118:LEU:O	6:F:122:MET:HG3	1.98	0.62
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.14	0.62
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.81	0.62
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.81	0.62
1:A:1385:THR:O	1:A:1387:HIS:N	2.32	0.62
2:B:446:LEU:O	2:B:447:ALA:HB3	1.99	0.62
3:C:66:ARG:NH2	10:J:3:VAL:O	2.32	0.62
8:H:128:ASN:CG	8:H:128:ASN:O	2.42	0.62
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.14	0.62
1:A:63:ARG:HA	1:A:74:MET:CE	2.29	0.62
3:C:18:VAL:O	3:C:20:PHE:HD2	1.83	0.62
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.64	0.62
3:C:226:ASP:O	3:C:227:THR:HB	2.00	0.62
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.80	0.62
1:A:482:PHE:C	1:A:484:GLY:H	2.07	0.62
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.30	0.62
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.80	0.62
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.64	0.62
2:B:916:THR:O	2:B:935:ARG:HG3	1.99	0.62
4:D:4:SER:O	4:D:5:THR:HB	1.98	0.62
5:E:22:MET:HE3	5:E:26:ARG:HE	1.64	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.00	0.62
12:L:58:LYS:O	12:L:58:LYS:HG2	2.00	0.62
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.80	0.62
1:A:714:PHE:CB	9:I:97:MET:HE1	2.30	0.62
2:B:185:THR:H	2:B:188:ASP:HB2	1.63	0.62
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.35	0.62
2:B:902:GLY:O	12:L:65:VAL:HG11	2.00	0.62
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.14	0.62
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.35	0.62
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.82	0.62
11:K:47:ARG:HD2	11:K:47:ARG:C	2.25	0.62
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.30	0.61
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.00	0.61
11:K:63:VAL:HG23	11:K:63:VAL:O	2.00	0.61
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.82	0.61
1:A:108:MET:SD	1:A:210:ILE:HD13	2.41	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.36	0.61
3:C:208:GLU:O	3:C:210:GLU:N	2.33	0.61
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.82	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.14	0.61
5:E:177:ARG:HD3	5:E:215:MET:CG	2.30	0.61
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.66	0.61
1:A:763:ALA:O	1:A:803:SER:HB3	1.99	0.61
1:A:765:VAL:HG23	1:A:802:ASN:O	2.00	0.61
1:A:858:ASN:C	1:A:858:ASN:ND2	2.54	0.61
2:B:770:GLN:CD	2:B:983:ARG:HA	2.24	0.61
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.35	0.61
3:C:34:ARG:HA	3:C:37:MET:HE3	1.81	0.61
4:D:130:LEU:O	4:D:132:GLN:N	2.33	0.61
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.63	0.61
1:A:144:THR:O	1:A:146:MET:HG3	2.00	0.61
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.29	0.61
4:D:66:ARG:HD2	4:D:133:THR:HB	1.83	0.61
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.82	0.61
6:F:76:LYS:O	6:F:79:ARG:HD3	2.01	0.61
8:H:63:LEU:HD22	8:H:90:ALA:HB3	1.82	0.61
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.15	0.61
10:J:48:ARG:HD2	10:J:49:MET:N	2.15	0.61
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.30	0.61
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.14	0.61
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.47	0.61
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.25	0.61
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.83	0.61
2:B:882:THR:HG21	2:B:935:ARG:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:THR:HG22	4:D:136:GLY:H	1.65	0.61
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.61
1:A:849:MET:HE1	1:A:1440:ALA:HB2	1.83	0.61
2:B:332:ASP:OD1	2:B:336:ARG:NE	2.34	0.61
2:B:344:LYS:O	2:B:345:LYS:HG3	2.01	0.61
2:B:464:GLY:HA2	2:B:479:VAL:O	2.01	0.61
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.81	0.61
5:E:15:ALA:O	5:E:19:VAL:HG23	2.01	0.61
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.66	0.61
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.82	0.61
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.16	0.61
2:B:281:PRO:O	2:B:283:VAL:N	2.34	0.61
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.48	0.61
2:B:975:GLN:HG2	2:B:976:ILE:H	1.64	0.61
3:C:179:GLU:HG2	3:C:180:TYR:N	2.16	0.61
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.30	0.61
2:B:185:THR:H	2:B:188:ASP:CB	2.13	0.61
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.61
3:C:73:GLN:HB3	3:C:131:HIS:H	1.66	0.61
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.14	0.61
10:J:8:PHE:H	10:J:49:MET:CE	2.14	0.61
10:J:44:TYR:HA	10:J:47:ARG:CB	2.31	0.61
11:K:67:PHE:C	11:K:68:PHE:CD2	2.79	0.61
11:K:69:ALA:O	11:K:70:ARG:HB3	2.00	0.61
1:A:58:LEU:HD11	1:A:80:HIS:H	1.65	0.60
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.83	0.60
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.64	0.60
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.07	0.60
2:B:176:SER:O	2:B:182:SER:HB3	2.01	0.60
2:B:842:ASN:HD22	2:B:845:SER:CB	2.14	0.60
4:D:17:LYS:CA	4:D:17:LYS:HE3	2.31	0.60
11:K:10:PHE:N	11:K:10:PHE:CD2	2.69	0.60
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.65	0.60
2:B:265:SER:O	2:B:266:ALA:HB3	2.01	0.60
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.84	0.60
2:B:525:ALA:O	2:B:768:THR:HA	2.02	0.60
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.60
1:A:33:ALA:O	1:A:83:HIS:HD2	1.84	0.60
1:A:742:ASN:O	1:A:745:GLN:HB2	2.01	0.60
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.31	0.60
2:B:25:ILE:HD11	2:B:653:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HE3	2:B:636:PRO:CG	2.32	0.60
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.82	0.60
10:J:44:TYR:H	10:J:44:TYR:HD2	1.47	0.60
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.60
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.46	0.60
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.01	0.60
2:B:1099:VAL:O	2:B:1101:ASP:N	2.35	0.60
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.31	0.60
1:A:130:ASP:O	1:A:131:SER:C	2.45	0.60
1:A:567:LYS:CB	1:A:568:PRO:CD	2.79	0.60
2:B:465:ASN:N	2:B:465:ASN:ND2	2.47	0.60
2:B:801:LYS:O	10:J:52:THR:HG23	2.01	0.60
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.84	0.60
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.17	0.60
1:A:709:THR:HB	1:A:712:GLU:HG3	1.84	0.60
1:A:829:VAL:C	1:A:831:THR:H	2.07	0.60
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.14	0.60
5:E:177:ARG:C	5:E:212:ARG:HD3	2.26	0.60
13:P:9:G:C2'	13:P:10:A:H5'	2.31	0.60
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.84	0.60
1:A:416:ARG:O	1:A:417:TYR:HD2	1.84	0.60
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.67	0.60
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.83	0.60
5:E:105:PHE:O	5:E:106:GLN:HB2	2.01	0.60
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.67	0.60
1:A:289:ILE:C	1:A:291:GLU:H	2.07	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
2:B:563:MET:CE	2:B:580:VAL:HB	2.32	0.60
3:C:133:ILE:CD1	3:C:237:SER:HA	2.31	0.60
7:G:1:MET:O	7:G:3:PHE:CD1	2.55	0.60
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	1.99	0.60
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.29	0.60
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.84	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.95	0.60
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60
1:A:466:SER:O	2:B:1103:ILE:HD11	2.01	0.60
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.18	0.60
2:B:34:ILE:O	2:B:37:PHE:N	2.34	0.60
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.83	0.60
2:B:753:ALA:O	2:B:756:ILE:HG13	2.02	0.60
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.83	0.59
1:A:244:PRO:O	1:A:247:ARG:N	2.35	0.59
1:A:596:THR:C	1:A:598:LEU:N	2.59	0.59
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.31	0.59
2:B:51:PHE:O	2:B:54:PHE:HB3	2.02	0.59
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.15	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.83	0.59
2:B:310:MET:HE1	2:B:387:LEU:CD1	2.32	0.59
2:B:637:LEU:O	2:B:690:VAL:HG13	2.01	0.59
2:B:744:HIS:HD2	2:B:746:SER:OG	1.85	0.59
11:K:42:LEU:O	11:K:46:ILE:HG13	2.02	0.59
1:A:446:ARG:HB2	1:A:487:MET:SD	2.41	0.59
2:B:557:PHE:C	2:B:557:PHE:HD2	2.10	0.59
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.02	0.59
2:B:822:ASN:O	10:J:48:ARG:NH1	2.35	0.59
2:B:843:GLN:O	2:B:846:ILE:N	2.35	0.59
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.67	0.59
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.71	0.59
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.84	0.59
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.84	0.59
10:J:32:GLU:CD	10:J:32:GLU:H	2.09	0.59
1:A:98:LYS:O	1:A:99:ILE:C	2.43	0.59
1:A:321:PRO:O	1:A:322:VAL:CB	2.49	0.59
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.37	0.59
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.37	0.59
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.32	0.59
2:B:531:GLN:HG3	2:B:532:ALA:H	1.67	0.59
2:B:737:THR:CG2	9:I:66:PRO:HA	2.31	0.59
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.84	0.59
1:A:164:ARG:HG3	1:A:165:GLY:H	1.65	0.59
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.37	0.59
2:B:310:MET:HE1	2:B:387:LEU:HD12	1.83	0.59
2:B:910:VAL:HG12	2:B:912:ILE:H	1.67	0.59
4:D:66:ARG:O	4:D:70:PHE:HB2	2.03	0.59
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.62	0.59
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.41	0.59
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.37	0.59
1:A:471:ASN:OD1	1:A:472:LEU:N	2.35	0.59
1:A:966:ASN:O	1:A:967:ALA:C	2.46	0.59
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.42	0.59
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.33	0.59
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.59
1:A:1444:MET:CG	7:G:60:ARG:HA	2.33	0.59
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.17	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.31	0.59
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.59	0.59
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.33	0.59
3:C:241:ASP:O	3:C:245:VAL:HG23	2.03	0.59
6:F:111:LEU:H	6:F:111:LEU:CD1	2.12	0.59
1:A:21:LEU:HG	1:A:1413:GLY:O	2.02	0.59
1:A:37:PHE:N	1:A:37:PHE:CD1	2.71	0.59
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.84	0.59
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.84	0.59
1:A:1171:GLN:HA	1:A:1174:PHE:HE1	1.66	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.85	0.59
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.50	0.59
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.30	0.59
8:H:82:PRO:C	8:H:84:ALA:H	2.10	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.33	0.59
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.02	0.59
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.03	0.59
1:A:853:ASP:OD1	1:A:855:THR:HB	2.03	0.59
1:A:867:ILE:HG22	1:A:872:GLY:N	2.18	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.59
1:A:1437:GLY:O	1:A:1439:GLY:N	2.36	0.59
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.27	0.59
3:C:174:ALA:O	10:J:10:CYS:O	2.20	0.59
10:J:2:ILE:HG22	10:J:3:VAL:O	2.03	0.59
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.85	0.59
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.67	0.59
1:A:504:LEU:HD12	1:A:504:LEU:N	2.17	0.59
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.68	0.59
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.38	0.59
5:E:78:LEU:HD23	5:E:78:LEU:C	2.27	0.59
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.38	0.59
8:H:93:TYR:HB3	8:H:144:ILE:O	2.03	0.59
1:A:107:CYS:N	1:A:114:LEU:HD21	2.18	0.59
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.25	0.59
3:C:41:ILE:HD11	3:C:247:GLY:HA2	1.84	0.59
3:C:69:LEU:HD12	3:C:69:LEU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.85	0.59
2:B:343:ILE:CB	2:B:348:ARG:HG3	2.32	0.58
2:B:360:PHE:C	2:B:360:PHE:CD2	2.80	0.58
2:B:705:MET:H	2:B:710:LEU:CD1	2.16	0.58
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.18	0.58
10:J:64:ASN:CB	10:J:65:PRO:CD	2.80	0.58
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.38	0.58
1:A:844:ALA:O	1:A:845:LEU:HD23	2.02	0.58
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.72	0.58
2:B:467:GLY:H	2:B:475:SER:CB	2.16	0.58
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.33	0.58
4:D:47:LEU:HD13	4:D:48:ILE:N	2.16	0.58
7:G:1:MET:O	7:G:3:PHE:CE1	2.56	0.58
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.18	0.58
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.39	0.58
1:A:974:ASP:C	1:A:976:THR:H	2.12	0.58
1:A:1279:ILE:HG22	1:A:1279:ILE:O	2.02	0.58
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.68	0.58
2:B:778:MET:CE	2:B:1094:ARG:CD	2.80	0.58
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.83	0.58
1:A:524:VAL:CG1	1:A:525:GLN:H	2.07	0.58
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.38	0.58
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.68	0.58
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.34	0.58
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.85	0.58
7:G:88:ASP:OD2	7:G:88:ASP:N	2.36	0.58
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.33	0.58
9:I:103:CYS:CB	9:I:106:CYS:SG	2.92	0.58
1:A:17:VAL:HA	2:B:1215:ARG:O	2.04	0.58
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.18	0.58
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.69	0.58
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.84	0.58
4:D:194:LEU:C	4:D:195:ILE:HG13	2.28	0.58
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.17	0.58
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.04	0.58
1:A:224:PHE:HD2	1:A:229:SER:O	1.85	0.58
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.28	0.58
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.38	0.58
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.43	0.58
2:B:1045:SER:O	2:B:1046:PRO:O	2.22	0.58
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:LEU:HD21	3:C:224:GLN:O	2.03	0.58
4:D:4:SER:OG	4:D:5:THR:N	2.33	0.58
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.86	0.58
5:E:157:SER:HG	5:E:160:GLU:HG3	1.67	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.84	0.58
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.85	0.58
1:A:1323:ASP:C	1:A:1325:THR:H	2.12	0.58
2:B:168:GLY:N	2:B:450:ALA:HB1	2.15	0.58
2:B:745:PRO:C	2:B:747:MET:H	2.12	0.58
2:B:830:TYR:O	2:B:831:SER:C	2.47	0.58
7:G:39:THR:HG22	7:G:40:GLY:H	1.69	0.58
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.69	0.58
1:A:58:LEU:HD21	1:A:243:PRO:CB	2.33	0.58
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.34	0.58
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.39	0.58
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.51	0.58
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.58
11:K:112:GLN:CB	11:K:112:GLN:C	2.74	0.58
1:A:783:THR:HG22	1:A:784:LEU:HG	1.86	0.58
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.38	0.58
1:A:853:ASP:OD1	1:A:855:THR:N	2.36	0.58
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.69	0.58
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.31	0.58
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.69	0.58
6:F:99:LEU:HD12	6:F:99:LEU:O	2.03	0.58
9:I:62:ILE:O	9:I:62:ILE:HG12	2.04	0.58
11:K:15:GLY:O	11:K:16:GLU:HG3	2.04	0.58
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.16	0.58
1:A:632:VAL:O	1:A:633:VAL:C	2.47	0.58
1:A:760:GLN:HG2	1:A:765:VAL:O	2.04	0.58
2:B:44:VAL:O	2:B:45:SER:C	2.46	0.58
2:B:122:LEU:O	2:B:206:ASN:HA	2.04	0.58
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.69	0.58
2:B:843:GLN:O	2:B:846:ILE:HB	2.04	0.58
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.33	0.58
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.86	0.58
7:G:17:PHE:N	7:G:17:PHE:CD2	2.72	0.58
10:J:27:GLU:C	10:J:29:GLU:H	2.10	0.58
11:K:46:ILE:O	11:K:46:ILE:HG22	2.03	0.58
1:A:68:GLN:O	1:A:70:CYS:N	2.36	0.57
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.17	0.57
1:A:782:ARG:NH2	2:B:699:GLU:O	2.36	0.57
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.39	0.57
2:B:466:TRP:O	2:B:468:GLU:N	2.37	0.57
4:D:57:LEU:O	4:D:61:GLU:HB2	2.04	0.57
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.04	0.57
14:T:19:DT:H2'	14:T:20:DC:C6	2.38	0.57
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.86	0.57
1:A:316:GLN:O	1:A:317:LYS:C	2.45	0.57
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.69	0.57
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.29	0.57
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.03	0.57
1:A:1369:ALA:O	1:A:1370:LEU:C	2.47	0.57
2:B:449:ASN:C	2:B:451:LYS:H	2.12	0.57
2:B:515:HIS:CD2	2:B:517:THR:H	2.21	0.57
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.30	0.57
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.57
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.87	0.57
1:A:1313:LEU:O	1:A:1315:GLU:N	2.37	0.57
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.03	0.57
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.05	0.57
1:A:629:LEU:O	1:A:633:VAL:HG23	2.05	0.57
1:A:1175:SER:O	1:A:1176:LEU:HB2	2.04	0.57
2:B:583:ASN:HD21	2:B:628:THR:HB	1.68	0.57
2:B:871:THR:HG22	2:B:872:GLU:O	2.03	0.57
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.18	0.57
3:C:263:THR:C	3:C:265:MET:H	2.12	0.57
1:A:364:VAL:O	1:A:364:VAL:HG13	2.03	0.57
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.85	0.57
2:B:278:GLN:NE2	2:B:337:ARG:HH21	2.02	0.57
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.69	0.57
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.85	0.57
8:H:123:MET:HG2	8:H:124:ARG:N	2.19	0.57
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.34	0.57
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.86	0.57
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.92	0.57
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.39	0.57
2:B:225:VAL:HA	2:B:237:VAL:O	2.05	0.57
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.29	0.57
3:C:129:ILE:HG23	3:C:130:GLY:N	2.18	0.57
1:A:1095:THR:O	1:A:1096:SER:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.35	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.05	0.57
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.87	0.57
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.35	0.57
2:B:705:MET:HA	2:B:705:MET:HE3	1.86	0.57
2:B:776:GLN:O	2:B:1095:LEU:HA	2.04	0.57
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.57
6:F:130:ILE:O	6:F:148:VAL:HG21	2.05	0.57
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.05	0.57
1:A:1001:ARG:O	1:A:1002:GLY:O	2.23	0.57
2:B:125:SER:HA	2:B:171:PRO:HA	1.86	0.57
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.85	0.57
2:B:337:ARG:C	2:B:338:GLY:N	2.62	0.57
2:B:843:GLN:O	2:B:844:SER:C	2.48	0.57
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.60	0.57
4:D:176:GLU:O	4:D:178:ALA:N	2.38	0.57
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.40	0.57
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.86	0.57
14:T:25:DT:C2'	14:T:26:DC:O5'	2.53	0.57
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.40	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.86	0.57
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.38	0.57
2:B:1010:LEU:HD23	2:B:1092:TYR:CD1	2.40	0.57
3:C:183:TRP:O	3:C:185:LYS:N	2.38	0.57
3:C:249:ASP:O	3:C:252:GLN:HB3	2.05	0.57
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.05	0.57
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.05	0.57
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.30	0.57
1:A:130:ASP:O	1:A:133:LYS:N	2.36	0.57
1:A:249:SER:O	1:A:250:ILE:HG13	2.04	0.57
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.87	0.57
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.19	0.57
2:B:654:ARG:O	2:B:656:GLY:N	2.38	0.57
2:B:1084:GLN:H	2:B:1084:GLN:HE21	1.51	0.57
2:B:1134:GLU:H	2:B:1134:GLU:CD	2.13	0.57
4:D:53:SER:HB3	4:D:152:SER:CA	2.35	0.57
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.39	0.57
5:E:157:SER:C	5:E:159:ASP:N	2.60	0.57
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.87	0.57
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.34	0.57
8:H:127:GLY:O	8:H:128:ASN:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:CG2	1:A:383:TYR:H	2.18	0.56
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.87	0.56
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.70	0.56
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.82	0.56
2:B:310:MET:CE	2:B:387:LEU:HD12	2.35	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.87	0.56
8:H:11:GLN:HA	8:H:53:ASP:O	2.05	0.56
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.40	0.56
8:H:111:LEU:HD23	8:H:127:GLY:O	2.04	0.56
1:A:528:LEU:C	1:A:528:LEU:HD12	2.30	0.56
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.71	0.56
1:A:1239:ARG:NH1	1:A:1239:ARG:HB3	2.19	0.56
2:B:217:ARG:HD2	2:B:217:ARG:C	2.30	0.56
3:C:35:ARG:HH11	11:K:41:THR:CA	2.18	0.56
4:D:18:VAL:HG13	4:D:18:VAL:O	2.05	0.56
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.40	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.24	0.56
7:G:143:ILE:CG2	7:G:144:ARG:N	2.68	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.35	0.56
10:J:12:LYS:O	10:J:14:VAL:HG23	2.05	0.56
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.87	0.56
1:A:392:VAL:HG22	1:A:432:VAL:HG11	1.87	0.56
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.87	0.56
1:A:438:ASP:O	1:A:439:ASN:HB2	2.06	0.56
1:A:840:ARG:O	1:A:841:LEU:C	2.48	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.37	0.56
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.38	0.56
2:B:102:VAL:HG12	2:B:104:GLU:HG2	1.86	0.56
2:B:224:GLN:O	2:B:238:ALA:HA	2.06	0.56
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.86	0.56
2:B:745:PRO:O	2:B:747:MET:N	2.38	0.56
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.31	0.56
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.35	0.56
3:C:77:ILE:O	3:C:79:GLN:N	2.38	0.56
4:D:7:THR:O	4:D:9:GLN:N	2.38	0.56
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.32	0.56
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.86	0.56
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.40	0.56
10:J:27:GLU:O	10:J:29:GLU:N	2.34	0.56
11:K:110:ASN:O	11:K:111:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.70	0.56
1:A:56:PRO:O	1:A:57:ARG:HG3	2.06	0.56
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.88	0.56
1:A:920:LEU:HD23	1:A:921:GLY:N	2.21	0.56
3:C:174:ALA:O	3:C:175:ALA:HB2	2.05	0.56
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.32	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.67	0.56
1:A:853:ASP:OD1	1:A:855:THR:CB	2.54	0.56
1:A:873:MET:C	1:A:1058:VAL:HG23	2.31	0.56
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.14	0.56
3:C:104:PHE:HD2	3:C:105:GLY:N	2.03	0.56
5:E:31:THR:O	5:E:35:VAL:HG23	2.05	0.56
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.86	0.56
9:I:106:CYS:O	9:I:107:SER:HB2	2.06	0.56
1:A:84:ILE:O	1:A:84:ILE:HG23	2.05	0.56
1:A:474:VAL:C	1:A:477:PRO:HD2	2.31	0.56
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.17	0.56
1:A:658:LEU:HD13	2:B:831:SER:N	2.21	0.56
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.05	0.56
9:I:112:SER:O	9:I:114:GLN:N	2.38	0.56
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.88	0.56
1:A:787:PHE:CE1	1:A:796:SER:HA	2.41	0.56
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.06	0.56
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.70	0.56
5:E:35:VAL:C	5:E:37:LEU:H	2.13	0.56
10:J:7:CYS:SG	10:J:49:MET:HE3	2.46	0.56
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.35	0.56
10:J:36:LEU:O	10:J:39:LEU:N	2.38	0.56
1:A:37:PHE:HD1	1:A:37:PHE:H	1.54	0.56
1:A:477:PRO:CG	1:A:521:MET:HG2	2.35	0.56
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.86	0.56
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56
1:A:1341:ILE:O	1:A:1344:GLY:N	2.39	0.56
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.39	0.56
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.56
2:B:954:VAL:O	12:L:55:ILE:O	2.24	0.56
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.88	0.56
3:C:18:VAL:O	3:C:18:VAL:HG12	2.06	0.56
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.69	0.56
4:D:198:LEU:O	4:D:200:ASN:N	2.39	0.56
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.40	0.56
1:A:720:ARG:O	1:A:724:GLU:HB2	2.06	0.56
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.41	0.56
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.06	0.56
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.14	0.56
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.71	0.56
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.19	0.56
6:F:99:LEU:HD12	6:F:99:LEU:C	2.31	0.56
7:G:91:VAL:HB	7:G:139:ILE:O	2.06	0.56
10:J:7:CYS:CB	10:J:46:CYS:HB3	2.36	0.56
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.88	0.56
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.88	0.56
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.88	0.56
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.69	0.56
13:P:4:A:H2'	13:P:5:C:H6	1.71	0.56
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.70	0.55
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.87	0.55
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.21	0.55
1:A:1329:THR:CG2	1:A:1331:SER:H	2.16	0.55
2:B:842:ASN:ND2	2:B:845:SER:OG	2.32	0.55
3:C:31:ASN:O	3:C:34:ARG:HB3	2.06	0.55
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.20	0.55
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.41	0.55
7:G:18:PHE:HA	7:G:22:MET:CE	2.36	0.55
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.88	0.55
1:A:639:PRO:HG2	1:A:640:GLN:H	1.70	0.55
1:A:834:THR:HG21	1:A:1077:THR:OG1	2.05	0.55
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.55
2:B:811:TYR:N	2:B:811:TYR:CD1	2.73	0.55
2:B:1023:VAL:O	2:B:1026:LEU:N	2.39	0.55
4:D:53:SER:CB	4:D:153:ARG:H	2.18	0.55
4:D:213:GLU:O	4:D:217:LEU:HG	2.06	0.55
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.55
9:I:15:TYR:N	9:I:15:TYR:CD1	2.74	0.55
1:A:166:GLY:O	1:A:167:CYS:SG	2.64	0.55
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.69	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.05	0.55
4:D:5:THR:O	4:D:5:THR:HG23	2.06	0.55
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.88	0.55
4:D:192:LYS:HB3	4:D:192:LYS:HZ3	1.72	0.55
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:41:ASP:O	8:H:42:ILE:HG13	2.06	0.55
8:H:102:TYR:N	8:H:102:TYR:CD2	2.73	0.55
1:A:42:ASP:C	1:A:44:THR:H	2.13	0.55
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.88	0.55
1:A:262:LEU:O	1:A:264:PHE:N	2.40	0.55
1:A:284:ALA:O	1:A:286:HIS:N	2.33	0.55
1:A:385:ILE:CG2	1:A:386:ASP:N	2.66	0.55
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.42	0.55
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.24	0.55
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.06	0.55
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.63	0.55
5:E:17:ARG:O	5:E:20:LYS:HB2	2.06	0.55
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.88	0.55
1:A:699:ALA:O	1:A:700:ASN:HB3	2.07	0.55
1:A:867:ILE:HG22	1:A:872:GLY:H	1.71	0.55
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.05	0.55
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.07	0.55
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.70	0.55
1:A:42:ASP:HB3	1:A:45:GLN:N	2.22	0.55
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.88	0.55
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.06	0.55
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.22	0.55
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.89	0.55
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.91	0.55
3:C:243:VAL:O	3:C:243:VAL:HG12	2.05	0.55
7:G:9:LEU:HD12	7:G:10:ASN:H	1.71	0.55
10:J:1:MET:H3	10:J:56:LEU:N	2.05	0.55
1:A:34:LYS:H	1:A:57:ARG:HH22	1.54	0.55
1:A:730:GLY:C	1:A:732:LEU:H	2.14	0.55
1:A:914:GLU:HB2	1:A:979:SER:O	2.07	0.55
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.89	0.55
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.42	0.55
3:C:73:GLN:NE2	3:C:75:MET:N	2.53	0.55
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.55
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.22	0.55
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	1.89	0.55
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.31	0.55
1:A:1213:GLY:O	1:A:1214:GLU:C	2.50	0.55
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.42	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.39	0.55
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:GLN:C	7:G:119:LEU:H	2.14	0.55
8:H:142:LEU:C	8:H:143:LEU:HD12	2.32	0.55
1:A:34:LYS:N	1:A:57:ARG:NH2	2.51	0.55
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.89	0.55
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.21	0.55
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.06	0.55
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.07	0.55
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.88	0.55
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.55
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.22	0.55
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.21	0.55
6:F:143:PHE:C	6:F:143:PHE:CD1	2.84	0.55
7:G:80:LYS:O	7:G:80:LYS:HG2	2.07	0.55
8:H:130:ARG:HD2	8:H:130:ARG:N	2.20	0.55
11:K:6:ARG:O	11:K:8:GLU:N	2.40	0.55
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.89	0.55
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.71	0.55
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.07	0.55
2:B:705:MET:N	2:B:710:LEU:HD12	2.22	0.55
2:B:745:PRO:C	2:B:747:MET:N	2.64	0.55
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.06	0.55
4:D:54:GLU:O	4:D:58:VAL:HG23	2.07	0.55
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.06	0.55
5:E:55:ARG:C	5:E:57:MET:N	2.65	0.55
8:H:4:THR:O	8:H:5:LEU:HD23	2.07	0.55
9:I:61:ASP:C	9:I:63:GLY:H	2.15	0.55
10:J:44:TYR:CD2	10:J:44:TYR:N	2.75	0.55
14:T:27:DA:H2''	14:T:28:DT:O4'	2.07	0.55
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.36	0.54
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.07	0.54
1:A:907:THR:CG2	1:A:908:LEU:N	2.70	0.54
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.89	0.54
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.36	0.54
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.19	0.54
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.25	0.54
4:D:134:THR:CG2	4:D:135:GLY:N	2.69	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.07	0.54
7:G:1:MET:O	7:G:1:MET:SD	2.65	0.54
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.37	0.54
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.50	0.54
1:A:506:ALA:C	1:A:508:PRO:HD2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.07	0.54
2:B:1102:LYS:O	2:B:1103:ILE:C	2.49	0.54
5:E:147:HIS:CD2	5:E:149:LEU:H	2.25	0.54
13:P:4:A:H2'	13:P:5:C:C6	2.42	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.54	0.54
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.20	0.54
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.86	0.54
1:A:965:GLN:O	1:A:968:GLN:HB2	2.07	0.54
2:B:337:ARG:C	2:B:338:GLY:CA	2.81	0.54
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.89	0.54
2:B:770:GLN:C	2:B:772:ALA:H	2.14	0.54
3:C:236:GLY:O	3:C:237:SER:C	2.51	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.69	0.54
12:L:55:ILE:O	12:L:56:LEU:HB2	2.06	0.54
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.37	0.54
1:A:317:LYS:O	1:A:318:SER:HB3	2.08	0.54
1:A:319:GLY:HA3	2:B:471:LYS:HA	1.89	0.54
1:A:362:ASP:HB3	1:A:508:PRO:HG3	1.89	0.54
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.89	0.54
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.54
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.08	0.54
2:B:344:LYS:O	2:B:345:LYS:CB	2.55	0.54
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.19	0.54
2:B:1165:ILE:HG12	4:D:17:LYS:HD2	1.89	0.54
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.72	0.54
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.72	0.54
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.37	0.54
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.90	0.54
1:A:433:GLU:OE1	2:B:1108:ARG:NH1	2.41	0.54
1:A:666:ILE:HD12	1:A:666:ILE:N	2.22	0.54
1:A:866:PHE:O	1:A:867:ILE:HD12	2.06	0.54
1:A:1332:PHE:O	1:A:1333:ILE:C	2.51	0.54
2:B:34:ILE:O	2:B:35:SER:C	2.50	0.54
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.35	0.54
8:H:40:LEU:HD12	8:H:122:LEU:O	2.08	0.54
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.54
1:A:71:GLN:C	1:A:73:GLY:H	2.14	0.54
1:A:222:LEU:O	1:A:224:PHE:N	2.41	0.54
1:A:1036:ARG:HH11	1:A:1036:ARG:CG	2.19	0.54
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.22	0.54
3:C:3:GLU:O	3:C:4:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.37	0.54
5:E:78:LEU:HD23	5:E:79:TRP:N	2.22	0.54
12:L:31:CYS:SG	12:L:34:CYS:N	2.79	0.54
1:A:567:LYS:CG	1:A:568:PRO:CD	2.79	0.54
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.54
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.48	0.54
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.08	0.54
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.89	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.43	0.54
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.12	0.54
2:B:386:LEU:O	2:B:388:CYS:N	2.41	0.54
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.22	0.54
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.20	0.54
6:F:82:THR:HG22	6:F:84:TYR:N	2.16	0.54
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.26	0.54
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.54
1:A:786:HIS:CD2	1:A:786:HIS:N	2.75	0.54
1:A:869:GLY:O	1:A:870:GLU:HB2	2.08	0.54
1:A:1053:PHE:O	1:A:1055:ARG:N	2.40	0.54
2:B:459:TYR:C	2:B:459:TYR:CD2	2.86	0.54
2:B:680:THR:O	2:B:684:LEU:HD12	2.08	0.54
2:B:1180:PHE:O	2:B:1181:GLU:O	2.26	0.54
5:E:29:PHE:O	5:E:30:ILE:HG13	2.07	0.54
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.40	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.90	0.54
9:I:111:THR:CG2	9:I:112:SER:H	2.19	0.54
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.89	0.54
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.37	0.54
2:B:525:ALA:O	2:B:768:THR:HG23	2.07	0.54
2:B:785:TYR:CD1	2:B:785:TYR:C	2.86	0.54
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.32	0.54
3:C:179:GLU:HG2	3:C:180:TYR:H	1.73	0.54
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.73	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.38	0.54
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.38	0.54
1:A:600:PRO:HG2	1:A:601:LYS:H	1.73	0.54
1:A:608:ILE:C	1:A:610:GLY:N	2.64	0.54
2:B:1099:VAL:HG22	2:B:1103:ILE:CD1	2.38	0.54
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.33	0.54
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.43	0.54
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:O	1:A:591:PHE:HB2	2.08	0.53
1:A:665:GLY:O	1:A:667:GLY:N	2.41	0.53
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.72	0.53
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.20	0.53
2:B:1121:GLY:C	2:B:1123:SER:N	2.62	0.53
2:B:1177:HIS:O	2:B:1179:GLN:N	2.41	0.53
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.89	0.53
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.38	0.53
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.08	0.53
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.55	0.53
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.72	0.53
2:B:310:MET:O	2:B:313:MET:HB2	2.09	0.53
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.90	0.53
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.33	0.53
3:C:112:ASN:HD22	3:C:112:ASN:N	2.05	0.53
3:C:254:LYS:C	3:C:256:ALA:N	2.66	0.53
6:F:69:LEU:N	6:F:70:LYS:CA	2.71	0.53
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.53
10:J:7:CYS:HB2	10:J:46:CYS:HB3	1.90	0.53
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.90	0.53
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.48	0.53
2:B:305:VAL:O	2:B:305:VAL:HG12	2.09	0.53
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.39	0.53
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.90	0.53
2:B:1017:ILE:HB	2:B:1018:PRO:CD	2.37	0.53
2:B:1174:LYS:O	2:B:1176:ASN:N	2.40	0.53
4:D:8:PHE:CZ	4:D:40:HIS:HA	2.42	0.53
6:F:69:LEU:N	6:F:70:LYS:HA	2.24	0.53
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.89	0.53
9:I:98:VAL:HG11	9:I:113:ASP:OD1	2.07	0.53
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.35	0.53
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.73	0.53
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.53
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.22	0.53
1:A:829:VAL:C	1:A:831:THR:N	2.67	0.53
2:B:27:ALA:O	2:B:29:ASP:N	2.42	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.39	0.53
2:B:797:TYR:HB2	2:B:852:ARG:O	2.09	0.53
5:E:213:ILE:HG12	5:E:214:CYS:N	2.23	0.53
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.24	0.53
9:I:13:MET:HG3	9:I:14:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:O	1:A:242:PRO:C	2.51	0.53
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.44	0.53
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.39	0.53
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.39	0.53
2:B:343:ILE:HG22	2:B:345:LYS:H	1.72	0.53
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.90	0.53
5:E:55:ARG:C	5:E:57:MET:H	2.15	0.53
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.42	0.53
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.39	0.53
2:B:911:ILE:O	2:B:911:ILE:HG22	2.08	0.53
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.49	0.53
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.67	0.53
4:D:208:GLU:O	4:D:212:LYS:HG3	2.08	0.53
6:F:109:VAL:HG12	6:F:110:ASP:N	2.23	0.53
9:I:14:LEU:HA	9:I:28:GLU:O	2.08	0.53
1:A:368:LYS:O	1:A:369:SER:C	2.52	0.53
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.90	0.53
2:B:408:LEU:HG	2:B:409:ALA:H	1.74	0.53
2:B:616:ILE:N	2:B:616:ILE:CD1	2.71	0.53
2:B:1013:ASN:OD1	2:B:1015:HIS:N	2.38	0.53
4:D:20:GLU:HA	4:D:20:GLU:OE2	2.08	0.53
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.90	0.53
10:J:44:TYR:HD2	10:J:44:TYR:N	2.07	0.53
1:A:335:ARG:O	1:A:336:ILE:C	2.52	0.53
1:A:547:LEU:HB3	11:K:58:PHE:HE1	1.74	0.53
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.53
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.22	0.53
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.39	0.53
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.72	0.53
2:B:794:ASN:C	2:B:795:ILE:HD12	2.34	0.53
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.91	0.53
7:G:154:VAL:HG12	7:G:155:SER:N	2.24	0.53
8:H:100:THR:HG22	8:H:101:ALA:N	2.22	0.53
11:K:109:TRP:O	11:K:111:LEU:N	2.36	0.53
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.53
1:A:71:GLN:O	1:A:73:GLY:N	2.37	0.53
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.09	0.53
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.38	0.53
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.44	0.53
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.73	0.53
2:B:955:THR:CG2	2:B:956:THR:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.00	0.53
3:C:35:ARG:HH11	11:K:41:THR:N	2.06	0.53
4:D:24:ALA:C	4:D:26:THR:H	2.16	0.53
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.91	0.53
1:A:341:MET:CE	1:A:843:LYS:NZ	2.70	0.53
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.42	0.53
1:A:1364:ASN:O	1:A:1365:TYR:C	2.52	0.53
2:B:365:THR:HG23	2:B:367:LEU:HG	1.90	0.53
2:B:515:HIS:O	2:B:518:HIS:HB2	2.08	0.53
2:B:758:PHE:N	2:B:759:PRO:CD	2.72	0.53
3:C:73:GLN:NE2	3:C:74:SER:N	2.57	0.53
3:C:104:PHE:HD2	3:C:105:GLY:H	1.55	0.53
4:D:130:LEU:C	4:D:132:GLN:N	2.67	0.53
13:P:6:C:H2'	13:P:7:A:H8	1.73	0.53
1:A:34:LYS:CB	1:A:36:ARG:HE	2.20	0.52
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.37	0.52
1:A:527:THR:CG2	1:A:650:GLN:HA	2.40	0.52
1:A:527:THR:HG23	1:A:650:GLN:HA	1.91	0.52
1:A:626:ASN:O	1:A:631:HIS:HD2	1.90	0.52
1:A:1151:GLU:HA	9:I:44:TYR:O	2.09	0.52
1:A:1334:ASP:O	1:A:1336:MET:N	2.42	0.52
2:B:114:PRO:O	2:B:116:GLU:N	2.42	0.52
2:B:814:PHE:C	2:B:816:GLU:H	2.16	0.52
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.09	0.52
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.38	0.52
2:B:1182:CYS:O	2:B:1183:LYS:C	2.52	0.52
10:J:43:ARG:O	10:J:47:ARG:HB2	2.09	0.52
1:A:282:ASN:O	1:A:284:ALA:N	2.43	0.52
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.43	0.52
1:A:871:ASP:O	1:A:873:MET:HE2	2.09	0.52
1:A:982:THR:N	1:A:985:ASP:HB2	2.24	0.52
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.74	0.52
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.44	0.52
4:D:176:GLU:C	4:D:178:ALA:N	2.63	0.52
5:E:163:GLU:O	5:E:164:LEU:C	2.53	0.52
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.75	0.52
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.73	0.52
1:A:442:VAL:O	1:A:457:ALA:HA	2.09	0.52
1:A:730:GLY:O	1:A:732:LEU:N	2.42	0.52
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.91	0.52
1:A:979:SER:OG	1:A:981:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HA	2:B:207:GLY:CA	2.39	0.52
2:B:1152:MET:HE1	2:B:1196:ILE:C	2.35	0.52
3:C:161:LYS:O	3:C:170:TRP:NE1	2.43	0.52
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.92	0.52
8:H:62:SER:C	8:H:64:ASN:H	2.18	0.52
1:A:26:GLU:O	1:A:27:VAL:C	2.52	0.52
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.24	0.52
1:A:603:ASN:O	1:A:604:GLY:C	2.52	0.52
1:A:817:ALA:O	1:A:818:MET:C	2.53	0.52
1:A:968:GLN:O	1:A:970:THR:N	2.43	0.52
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.44	0.52
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.38	0.52
2:B:54:PHE:O	2:B:58:THR:HB	2.09	0.52
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.92	0.52
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.26	0.52
3:C:29:MET:HE2	11:K:98:LEU:HD21	1.91	0.52
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.45	0.52
1:A:231:PRO:HA	1:A:234:MET:HE2	1.91	0.52
1:A:332:LYS:C	1:A:334:GLY:H	2.17	0.52
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.10	0.52
1:A:687:LYS:O	1:A:690:VAL:HB	2.09	0.52
1:A:867:ILE:CG2	1:A:872:GLY:N	2.72	0.52
1:A:901:LEU:H	1:A:926:GLN:HE21	1.55	0.52
1:A:1424:VAL:CG1	1:A:1436:ILE:HD11	2.33	0.52
2:B:981:ALA:CB	2:B:987:LYS:HA	2.39	0.52
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.90	0.52
3:C:88:CYS:SG	3:C:91:HIS:HA	2.50	0.52
6:F:96:THR:O	6:F:100:GLN:HG3	2.09	0.52
8:H:64:ASN:O	8:H:65:LEU:HB2	2.08	0.52
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.24	0.52
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.52
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.40	0.52
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.35	0.52
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.90	0.52
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.75	0.52
2:B:357:GLN:O	2:B:366:GLN:HA	2.09	0.52
2:B:979:LYS:HG2	2:B:1095:LEU:HD13	1.92	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.41	0.52
4:D:59:ILE:O	4:D:60:LYS:C	2.50	0.52
11:K:40:HIS:O	11:K:41:THR:C	2.52	0.52
13:P:6:C:O2'	13:P:7:A:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:CB	1:A:458:HIS:CD2	2.91	0.52
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.92	0.52
2:B:25:ILE:HD11	2:B:653:VAL:C	2.35	0.52
2:B:343:ILE:CG2	2:B:348:ARG:N	2.68	0.52
2:B:542:MET:HG2	2:B:747:MET:HB3	1.91	0.52
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.90	0.52
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.38	0.52
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.45	0.52
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.40	0.52
1:A:42:ASP:HA	1:A:46:THR:O	2.10	0.52
1:A:58:LEU:CD1	1:A:59:GLY:N	2.68	0.52
1:A:982:THR:H	1:A:985:ASP:HB2	1.74	0.52
1:A:982:THR:O	1:A:985:ASP:HB2	2.09	0.52
2:B:388:CYS:C	2:B:390:LEU:H	2.15	0.52
2:B:654:ARG:C	2:B:656:GLY:N	2.68	0.52
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.52
2:B:1182:CYS:O	2:B:1183:LYS:O	2.28	0.52
3:C:59:ALA:O	3:C:60:ASP:C	2.53	0.52
3:C:254:LYS:C	3:C:256:ALA:H	2.16	0.52
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.91	0.52
5:E:84:ASP:O	5:E:86:PRO:HD3	2.10	0.52
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.92	0.52
1:A:485:ASP:OD1	13:P:10:A:H4'	2.10	0.52
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.75	0.52
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.97	0.52
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.10	0.52
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.91	0.52
2:B:549:THR:HG22	2:B:550:ASP:N	2.17	0.52
2:B:770:GLN:HG2	2:B:983:ARG:O	2.09	0.52
2:B:863:GLU:O	2:B:961:LEU:HD22	2.10	0.52
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.40	0.52
2:B:1034:VAL:O	2:B:1037:LEU:N	2.39	0.52
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.92	0.52
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.57	0.52
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.25	0.52
1:A:50:ILE:C	1:A:52:GLY:N	2.66	0.52
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.45	0.52
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.38	0.52
1:A:414:ASP:OD1	1:A:414:ASP:C	2.53	0.52
1:A:857:ARG:HD3	1:A:861:GLY:O	2.10	0.52
1:A:1265:ASN:C	1:A:1267:MET:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLY:C	2:B:249:ARG:N	2.65	0.52
2:B:731:VAL:HG12	2:B:732:SER:N	2.24	0.52
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.58	0.52
3:C:76:ASP:O	3:C:79:GLN:HG2	2.11	0.52
3:C:100:THR:HG22	3:C:101:LEU:N	2.24	0.52
3:C:215:GLU:O	3:C:216:GLY:C	2.53	0.52
7:G:1:MET:SD	7:G:1:MET:C	2.93	0.52
10:J:31:ASP:O	10:J:32:GLU:C	2.53	0.52
13:P:4:A:O2'	13:P:5:C:H5'	2.10	0.52
1:A:243:PRO:O	1:A:244:PRO:C	2.53	0.51
1:A:551:TYR:CZ	11:K:62:LYS:HE2	2.45	0.51
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.40	0.51
1:A:1437:GLY:O	1:A:1438:THR:C	2.53	0.51
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.98	0.51
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.90	0.51
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.40	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.27	0.51
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.90	0.51
5:E:178:ILE:HG22	5:E:213:ILE:O	2.10	0.51
6:F:103:MET:CE	7:G:66:GLY:H	2.21	0.51
1:A:584:ASN:O	1:A:637:LYS:HE3	2.11	0.51
1:A:1095:THR:O	1:A:1096:SER:CB	2.58	0.51
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.46	0.51
3:C:143:LEU:C	3:C:143:LEU:HD12	2.35	0.51
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.11	0.51
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.91	0.51
11:K:46:ILE:O	11:K:50:LEU:HB2	2.10	0.51
11:K:111:LEU:C	11:K:112:GLN:CG	2.83	0.51
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.08	0.51
1:A:53:LEU:O	1:A:54:ASN:C	2.51	0.51
1:A:116:ASP:C	1:A:118:HIS:N	2.66	0.51
1:A:317:LYS:O	1:A:318:SER:CB	2.59	0.51
1:A:920:LEU:HD23	1:A:920:LEU:C	2.35	0.51
1:A:1074:GLU:C	1:A:1076:ALA:H	2.18	0.51
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.25	0.51
2:B:343:ILE:HB	2:B:348:ARG:HE	1.75	0.51
2:B:498:THR:HB	2:B:537:LYS:O	2.10	0.51
2:B:1072:MET:HE1	2:B:1085:ILE:HB	1.87	0.51
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.45	0.51
7:G:117:GLN:C	7:G:119:LEU:N	2.69	0.51
11:K:6:ARG:C	11:K:8:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.74	0.51
1:A:60:SER:C	1:A:61:ILE:HG13	2.34	0.51
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.92	0.51
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.51
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.75	0.51
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.91	0.51
2:B:797:TYR:O	10:J:1:MET:HG2	2.10	0.51
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.41	0.51
4:D:53:SER:HB3	4:D:153:ARG:H	1.75	0.51
4:D:156:ASP:C	4:D:158:GLU:H	2.16	0.51
6:F:99:LEU:O	6:F:103:MET:HG2	2.09	0.51
8:H:84:ALA:HA	8:H:87:ARG:CB	2.35	0.51
9:I:101:PHE:N	9:I:101:PHE:CD1	2.78	0.51
1:A:7:SER:C	1:A:9:ALA:H	2.19	0.51
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.45	0.51
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.92	0.51
1:A:699:ALA:O	1:A:700:ASN:CB	2.58	0.51
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.92	0.51
1:A:870:GLU:HG2	5:E:208:TYR:CD1	2.46	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.92	0.51
2:B:112:LEU:HD12	2:B:113:TYR:N	2.24	0.51
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.92	0.51
2:B:213:ILE:O	2:B:215:GLN:HG2	2.10	0.51
2:B:220:GLY:O	2:B:222:ILE:HG13	2.11	0.51
2:B:1064:TYR:O	2:B:1065:GLN:C	2.54	0.51
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.29	0.51
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.43	0.51
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.40	0.51
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.40	0.51
9:I:111:THR:CG2	9:I:112:SER:N	2.71	0.51
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.40	0.51
1:A:264:PHE:O	1:A:267:ALA:HB3	2.11	0.51
1:A:418:SER:C	1:A:420:ARG:N	2.68	0.51
1:A:587:HIS:ND1	1:A:965:GLN:OE1	2.44	0.51
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.75	0.51
2:B:498:THR:CG2	2:B:499:ASN:N	2.74	0.51
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.51
4:D:17:LYS:HE3	4:D:17:LYS:HA	1.91	0.51
6:F:123:LYS:O	6:F:124:GLU:C	2.54	0.51
7:G:29:LYS:O	7:G:30:LEU:C	2.54	0.51
7:G:115:MET:CB	7:G:116:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:ILE:HG22	7:G:140:LYS:N	2.24	0.51
1:A:41:MET:HB3	1:A:48:ALA:O	2.11	0.51
1:A:107:CYS:H	1:A:114:LEU:HD21	1.75	0.51
1:A:384:ASN:O	1:A:386:ASP:N	2.43	0.51
1:A:399:HIS:CB	1:A:400:PRO:CD	2.85	0.51
1:A:549:MET:SD	1:A:577:ILE:CD1	2.98	0.51
1:A:832:ALA:HB2	14:T:18:DT:C7	2.41	0.51
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	2.99	0.51
1:A:1259:MET:C	1:A:1261:LYS:H	2.18	0.51
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.39	0.51
2:B:731:VAL:HG12	2:B:732:SER:H	1.76	0.51
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.93	0.51
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.39	0.51
2:B:1023:VAL:O	2:B:1024:ALA:C	2.54	0.51
3:C:77:ILE:C	3:C:79:GLN:H	2.19	0.51
5:E:134:THR:C	5:E:135:PHE:HD1	2.17	0.51
7:G:145:VAL:CG1	7:G:146:LYS:N	2.73	0.51
8:H:4:THR:CA	8:H:60:ALA:HB2	2.35	0.51
11:K:40:HIS:O	11:K:43:GLY:N	2.44	0.51
12:L:58:LYS:O	12:L:59:ALA:O	2.29	0.51
14:T:18:DT:H2''	14:T:19:DT:O5'	2.11	0.51
1:A:40:THR:HG22	1:A:41:MET:CG	2.29	0.51
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.46	0.51
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.40	0.51
2:B:434:ARG:HA	2:B:437:GLU:CD	2.35	0.51
4:D:51:ASN:C	4:D:52:LEU:O	2.53	0.51
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.22	0.51
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.46	0.51
1:A:913:LEU:HD23	1:A:919:ILE:HD12	1.92	0.51
1:A:1211:GLN:O	1:A:1212:VAL:C	2.53	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.10	0.51
3:C:82:TYR:O	3:C:83:SER:C	2.53	0.51
4:D:118:THR:HB	4:D:121:LYS:HB2	1.93	0.51
1:A:61:ILE:O	1:A:63:ARG:N	2.44	0.51
1:A:499:ALA:O	1:A:503:GLN:HG2	2.11	0.51
1:A:577:ILE:O	1:A:580:VAL:HG23	2.12	0.51
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.10	0.51
1:A:1385:THR:C	1:A:1387:HIS:N	2.67	0.51
2:B:226:PHE:CD1	2:B:398:ARG:NH2	2.79	0.51
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.92	0.51
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1121:GLY:O	2:B:1123:SER:N	2.43	0.51
3:C:189:THR:HG22	3:C:190:ASP:H	1.76	0.51
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.45	0.51
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.46	0.51
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.20	0.50
1:A:356:ASP:C	1:A:358:ASN:H	2.19	0.50
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.32	0.50
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.41	0.50
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.92	0.50
1:A:1114:PRO:O	1:A:1115:SER:O	2.28	0.50
2:B:274:PRO:O	2:B:275:TYR:HB2	2.12	0.50
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.33	0.50
2:B:758:PHE:O	2:B:760:ASP:N	2.44	0.50
2:B:841:MET:SD	2:B:846:ILE:HD11	2.50	0.50
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.92	0.50
2:B:1099:VAL:C	2:B:1101:ASP:H	2.19	0.50
2:B:1177:HIS:C	2:B:1179:GLN:H	2.19	0.50
3:C:8:VAL:HG12	3:C:9:LYS:H	1.75	0.50
7:G:112:LYS:NZ	7:G:120:THR:HA	2.27	0.50
9:I:59:VAL:C	9:I:61:ASP:H	2.17	0.50
10:J:48:ARG:HE	10:J:49:MET:HE2	1.76	0.50
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.39	0.50
1:A:64:ASN:O	1:A:65:LEU:C	2.54	0.50
1:A:535:THR:CG2	1:A:616:VAL:HA	2.38	0.50
1:A:718:VAL:O	1:A:721:PHE:HB2	2.11	0.50
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.23	0.50
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.76	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.12	0.50
5:E:22:MET:HE3	5:E:26:ARG:NE	2.25	0.50
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.46	0.50
8:H:58:THR:HG22	8:H:59:ILE:H	1.77	0.50
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.93	0.50
1:A:44:THR:O	1:A:45:GLN:HB2	2.12	0.50
2:B:46:GLN:HG3	2:B:47:GLN:N	2.16	0.50
2:B:841:MET:O	2:B:993:THR:HA	2.11	0.50
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.10	0.50
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.75	0.50
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.50
6:F:77:ASP:C	6:F:79:ARG:N	2.69	0.50
8:H:39:THR:O	8:H:123:MET:HA	2.11	0.50
1:A:472:LEU:O	1:A:475:THR:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:O	1:A:493:GLN:NE2	2.44	0.50
1:A:532:ARG:NH2	1:A:748:MET:HE3	2.26	0.50
2:B:486:TYR:CE1	2:B:1096:ARG:HD3	2.45	0.50
2:B:597:MET:O	2:B:599:THR:N	2.44	0.50
2:B:787:VAL:O	2:B:787:VAL:HG12	2.10	0.50
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.50
3:C:58:LEU:HD22	3:C:58:LEU:N	2.26	0.50
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.50
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.50
12:L:39:SER:O	12:L:40:LEU:HG	2.10	0.50
1:A:71:GLN:C	1:A:73:GLY:N	2.70	0.50
1:A:117:GLU:H	1:A:117:GLU:CD	2.20	0.50
1:A:262:LEU:C	1:A:264:PHE:N	2.66	0.50
1:A:447:GLN:NE2	14:T:20:DC:H4'	2.26	0.50
1:A:503:GLN:C	1:A:504:LEU:HD12	2.35	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
1:A:1423:GLY:O	1:A:1424:VAL:C	2.55	0.50
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.77	0.50
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.58	0.50
2:B:1176:ASN:C	2:B:1178:ASN:H	2.17	0.50
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.88	0.50
4:D:68:ARG:C	4:D:70:PHE:H	2.19	0.50
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.50
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.50
1:A:75:ASN:O	1:A:76:GLU:HB2	2.12	0.50
1:A:195:ASP:O	1:A:196:GLU:HB3	2.12	0.50
1:A:566:ILE:O	1:A:567:LYS:O	2.30	0.50
2:B:343:ILE:HB	2:B:348:ARG:HG3	1.92	0.50
2:B:531:GLN:CG	2:B:532:ALA:H	2.20	0.50
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.50
2:B:850:LEU:HD12	2:B:851:PHE:H	1.76	0.50
5:E:13:TRP:O	5:E:16:PHE:HB3	2.11	0.50
9:I:4:PHE:CD1	9:I:4:PHE:C	2.89	0.50
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.46	0.50
11:K:65:HIS:CD2	11:K:65:HIS:C	2.89	0.50
13:P:9:G:H2'	13:P:10:A:H5'	1.93	0.50
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.41	0.50
1:A:187:LYS:HE3	1:A:198:GLU:OE2	2.12	0.50
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.93	0.50
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.94	0.50
1:A:909:ASP:C	1:A:911:SER:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.12	0.50
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.50
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.50
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.94	0.50
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.12	0.50
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.50
3:C:31:ASN:O	3:C:32:SER:C	2.53	0.50
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.92	0.50
4:D:19:GLU:O	4:D:21:GLU:N	2.45	0.50
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.38	0.50
9:I:32:CYS:SG	9:I:33:SER:N	2.85	0.50
10:J:28:ASP:O	10:J:30:LEU:HG	2.12	0.50
13:P:10:A:C8	13:P:10:A:H3'	2.46	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.42	0.50
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.92	0.50
2:B:102:VAL:O	2:B:109:THR:HA	2.11	0.50
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.25	0.50
2:B:327:ARG:O	2:B:331:LEU:HD13	2.12	0.50
2:B:778:MET:HE2	2:B:1094:ARG:CD	2.42	0.50
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.70	0.50
7:G:99:PHE:CD1	7:G:99:PHE:C	2.89	0.50
7:G:111:THR:HG22	7:G:113:HIS:N	2.25	0.50
10:J:8:PHE:H	10:J:49:MET:HE3	1.75	0.50
1:A:427:GLN:O	1:A:428:TYR:C	2.53	0.50
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.47	0.50
1:A:730:GLY:C	1:A:732:LEU:N	2.69	0.50
1:A:817:ALA:O	1:A:820:GLY:N	2.45	0.50
1:A:913:LEU:HD21	1:A:915:SER:OG	2.12	0.50
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.27	0.50
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.41	0.50
2:B:388:CYS:C	2:B:390:LEU:N	2.69	0.50
2:B:519:TRP:C	2:B:519:TRP:CD1	2.90	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.42	0.50
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.94	0.50
4:D:64:VAL:C	4:D:66:ARG:H	2.19	0.50
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.94	0.49
1:A:449:SER:O	2:B:1133:MET:HB3	2.11	0.49
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.93	0.49
2:B:19:GLU:O	2:B:20:ASP:C	2.55	0.49
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:SER:HB3	2:B:994:TYR:OH	2.12	0.49
2:B:1202:LEU:O	2:B:1203:LEU:C	2.54	0.49
4:D:191:ALA:C	4:D:193:THR:H	2.20	0.49
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.94	0.49
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.11	0.49
10:J:32:GLU:O	10:J:33:GLY:C	2.54	0.49
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.60	0.49
2:B:185:THR:O	2:B:188:ASP:HB2	2.12	0.49
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.49
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.49
5:E:67:GLU:O	5:E:70:SER:HB3	2.11	0.49
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.94	0.49
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.77	0.49
1:A:95:PHE:O	1:A:96:ILE:C	2.54	0.49
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.94	0.49
2:B:382:ILE:O	2:B:386:LEU:HG	2.12	0.49
2:B:654:ARG:N	2:B:657:HIS:HD2	1.98	0.49
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.94	0.49
2:B:990:ILE:HG22	2:B:991:GLY:N	2.27	0.49
7:G:1:MET:SD	7:G:79:PHE:HD1	2.35	0.49
9:I:99:LEU:O	9:I:111:THR:HG23	2.12	0.49
9:I:110:PHE:H	9:I:110:PHE:HD2	1.59	0.49
1:A:23:SER:O	1:A:24:PRO:C	2.54	0.49
1:A:92:HIS:O	1:A:93:VAL:C	2.54	0.49
1:A:166:GLY:O	1:A:167:CYS:CB	2.60	0.49
1:A:203:SER:OG	1:A:206:GLU:HB2	2.13	0.49
1:A:832:ALA:CB	14:T:18:DT:H71	2.41	0.49
1:A:920:LEU:C	1:A:920:LEU:CD2	2.86	0.49
2:B:126:SER:O	2:B:169:ARG:HA	2.13	0.49
2:B:558:LEU:O	2:B:561:TRP:N	2.45	0.49
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.93	0.49
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.12	0.49
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.48	0.49
9:I:85:PHE:CD2	9:I:85:PHE:N	2.65	0.49
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.94	0.49
1:A:208:LEU:O	1:A:208:LEU:HD23	2.13	0.49
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.39	0.49
1:A:577:ILE:O	1:A:578:LEU:C	2.52	0.49
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.95	0.49
1:A:1096:SER:O	1:A:1100:ARG:HB3	2.11	0.49
2:B:34:ILE:HD13	2:B:747:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:O	2:B:121:ASN:HB2	2.13	0.49
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.47	0.49
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.43	0.49
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.49
2:B:763:GLN:O	2:B:764:SER:C	2.55	0.49
2:B:882:THR:O	2:B:883:LEU:HB2	2.11	0.49
2:B:893:LEU:HD22	2:B:897:GLY:C	2.37	0.49
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.49
13:P:10:A:C8	13:P:10:A:C3'	2.95	0.49
1:A:115:LEU:CB	1:A:122:MET:HE2	2.37	0.49
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.75	0.49
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.94	0.49
2:B:244:LEU:C	2:B:246:LYS:N	2.68	0.49
2:B:365:THR:HG23	2:B:367:LEU:N	2.21	0.49
2:B:372:SER:O	2:B:376:PHE:HD1	1.96	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.28	0.49
2:B:992:ILE:HG12	2:B:993:THR:N	2.27	0.49
3:C:168:ALA:C	3:C:170:TRP:N	2.69	0.49
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.47	0.49
4:D:177:VAL:O	4:D:177:VAL:HG12	2.11	0.49
5:E:23:VAL:O	5:E:28:TYR:HB2	2.13	0.49
7:G:1:MET:HE1	7:G:80:LYS:H	1.78	0.49
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.38	0.49
11:K:31:VAL:HG12	11:K:32:VAL:H	1.75	0.49
14:T:23:DG:H2'	14:T:24:DG:C8	2.48	0.49
1:A:351:THR:CB	2:B:1103:ILE:HD12	2.36	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.43	0.49
1:A:418:SER:C	1:A:420:ARG:H	2.21	0.49
1:A:418:SER:O	1:A:420:ARG:N	2.46	0.49
1:A:647:GLY:O	1:A:651:LYS:HG3	2.12	0.49
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.60	0.49
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.47	0.49
1:A:1334:ASP:O	1:A:1337:GLU:N	2.45	0.49
2:B:281:PRO:O	2:B:282:ILE:C	2.56	0.49
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.47	0.49
2:B:792:MET:HA	2:B:856:PHE:O	2.13	0.49
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.41	0.49
2:B:1142:GLY:O	2:B:1144:ALA:N	2.45	0.49
2:B:1156:ASP:O	2:B:1157:ALA:O	2.31	0.49
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.46	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:THR:O	1:A:1209:MET:C	2.55	0.49
2:B:223:VAL:HG21	2:B:380:TYR:CE2	2.47	0.49
2:B:797:TYR:O	2:B:799:PRO:HD3	2.13	0.49
5:E:161:LYS:C	5:E:163:GLU:N	2.69	0.49
1:A:278:THR:O	1:A:278:THR:HG22	2.12	0.49
1:A:500:GLU:O	1:A:504:LEU:HD13	2.13	0.49
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.95	0.49
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.47	0.49
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.43	0.49
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.42	0.49
2:B:189:LEU:O	2:B:190:TYR:C	2.55	0.49
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.61	0.49
2:B:597:MET:O	2:B:600:LEU:N	2.43	0.49
2:B:909:ASP:OD1	2:B:909:ASP:N	2.41	0.49
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.43	0.49
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.49
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.94	0.49
7:G:1:MET:O	7:G:1:MET:HE2	2.13	0.49
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.43	0.49
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.96	0.49
1:A:34:LYS:NZ	1:A:57:ARG:CZ	2.76	0.49
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.94	0.49
1:A:577:ILE:C	1:A:579:SER:N	2.68	0.49
1:A:606:LEU:HD23	1:A:614:PHE:HE2	1.78	0.49
1:A:666:ILE:CD1	1:A:667:GLY:H	2.26	0.49
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.49
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.94	0.49
2:B:683:SER:O	2:B:687:GLU:HB2	2.13	0.49
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.48	0.49
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.49
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.94	0.48
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.95	0.48
2:B:467:GLY:N	2:B:475:SER:CB	2.71	0.48
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.54	0.48
2:B:979:LYS:HG2	2:B:1095:LEU:CD1	2.43	0.48
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.77	0.48
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.47	0.48
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.46	0.48
5:E:90:VAL:O	5:E:90:VAL:HG22	2.13	0.48
5:E:205:SER:O	5:E:206:GLY:C	2.56	0.48
7:G:1:MET:O	7:G:1:MET:CE	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.92	0.48
7:G:91:VAL:HA	7:G:101:VAL:HA	1.96	0.48
10:J:13:VAL:C	10:J:14:VAL:HG23	2.38	0.48
1:A:32:VAL:O	1:A:32:VAL:HG23	2.13	0.48
1:A:50:ILE:O	1:A:52:GLY:N	2.44	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
1:A:417:TYR:O	1:A:418:SER:C	2.55	0.48
1:A:608:ILE:C	1:A:610:GLY:H	2.21	0.48
1:A:779:PHE:O	1:A:780:VAL:C	2.55	0.48
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.95	0.48
1:A:982:THR:HG22	1:A:984:LYS:H	1.76	0.48
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.13	0.48
2:B:785:TYR:CD1	2:B:786:ASN:N	2.81	0.48
2:B:950:ASP:O	2:B:951:GLN:HB2	2.13	0.48
2:B:1010:LEU:HD23	2:B:1092:TYR:CE1	2.49	0.48
2:B:1121:GLY:O	2:B:1124:ARG:N	2.41	0.48
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.44	0.48
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.41	0.48
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.13	0.48
6:F:111:LEU:C	6:F:113:GLY:N	2.70	0.48
6:F:132:LEU:O	6:F:148:VAL:HG22	2.13	0.48
7:G:51:TYR:CD2	7:G:51:TYR:O	2.65	0.48
7:G:149:GLY:O	7:G:159:ALA:HB1	2.13	0.48
8:H:103:LYS:HG2	8:H:104:PHE:N	2.29	0.48
9:I:84:VAL:HG13	9:I:84:VAL:O	2.13	0.48
12:L:34:CYS:O	12:L:36:SER:N	2.46	0.48
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.12	0.48
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.68	0.48
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.38	0.48
1:A:298:PHE:O	1:A:301:ALA:HB3	2.13	0.48
1:A:367:PRO:O	1:A:368:LYS:C	2.57	0.48
1:A:809:THR:O	1:A:810:PRO:C	2.56	0.48
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.48	0.48
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.82	0.48
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.43	0.48
2:B:591:ARG:O	2:B:592:ASN:C	2.56	0.48
2:B:614:SER:C	2:B:615:MET:HG3	2.37	0.48
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.13	0.48
2:B:1121:GLY:C	2:B:1123:SER:H	2.21	0.48
4:D:156:ASP:C	4:D:158:GLU:N	2.71	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.47	0.48
11:K:68:PHE:CD2	11:K:68:PHE:N	2.78	0.48
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.95	0.48
1:A:577:ILE:HG13	1:A:578:LEU:N	2.27	0.48
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.77	0.48
1:A:763:ALA:C	1:A:803:SER:HB3	2.39	0.48
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.43	0.48
1:A:1036:ARG:CG	1:A:1036:ARG:NH1	2.77	0.48
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.37	0.48
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.20	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.27	0.48
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.26	0.48
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.26	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.61	0.48
9:I:52:ILE:HG13	9:I:52:ILE:O	2.13	0.48
9:I:112:SER:O	9:I:114:GLN:HG3	2.12	0.48
1:A:4:GLN:O	1:A:5:GLN:HB2	2.11	0.48
1:A:845:LEU:O	1:A:846:GLU:C	2.55	0.48
1:A:1265:ASN:C	1:A:1267:MET:H	2.21	0.48
1:A:1385:THR:C	1:A:1387:HIS:H	2.22	0.48
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.95	0.48
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.13	0.48
2:B:847:ASP:C	2:B:849:GLY:N	2.70	0.48
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.43	0.48
1:A:34:LYS:H	1:A:57:ARG:HH21	1.55	0.48
1:A:289:ILE:C	1:A:291:GLU:N	2.71	0.48
1:A:532:ARG:O	1:A:535:THR:HB	2.14	0.48
1:A:634:THR:HG1	1:A:642:CYS:HG	1.61	0.48
1:A:663:SER:HB2	2:B:827:ILE:O	2.13	0.48
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.95	0.48
1:A:1118:VAL:HG12	1:A:1327:ILE:CD1	2.44	0.48
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.48
2:B:597:MET:C	2:B:599:THR:H	2.21	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
9:I:33:SER:O	9:I:35:VAL:HG23	2.13	0.48
1:A:67:CYS:O	1:A:68:GLN:HB2	2.14	0.48
1:A:116:ASP:C	1:A:118:HIS:H	2.22	0.48
1:A:135:PHE:HB2	1:A:223:GLY:H	1.79	0.48
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.48
1:A:408:ASP:C	1:A:410:GLY:H	2.22	0.48
1:A:420:ARG:O	1:A:421:ALA:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ALA:C	1:A:699:ALA:H	2.21	0.48
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.61	0.48
1:A:1067:LEU:C	1:A:1067:LEU:CD1	2.87	0.48
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.95	0.48
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.78	0.48
2:B:758:PHE:N	2:B:759:PRO:HD2	2.29	0.48
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.73	0.48
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.96	0.48
4:D:137:ASN:C	4:D:137:ASN:HD22	2.21	0.48
7:G:25:TYR:O	7:G:28:THR:HB	2.14	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.47	0.48
12:L:47:ARG:HH21	12:L:54:ARG:NH2	2.11	0.48
1:A:95:PHE:CZ	1:A:1414:ALA:HB2	2.48	0.48
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.95	0.48
1:A:475:THR:CG2	1:A:476:SER:H	2.26	0.48
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.62	0.48
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.48	0.48
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.48
2:B:337:ARG:C	2:B:338:GLY:HA2	2.39	0.48
2:B:386:LEU:O	2:B:387:LEU:C	2.57	0.48
2:B:1040:ASN:O	2:B:1041:GLU:C	2.55	0.48
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.47	0.48
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.49	0.48
5:E:48:ASP:CG	5:E:49:SER:N	2.70	0.48
9:I:60:GLN:NE2	9:I:107:SER:OG	2.47	0.48
9:I:71:SER:OG	9:I:83:ASN:HB2	2.13	0.48
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.96	0.48
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.61	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.13	0.48
1:A:470:LEU:HD22	1:A:487:MET:CE	2.43	0.48
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.57	0.48
1:A:528:LEU:O	1:A:528:LEU:HD12	2.13	0.48
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.48
1:A:728:LYS:HA	1:A:731:ARG:HB2	1.95	0.48
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.96	0.48
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.14	0.48
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.48
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.14	0.48
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.14	0.48
2:B:363:HIS:O	2:B:364:ILE:CB	2.54	0.48
2:B:388:CYS:O	2:B:390:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.29	0.48
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.13	0.48
8:H:91:ASP:C	8:H:93:TYR:N	2.71	0.48
14:T:18:DT:C2'	14:T:19:DT:O5'	2.62	0.48
1:A:23:SER:CB	1:A:233:TRP:NE1	2.77	0.48
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.78	0.48
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.48
1:A:915:SER:O	1:A:919:ILE:HG13	2.14	0.48
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.13	0.48
2:B:24:PRO:O	2:B:655:LYS:HB2	2.14	0.48
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.14	0.48
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.29	0.48
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.96	0.48
2:B:910:VAL:HG12	2:B:911:ILE:N	2.29	0.48
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.81	0.48
3:C:213:PRO:O	3:C:214:ASN:CB	2.61	0.48
3:C:236:GLY:C	3:C:238:ILE:N	2.69	0.48
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.95	0.48
7:G:15:PRO:O	7:G:16:SER:C	2.56	0.48
11:K:103:THR:C	11:K:105:PHE:H	2.20	0.48
1:A:42:ASP:C	1:A:44:THR:N	2.70	0.47
1:A:339:ASN:O	1:A:343:LYS:HG2	2.13	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
1:A:574:GLY:O	1:A:575:LYS:C	2.57	0.47
1:A:960:ILE:O	1:A:961:ARG:C	2.55	0.47
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.14	0.47
2:B:344:LYS:O	2:B:345:LYS:HB2	2.13	0.47
2:B:502:ILE:H	2:B:502:ILE:CD1	2.01	0.47
2:B:552:MET:C	2:B:554:ILE:H	2.21	0.47
2:B:642:ASP:CA	2:B:649:LYS:HA	2.40	0.47
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.14	0.47
2:B:874:PHE:HA	2:B:913:GLY:O	2.14	0.47
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.96	0.47
2:B:1208:MET:O	2:B:1211:ASN:N	2.46	0.47
3:C:99:LEU:HD23	3:C:99:LEU:N	2.28	0.47
3:C:123:ASN:ND2	3:C:125:MET:CG	2.77	0.47
4:D:170:THR:CG2	4:D:172:LEU:HG	2.43	0.47
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.96	0.47
1:A:262:LEU:C	1:A:264:PHE:H	2.21	0.47
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.43	0.47
1:A:1121:GLU:O	1:A:1122:PRO:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	1.96	0.47
1:A:1377:THR:O	1:A:1379:GLY:N	2.47	0.47
2:B:311:LEU:O	2:B:312:GLU:C	2.57	0.47
2:B:383:ASN:O	2:B:384:ARG:C	2.57	0.47
2:B:1198:TYR:C	2:B:1198:TYR:CD2	2.92	0.47
3:C:242:GLN:C	3:C:244:VAL:H	2.20	0.47
4:D:46:GLU:C	4:D:47:LEU:O	2.57	0.47
5:E:10:SER:O	5:E:14:ARG:HG3	2.14	0.47
5:E:30:ILE:HG22	5:E:31:THR:N	2.27	0.47
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.14	0.47
7:G:106:MET:HG2	7:G:107:LYS:N	2.28	0.47
9:I:34:TYR:CD2	9:I:34:TYR:C	2.91	0.47
12:L:31:CYS:HB3	12:L:34:CYS:C	2.39	0.47
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.79	0.47
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.96	0.47
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.13	0.47
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.97	0.47
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.44	0.47
2:B:683:SER:C	2:B:685:LEU:N	2.72	0.47
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.79	0.47
2:B:1005:GLY:HA2	3:C:176:ILE:O	2.13	0.47
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.95	0.47
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.79	0.47
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.96	0.47
6:F:94:LEU:HD21	6:F:122:MET:HA	1.95	0.47
8:H:38:LEU:HD12	8:H:124:ARG:O	2.14	0.47
10:J:34:THR:O	10:J:35:ALA:C	2.57	0.47
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.26	0.47
1:A:98:LYS:O	1:A:100:LYS:N	2.47	0.47
1:A:335:ARG:N	1:A:339:ASN:HD22	2.12	0.47
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.45	0.47
1:A:639:PRO:HG2	1:A:640:GLN:N	2.29	0.47
1:A:809:THR:H	1:A:812:GLU:HB2	1.80	0.47
1:A:873:MET:C	1:A:1058:VAL:CG2	2.88	0.47
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.47
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.49	0.47
2:B:329:THR:O	2:B:332:ASP:HB3	2.15	0.47
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.43	0.47
2:B:658:ILE:O	2:B:661:LEU:HB2	2.14	0.47
2:B:1138:MET:HA	2:B:1138:MET:CE	2.40	0.47
3:C:18:VAL:O	3:C:20:PHE:CD2	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:N	3:C:58:LEU:CD2	2.77	0.47
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.47
3:C:254:LYS:O	3:C:256:ALA:N	2.47	0.47
6:F:143:PHE:C	6:F:143:PHE:HD1	2.21	0.47
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.45	0.47
9:I:51:ASN:O	9:I:54:GLU:HG3	2.15	0.47
9:I:55:THR:HG22	9:I:55:THR:O	2.14	0.47
1:A:92:HIS:HD2	1:A:304:MET:CE	2.27	0.47
1:A:98:LYS:O	1:A:101:LYS:N	2.47	0.47
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.29	0.47
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.45	0.47
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.75	0.47
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.49	0.47
1:A:646:PHE:O	1:A:647:GLY:C	2.57	0.47
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.44	0.47
1:A:1405:THR:HB	1:A:1406:VAL:H	1.50	0.47
2:B:123:THR:O	2:B:125:SER:N	2.47	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
2:B:1060:ARG:C	2:B:1062:HIS:H	2.21	0.47
2:B:1162:ILE:C	2:B:1171:VAL:HG21	2.38	0.47
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.95	0.47
8:H:89:LEU:C	8:H:91:ASP:N	2.73	0.47
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.49	0.47
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.50	0.47
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.49	0.47
10:J:1:MET:H3	10:J:56:LEU:H	1.62	0.47
1:A:248:PRO:O	1:A:260:ASP:HB2	2.14	0.47
1:A:325:ILE:O	1:A:326:ARG:C	2.57	0.47
1:A:332:LYS:O	1:A:334:GLY:N	2.48	0.47
1:A:877:HIS:O	1:A:878:ILE:HG12	2.14	0.47
1:A:921:GLY:O	1:A:922:ASP:C	2.58	0.47
1:A:947:PHE:HD2	1:A:954:TRP:CZ2	2.32	0.47
1:A:1013:ASP:C	1:A:1015:VAL:H	2.22	0.47
2:B:55:VAL:O	2:B:56:ASP:C	2.58	0.47
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.96	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.49	0.47
2:B:597:MET:C	2:B:599:THR:N	2.70	0.47
2:B:710:LEU:C	2:B:711:GLU:HG2	2.40	0.47
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.96	0.47
2:B:1084:GLN:N	2:B:1084:GLN:HE21	2.10	0.47
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.39	0.47
3:C:47:ASP:CA	12:L:69:ALA:CB	2.90	0.47
3:C:168:ALA:O	3:C:170:TRP:N	2.48	0.47
4:D:153:ARG:C	4:D:154:PHE:CD1	2.92	0.47
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.80	0.47
7:G:1:MET:HG2	7:G:85:GLU:CD	2.40	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47
10:J:7:CYS:SG	10:J:8:PHE:N	2.87	0.47
11:K:24:ASP:OD1	11:K:26:LYS:N	2.48	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
1:A:308:ILE:HG22	1:A:309:ALA:N	2.19	0.47
1:A:381:THR:HG23	1:A:383:TYR:H	1.80	0.47
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.64	0.47
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.96	0.47
1:A:958:VAL:O	1:A:958:VAL:HG12	2.13	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.71	0.47
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.28	0.47
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.14	0.47
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.15	0.47
2:B:558:LEU:C	2:B:560:GLU:N	2.72	0.47
2:B:590:HIS:HD2	2:B:593:PRO:HB3	1.79	0.47
2:B:729:ILE:O	2:B:729:ILE:HG22	2.13	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.58	0.47
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.15	0.47
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.79	0.47
2:B:1106:ARG:HH11	2:B:1110:PRO:HG2	1.80	0.47
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.96	0.47
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.50	0.47
8:H:18:GLY:O	8:H:19:ARG:HB2	2.14	0.47
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.95	0.47
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.15	0.47
9:I:61:ASP:C	9:I:63:GLY:N	2.71	0.47
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.50	0.47
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.95	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.47	0.47
11:K:89:ASN:O	11:K:90:ALA:C	2.57	0.47
13:P:2:C:C2'	13:P:3:G:H5'	2.44	0.47
1:A:3:GLY:O	1:A:4:GLN:HB2	2.15	0.47
1:A:381:THR:HG23	1:A:382:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:O	1:A:404:TYR:CG	2.67	0.47
1:A:844:ALA:HB2	1:A:1389:PHE:CE2	2.50	0.47
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.44	0.47
2:B:210:LYS:HG3	2:B:461:LEU:O	2.14	0.47
2:B:294:ASP:C	2:B:296:GLU:H	2.22	0.47
2:B:343:ILE:HG23	2:B:347:LYS:CB	2.13	0.47
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.49	0.47
3:C:99:LEU:HA	3:C:119:VAL:O	2.14	0.47
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.15	0.47
11:K:67:PHE:O	11:K:68:PHE:HD2	1.98	0.47
12:L:43:THR:C	12:L:45:ALA:H	2.23	0.47
13:P:10:A:H3'	13:P:10:A:H8	1.80	0.47
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.15	0.47
1:A:230:ARG:N	1:A:233:TRP:CE3	2.64	0.47
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.30	0.47
1:A:482:PHE:C	1:A:484:GLY:N	2.73	0.47
1:A:780:VAL:O	1:A:782:ARG:HG2	2.15	0.47
1:A:1097:GLY:O	1:A:1100:ARG:N	2.46	0.47
2:B:263:GLY:O	2:B:264:SER:C	2.57	0.47
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.15	0.47
2:B:763:GLN:O	2:B:765:PRO:N	2.48	0.47
2:B:955:THR:CG2	2:B:956:THR:N	2.72	0.47
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.80	0.47
2:B:1166:CYS:O	2:B:1168:LEU:N	2.48	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.33	0.47
7:G:138:THR:CG2	7:G:139:ILE:H	2.02	0.47
9:I:56:ALA:O	9:I:57:GLY:C	2.57	0.47
1:A:43:GLU:O	1:A:44:THR:CB	2.63	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.29	0.47
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.78	0.47
1:A:409:SER:O	1:A:410:GLY:C	2.58	0.47
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.47
1:A:903:ASN:ND2	1:A:903:ASN:C	2.58	0.47
1:A:1157:ASP:C	1:A:1159:ARG:H	2.23	0.47
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.15	0.47
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.38	0.47
2:B:45:SER:O	2:B:46:GLN:C	2.57	0.47
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.42	0.47
2:B:446:LEU:O	2:B:447:ALA:CB	2.63	0.47
2:B:710:LEU:O	2:B:711:GLU:HG2	2.15	0.47
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.30	0.47
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.56	0.47
5:E:42:PHE:HZ	5:E:58:MET:HE3	1.80	0.47
5:E:124:VAL:HB	5:E:125:PRO:CD	2.45	0.47
5:E:131:THR:HG21	5:E:191:LYS:HZ3	1.80	0.47
5:E:147:HIS:HD2	5:E:149:LEU:H	1.62	0.47
10:J:16:ASP:O	10:J:18:TRP:N	2.48	0.47
1:A:399:HIS:O	1:A:400:PRO:C	2.56	0.46
1:A:474:VAL:HG22	1:A:474:VAL:O	2.15	0.46
1:A:595:THR:O	1:A:596:THR:HG23	2.14	0.46
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.49	0.46
1:A:1074:GLU:C	1:A:1076:ALA:N	2.72	0.46
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.96	0.46
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.50	0.46
3:C:239:PRO:O	3:C:241:ASP:N	2.48	0.46
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.80	0.46
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.98	0.46
8:H:7:ASP:O	8:H:8:ASP:HB2	2.14	0.46
1:A:24:PRO:HB3	1:A:237:THR:HB	1.97	0.46
1:A:89:PRO:C	1:A:204:THR:HG21	2.39	0.46
1:A:92:HIS:O	1:A:95:PHE:N	2.40	0.46
1:A:722:LEU:O	1:A:725:ALA:HB3	2.15	0.46
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.45	0.46
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.46	0.46
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.96	0.46
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.48	0.46
2:B:259:TYR:HD1	2:B:259:TYR:H	1.62	0.46
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.97	0.46
2:B:1151:LEU:N	2:B:1151:LEU:CD1	2.78	0.46
4:D:56:ARG:HD3	4:D:149:THR:HA	1.98	0.46
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.50	0.46
7:G:20:PRO:HG2	7:G:21:ARG:H	1.79	0.46
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.30	0.46
1:A:450:LEU:HB3	1:A:838:GLN:HE21	1.78	0.46
1:A:567:LYS:HE3	8:H:46:LEU:CB	2.45	0.46
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.59	0.46
1:A:1070:GLN:O	1:A:1071:SER:C	2.56	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.97	0.46
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.96	0.46
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.96	0.46
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:O	7:G:67:SER:HA	2.16	0.46
8:H:10:PHE:CE1	8:H:57:VAL:HB	2.50	0.46
8:H:10:PHE:HA	8:H:29:ALA:O	2.15	0.46
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.46
1:A:299:HIS:C	1:A:301:ALA:H	2.24	0.46
1:A:416:ARG:C	1:A:417:TYR:CD2	2.94	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.15	0.46
1:A:1205:LYS:O	1:A:1206:ASP:C	2.57	0.46
1:A:1239:ARG:CB	1:A:1239:ARG:HH11	2.28	0.46
1:A:1447:GLU:C	1:A:1447:GLU:OE1	2.59	0.46
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.98	0.46
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.50	0.46
2:B:640:VAL:O	2:B:640:VAL:HG12	2.16	0.46
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.30	0.46
3:C:11:ARG:HD3	3:C:209:TYR:CZ	2.51	0.46
3:C:73:GLN:HE21	3:C:74:SER:N	2.14	0.46
4:D:52:LEU:C	4:D:54:GLU:N	2.68	0.46
5:E:153:HIS:C	5:E:154:ILE:HG13	2.40	0.46
7:G:91:VAL:HG23	7:G:141:SER:O	2.16	0.46
1:A:56:PRO:O	1:A:57:ARG:CG	2.64	0.46
1:A:84:ILE:O	1:A:84:ILE:CG2	2.63	0.46
1:A:270:LEU:O	1:A:271:LYS:C	2.58	0.46
1:A:344:ARG:C	1:A:345:VAL:CG1	2.89	0.46
1:A:534:LEU:HD13	1:A:656:TRP:CD2	2.50	0.46
1:A:541:ILE:HD13	1:A:549:MET:CE	2.30	0.46
1:A:862:ASN:O	1:A:864:ILE:HG13	2.15	0.46
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.46	0.46
1:A:975:HIS:HA	1:A:1036:ARG:HG3	1.97	0.46
2:B:361:LEU:N	2:B:362:PRO:CD	2.78	0.46
2:B:510:LYS:CG	2:B:511:PRO:CD	2.85	0.46
2:B:899:ILE:HG22	2:B:900:ALA:N	2.30	0.46
2:B:957:ASN:O	2:B:960:GLY:N	2.47	0.46
3:C:77:ILE:HG22	3:C:78:GLU:N	2.31	0.46
3:C:263:THR:C	3:C:265:MET:N	2.74	0.46
4:D:53:SER:CB	4:D:152:SER:HB2	2.44	0.46
5:E:42:PHE:O	5:E:43:LYS:C	2.58	0.46
5:E:136:ASN:OD1	5:E:138:ALA:N	2.49	0.46
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.97	0.46
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.45	0.46
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.46
8:H:93:TYR:N	8:H:93:TYR:CD1	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.98	0.46
11:K:52:ASN:O	11:K:53:ASP:C	2.58	0.46
11:K:55:LYS:CB	11:K:81:TYR:HE1	2.28	0.46
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.51	0.46
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.97	0.46
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.45	0.46
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.44	0.46
1:A:370:ILE:O	1:A:372:LYS:N	2.48	0.46
1:A:536:LEU:O	1:A:537:ARG:C	2.57	0.46
1:A:570:PRO:C	1:A:571:LEU:HD12	2.40	0.46
1:A:672:ASP:O	1:A:673:GLY:C	2.59	0.46
1:A:735:VAL:O	1:A:735:VAL:HG12	2.14	0.46
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.96	0.46
1:A:1280:GLU:O	1:A:1281:ARG:C	2.58	0.46
1:A:1349:TYR:CB	1:A:1372:VAL:HG21	2.46	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.81	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.51	0.46
2:B:479:VAL:O	2:B:480:SER:HB3	2.14	0.46
2:B:801:LYS:O	10:J:52:THR:CG2	2.63	0.46
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.80	0.46
7:G:1:MET:HE1	7:G:80:LYS:C	2.41	0.46
1:A:53:LEU:CD2	1:A:54:ASN:N	2.52	0.46
1:A:92:HIS:HD2	1:A:304:MET:HE1	1.80	0.46
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.49	0.46
1:A:471:ASN:O	1:A:474:VAL:HG12	2.15	0.46
1:A:695:LYS:C	1:A:697:ALA:H	2.22	0.46
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.46
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.13	0.46
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.97	0.46
1:A:996:ASN:O	1:A:998:LEU:HD12	2.15	0.46
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.29	0.46
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.45	0.46
1:A:1325:THR:O	1:A:1325:THR:CG2	2.63	0.46
2:B:971:THR:HG1	3:C:61:GLU:HG3	1.81	0.46
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.16	0.46
3:C:34:ARG:O	3:C:38:ILE:HG13	2.16	0.46
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.45	0.46
3:C:168:ALA:O	3:C:169:LYS:C	2.58	0.46
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.45	0.46
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.50	0.46
1:A:356:ASP:O	1:A:358:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LYS:CB	1:A:641:VAL:HG11	2.45	0.46
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.14	0.46
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.97	0.46
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.98	0.46
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.15	0.46
2:B:658:ILE:O	2:B:661:LEU:N	2.38	0.46
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.79	0.46
2:B:798:TYR:CE2	3:C:62:PHE:HZ	2.29	0.46
2:B:861:ASP:OD1	2:B:862:GLN:N	2.49	0.46
2:B:865:LYS:C	2:B:866:TYR:CD1	2.94	0.46
2:B:1017:ILE:CB	2:B:1018:PRO:CD	2.94	0.46
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.16	0.46
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.46
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.97	0.46
4:D:151:PHE:CD1	4:D:151:PHE:N	2.84	0.46
10:J:28:ASP:O	10:J:29:GLU:C	2.59	0.46
1:A:261:ASP:O	1:A:264:PHE:HB2	2.16	0.46
1:A:399:HIS:CG	1:A:400:PRO:N	2.83	0.46
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.15	0.46
1:A:630:ILE:O	1:A:631:HIS:C	2.57	0.46
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.97	0.46
1:A:841:LEU:O	1:A:845:LEU:HG	2.15	0.46
1:A:1027:ALA:O	1:A:1028:THR:C	2.58	0.46
1:A:1134:ILE:O	1:A:1135:ARG:C	2.58	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.46
2:B:618:ASP:O	2:B:619:ILE:C	2.58	0.46
2:B:661:LEU:C	2:B:663:ALA:N	2.74	0.46
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.46	0.46
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.46	0.46
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.81	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.60	0.46
4:D:27:LEU:HD22	4:D:173:HIS:HD2	1.79	0.46
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.51	0.46
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.80	0.46
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.49	0.46
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.42	0.46
2:B:53:GLN:HG3	2:B:53:GLN:O	2.15	0.46
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.98	0.46
2:B:410:GLY:O	2:B:412:LEU:N	2.49	0.46
2:B:530:GLY:O	2:B:531:GLN:HG3	2.16	0.46
3:C:123:ASN:ND2	3:C:125:MET:SD	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLU:O	3:C:167:HIS:HB2	2.16	0.46
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.51	0.46
6:F:121:ALA:O	6:F:122:MET:C	2.59	0.46
12:L:36:SER:O	12:L:37:LYS:C	2.58	0.46
1:A:89:PRO:HB3	1:A:208:LEU:HD12	1.99	0.45
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.98	0.45
1:A:437:MET:O	1:A:438:ASP:C	2.58	0.45
1:A:524:VAL:O	1:A:525:GLN:C	2.59	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.98	0.45
1:A:608:ILE:O	1:A:610:GLY:N	2.50	0.45
2:B:53:GLN:CB	2:B:547:VAL:HG21	2.45	0.45
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.51	0.45
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.98	0.45
2:B:386:LEU:C	2:B:388:CYS:N	2.72	0.45
2:B:449:ASN:O	2:B:451:LYS:N	2.49	0.45
2:B:591:ARG:O	2:B:593:PRO:HD3	2.15	0.45
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.51	0.45
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.31	0.45
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.45
4:D:7:THR:O	4:D:7:THR:HG23	2.15	0.45
5:E:55:ARG:O	5:E:57:MET:N	2.49	0.45
5:E:161:LYS:C	5:E:163:GLU:H	2.23	0.45
8:H:59:ILE:CG2	8:H:60:ALA:H	2.23	0.45
9:I:56:ALA:O	9:I:57:GLY:O	2.33	0.45
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.97	0.45
1:A:230:ARG:HB2	1:A:233:TRP:CE3	2.51	0.45
1:A:370:ILE:O	1:A:371:ALA:C	2.55	0.45
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.45
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.82	0.45
2:B:29:ASP:O	2:B:30:SER:C	2.59	0.45
2:B:189:LEU:O	2:B:192:LEU:HB2	2.16	0.45
2:B:303:TYR:CD2	2:B:303:TYR:N	2.82	0.45
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.52	0.45
2:B:757:PRO:HD3	2:B:983:ARG:NH2	2.31	0.45
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.51	0.45
4:D:17:LYS:HE3	4:D:17:LYS:N	2.31	0.45
7:G:1:MET:HE1	7:G:80:LYS:N	2.32	0.45
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.16	0.45
8:H:61:SER:O	8:H:62:SER:CB	2.58	0.45
8:H:83:GLN:C	8:H:85:GLY:N	2.75	0.45
9:I:15:TYR:N	9:I:15:TYR:HD1	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:6:C:H2'	13:P:7:A:C8	2.51	0.45
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.50	0.45
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.97	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.80	0.45
1:A:1438:THR:CB	2:B:1144:ALA:HB3	2.38	0.45
2:B:210:LYS:HA	2:B:481:GLN:O	2.17	0.45
2:B:237:VAL:HG12	2:B:238:ALA:N	2.31	0.45
2:B:294:ASP:O	2:B:296:GLU:N	2.46	0.45
2:B:806:THR:C	2:B:808:ALA:N	2.74	0.45
2:B:860:MET:CG	2:B:861:ASP:N	2.78	0.45
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.41	0.45
3:C:8:VAL:HG12	3:C:9:LYS:N	2.31	0.45
4:D:195:ILE:HG22	4:D:195:ILE:O	2.17	0.45
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.50	0.45
6:F:92:ARG:O	6:F:93:ILE:C	2.58	0.45
10:J:23:ASN:O	10:J:25:LEU:N	2.49	0.45
11:K:31:VAL:CG1	11:K:32:VAL:H	2.29	0.45
1:A:331:GLY:O	1:A:332:LYS:HB3	2.16	0.45
1:A:968:GLN:C	1:A:970:THR:H	2.24	0.45
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.45
2:B:37:PHE:HD2	2:B:542:MET:SD	2.39	0.45
2:B:199:MET:N	2:B:199:MET:SD	2.86	0.45
2:B:234:ILE:O	2:B:261:ARG:NH2	2.48	0.45
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.16	0.45
2:B:583:ASN:OD1	2:B:628:THR:N	2.43	0.45
3:C:242:GLN:C	3:C:244:VAL:N	2.74	0.45
4:D:9:GLN:OE1	4:D:38:ILE:HD12	2.16	0.45
5:E:18:THR:O	5:E:19:VAL:C	2.58	0.45
5:E:177:ARG:HG2	5:E:213:ILE:HG22	1.99	0.45
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.45
14:T:24:DG:H2''	14:T:25:DT:C5'	2.42	0.45
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.98	0.45
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.97	0.45
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.99	0.45
1:A:535:THR:HG21	1:A:617:VAL:H	1.80	0.45
1:A:688:LYS:C	1:A:690:VAL:H	2.24	0.45
1:A:823:GLY:O	1:A:824:LEU:C	2.60	0.45
1:A:832:ALA:HA	14:T:18:DT:C6	2.52	0.45
2:B:226:PHE:HA	2:B:395:GLN:CG	2.45	0.45
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.43	0.45
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:TRP:O	2:B:684:LEU:N	2.50	0.45
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.99	0.45
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.97	0.45
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.14	0.45
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.32	0.45
4:D:187:THR:HG22	4:D:188:ALA:H	1.82	0.45
5:E:72:PHE:CE2	5:E:155:ARG:NH2	2.84	0.45
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.98	0.45
9:I:115:LYS:HD3	9:I:117:LYS:CE	2.39	0.45
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.98	0.45
1:A:472:LEU:CD2	2:B:836:GLU:HG3	2.46	0.45
1:A:673:GLY:O	1:A:676:MET:HB2	2.17	0.45
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.16	0.45
2:B:458:LYS:O	2:B:459:TYR:C	2.59	0.45
2:B:763:GLN:C	2:B:765:PRO:HD2	2.41	0.45
2:B:913:GLY:HA2	2:B:938:SER:OG	2.17	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.31	0.45
3:C:27:LEU:O	3:C:28:ALA:C	2.59	0.45
3:C:107:SER:C	3:C:109:SER:H	2.24	0.45
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.76	0.45
8:H:10:PHE:HE1	8:H:57:VAL:HB	1.81	0.45
8:H:58:THR:HB	8:H:143:LEU:HD13	1.99	0.45
8:H:91:ASP:O	8:H:93:TYR:N	2.49	0.45
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.18	0.45
12:L:49:LYS:O	12:L:50:ASP:CB	2.63	0.45
1:A:43:GLU:O	1:A:44:THR:HB	2.16	0.45
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.99	0.45
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.44	0.45
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.97	0.45
1:A:723:ASN:C	1:A:725:ALA:N	2.72	0.45
1:A:818:MET:HA	2:B:514:LEU:HB3	1.98	0.45
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.52	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.16	0.45
2:B:866:TYR:HD1	2:B:870:ILE:O	1.99	0.45
2:B:903:VAL:HG12	2:B:904:ARG:N	2.32	0.45
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.49	0.45
3:C:69:LEU:O	10:J:6:ARG:HD2	2.16	0.45
3:C:172:PRO:O	3:C:235:VAL:HG23	2.17	0.45
9:I:8:ARG:O	9:I:10:CYS:N	2.50	0.45
9:I:75:CYS:SG	9:I:78:CYS:C	3.00	0.45
10:J:52:THR:O	10:J:53:HIS:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.52	0.45
1:A:219:PHE:O	1:A:222:LEU:O	2.34	0.45
1:A:313:GLN:O	1:A:314:ALA:HB3	2.17	0.45
1:A:688:LYS:C	1:A:690:VAL:N	2.75	0.45
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.27	0.45
1:A:821:ARG:O	1:A:825:ILE:HG13	2.16	0.45
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.47	0.45
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.45
3:C:251:LEU:O	3:C:251:LEU:HD12	2.16	0.45
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.52	0.45
11:K:59:ALA:HA	11:K:74:ARG:O	2.17	0.45
1:A:41:MET:O	1:A:42:ASP:C	2.59	0.45
1:A:218:ASP:O	1:A:219:PHE:C	2.60	0.45
1:A:230:ARG:N	1:A:233:TRP:HE3	2.07	0.45
1:A:666:ILE:HG12	2:B:1030:LEU:HD22	1.99	0.45
1:A:698:GLN:HA	9:I:97:MET:O	2.16	0.45
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.17	0.45
1:A:1334:ASP:C	1:A:1336:MET:N	2.74	0.45
1:A:1396:ALA:O	1:A:1397:LEU:C	2.60	0.45
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.45
1:A:1418:LEU:HD12	1:A:1419:ASP:H	1.81	0.45
2:B:180:TYR:CD1	2:B:180:TYR:N	2.78	0.45
2:B:244:LEU:O	2:B:246:LYS:N	2.50	0.45
2:B:487:THR:O	2:B:490:SER:HB3	2.17	0.45
2:B:558:LEU:O	2:B:560:GLU:N	2.49	0.45
2:B:1155:SER:OG	2:B:1156:ASP:N	2.42	0.45
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.47	0.45
7:G:14:HIS:CD2	7:G:16:SER:CB	2.90	0.45
8:H:40:LEU:HD22	8:H:123:MET:CE	2.46	0.45
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.99	0.45
1:A:55:ASP:C	1:A:57:ARG:N	2.72	0.45
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.57	0.45
1:A:285:PRO:O	1:A:287:HIS:N	2.49	0.45
1:A:534:LEU:O	1:A:534:LEU:HG	2.15	0.45
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.52	0.45
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.82	0.45
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.17	0.45
2:B:315:LYS:N	2:B:316:PRO:CD	2.79	0.45
2:B:552:MET:C	2:B:554:ILE:N	2.75	0.45
2:B:615:MET:HE3	2:B:615:MET:HB2	1.85	0.45
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:PRO:O	2:B:766:ARG:C	2.60	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.97	0.45
3:C:44:LEU:HD21	3:C:159:ALA:HB1	1.98	0.45
3:C:209:TYR:H	3:C:209:TYR:HD1	1.63	0.45
4:D:59:ILE:HG21	4:D:145:MET:SD	2.57	0.45
6:F:97:ARG:NH2	6:F:106:PRO:O	2.50	0.45
8:H:82:PRO:C	8:H:84:ALA:N	2.74	0.45
11:K:5:ASP:O	11:K:6:ARG:C	2.60	0.45
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.04	0.45
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.33	0.44
1:A:58:LEU:HD11	1:A:243:PRO:HB2	1.99	0.44
1:A:381:THR:O	1:A:382:PRO:C	2.60	0.44
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.99	0.44
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.32	0.44
1:A:1439:GLY:C	1:A:1441:PHE:H	2.25	0.44
2:B:531:GLN:HG3	2:B:532:ALA:N	2.30	0.44
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.32	0.44
4:D:10:THR:HG23	4:D:10:THR:O	2.17	0.44
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.83	0.44
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.46	0.44
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.98	0.44
8:H:95:TYR:HE2	8:H:97:MET:CG	2.30	0.44
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.81	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.44
1:A:392:VAL:O	1:A:393:ARG:C	2.60	0.44
1:A:506:ALA:C	1:A:508:PRO:CD	2.91	0.44
1:A:653:VAL:O	1:A:654:ASN:C	2.59	0.44
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.17	0.44
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.98	0.44
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.18	0.44
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.34	0.44
2:B:166:PHE:C	2:B:167:ILE:HG13	2.43	0.44
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.98	0.44
2:B:730:ARG:O	2:B:731:VAL:O	2.35	0.44
2:B:744:HIS:HD2	2:B:746:SER:CB	2.30	0.44
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.44
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.98	0.44
3:C:9:LYS:O	3:C:10:ILE:C	2.59	0.44
10:J:21:TYR:HB2	10:J:39:LEU:HD13	1.98	0.44
12:L:40:LEU:HB3	12:L:41:SER:H	1.69	0.44
12:L:61:THR:HG22	12:L:63:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.56	0.44
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.51	0.44
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.32	0.44
1:A:794:PRO:C	1:A:796:SER:H	2.25	0.44
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.31	0.44
1:A:1013:ASP:O	1:A:1015:VAL:N	2.51	0.44
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.44
2:B:258:LEU:HG	2:B:258:LEU:O	2.17	0.44
2:B:259:TYR:N	2:B:259:TYR:CD1	2.85	0.44
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.98	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
2:B:895:ASP:C	2:B:897:GLY:N	2.75	0.44
2:B:1017:ILE:O	2:B:1018:PRO:C	2.60	0.44
2:B:1076:HIS:CD2	11:K:40:HIS:CE1	3.05	0.44
2:B:1138:MET:HE3	2:B:1143:ALA:HB3	2.00	0.44
3:C:252:GLN:O	3:C:253:LYS:C	2.59	0.44
7:G:79:PHE:HZ	7:G:106:MET:CE	2.25	0.44
7:G:115:MET:HB3	7:G:163:ILE:HD11	1.99	0.44
11:K:89:ASN:O	11:K:92:ASN:N	2.50	0.44
1:A:61:ILE:HG22	1:A:62:ASP:N	2.28	0.44
1:A:453:MET:O	1:A:456:MET:HE2	2.17	0.44
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.98	0.44
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.33	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.33	0.44
2:B:27:ALA:C	2:B:29:ASP:N	2.74	0.44
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.18	0.44
3:C:187:LYS:C	3:C:189:THR:H	2.24	0.44
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.16	0.44
4:D:35:LEU:HD13	4:D:173:HIS:ND1	2.33	0.44
4:D:146:GLN:O	4:D:147:TYR:C	2.60	0.44
5:E:129:PRO:O	5:E:130:ALA:C	2.61	0.44
7:G:27:LYS:O	7:G:28:THR:C	2.58	0.44
8:H:31:THR:O	8:H:31:THR:HG22	2.16	0.44
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.18	0.44
11:K:103:THR:O	11:K:105:PHE:N	2.51	0.44
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.14	0.44
1:A:274:ILE:O	1:A:275:SER:C	2.61	0.44
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.31	0.44
1:A:353:ILE:HG21	1:A:487:MET:CE	2.48	0.44
1:A:971:PHE:O	1:A:972:HIS:C	2.61	0.44
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:336:ARG:NH2	2:B:345:LYS:CG	2.73	0.44
2:B:343:ILE:HG21	2:B:348:ARG:CA	2.46	0.44
2:B:344:LYS:O	2:B:345:LYS:CG	2.65	0.44
2:B:549:THR:N	2:B:628:THR:HG23	2.31	0.44
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.44
3:C:167:HIS:HA	11:K:6:ARG:NH1	2.32	0.44
4:D:71:LYS:HA	4:D:74:GLN:CB	2.44	0.44
5:E:55:ARG:HD2	5:E:83:CYS:O	2.18	0.44
5:E:128:PRO:HA	5:E:129:PRO:C	2.43	0.44
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.83	0.44
8:H:56:THR:HB	8:H:145:ARG:CG	2.42	0.44
10:J:21:TYR:CD2	10:J:21:TYR:C	2.95	0.44
10:J:48:ARG:HD2	10:J:48:ARG:C	2.43	0.44
11:K:88:LYS:O	11:K:89:ASN:C	2.60	0.44
11:K:89:ASN:O	11:K:91:CYS:N	2.51	0.44
1:A:652:VAL:O	1:A:653:VAL:C	2.61	0.44
1:A:719:VAL:C	1:A:721:PHE:N	2.75	0.44
1:A:825:ILE:O	1:A:826:ASP:C	2.60	0.44
2:B:230:ALA:N	2:B:231:PRO:CD	2.80	0.44
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.82	0.44
3:C:189:THR:CG2	3:C:190:ASP:N	2.80	0.44
6:F:116:ASP:C	6:F:116:ASP:OD1	2.61	0.44
1:A:371:ALA:O	1:A:435:HIS:HB3	2.18	0.44
1:A:470:LEU:HD22	1:A:487:MET:HE3	2.00	0.44
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.83	0.44
1:A:936:LEU:O	1:A:939:ASP:HB2	2.17	0.44
2:B:185:THR:N	2:B:188:ASP:HB2	2.29	0.44
2:B:765:PRO:C	2:B:767:ASN:N	2.74	0.44
2:B:903:VAL:CG1	2:B:904:ARG:N	2.81	0.44
2:B:997:GLU:CD	2:B:997:GLU:H	2.24	0.44
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.00	0.44
3:C:239:PRO:O	3:C:240:VAL:C	2.61	0.44
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.81	0.44
6:F:86:THR:HG23	6:F:89:GLU:CD	2.43	0.44
7:G:9:LEU:HD12	7:G:10:ASN:N	2.32	0.44
7:G:17:PHE:C	7:G:19:GLY:H	2.25	0.44
7:G:83:LYS:HE2	7:G:150:CYS:H	1.83	0.44
1:A:225:ASN:ND2	1:A:227:VAL:H	2.16	0.44
1:A:606:LEU:HD23	1:A:614:PHE:CE2	2.52	0.44
1:A:711:ARG:O	1:A:712:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.48	0.44
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.33	0.44
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.18	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HG13	1.99	0.44
1:A:1396:ALA:O	1:A:1398:MET:N	2.51	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.51	0.44
2:B:711:GLU:H	2:B:712:PRO:HD2	1.82	0.44
2:B:877:PRO:C	2:B:878:GLN:HG3	2.42	0.44
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.00	0.44
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.16	0.44
2:B:1177:HIS:C	2:B:1179:GLN:N	2.76	0.44
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.99	0.44
3:C:255:VAL:HG12	11:K:91:CYS:HB3	2.00	0.44
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.53	0.44
4:D:64:VAL:O	4:D:66:ARG:N	2.51	0.44
4:D:153:ARG:C	4:D:154:PHE:CG	2.96	0.44
7:G:115:MET:CB	7:G:116:PRO:CD	2.96	0.44
10:J:32:GLU:O	10:J:35:ALA:N	2.51	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
1:A:349:ALA:HB2	2:B:1105:ALA:HA	1.98	0.44
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.17	0.44
2:B:247:GLY:O	2:B:249:ARG:N	2.50	0.44
2:B:460:ALA:C	2:B:462:ALA:H	2.25	0.44
2:B:710:LEU:O	2:B:711:GLU:OE2	2.35	0.44
2:B:770:GLN:C	2:B:772:ALA:N	2.76	0.44
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.99	0.44
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.81	0.44
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.47	0.44
3:C:86:CYS:O	3:C:88:CYS:N	2.51	0.44
5:E:73:PRO:O	5:E:75:MET:N	2.46	0.44
8:H:26:ILE:CG2	8:H:27:GLU:N	2.81	0.44
8:H:59:ILE:CG2	8:H:60:ALA:N	2.66	0.44
8:H:84:ALA:C	8:H:86:ASP:N	2.73	0.44
11:K:103:THR:C	11:K:105:PHE:N	2.76	0.44
1:A:442:VAL:CG2	1:A:460:VAL:HG23	2.48	0.43
1:A:853:ASP:O	1:A:854:ASN:CB	2.65	0.43
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.33	0.43
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.74	0.43
1:A:1313:LEU:HB3	1:A:1338:VAL:HG21	1.99	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.43
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.47	0.43
2:B:276:ILE:HD13	2:B:334:ILE:HG23	2.00	0.43
2:B:388:CYS:O	2:B:391:ASP:N	2.42	0.43
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.83	0.43
2:B:566:LEU:O	2:B:567:GLU:C	2.61	0.43
2:B:575:PRO:HG2	2:B:576:ASP:H	1.83	0.43
2:B:707:PRO:O	2:B:711:GLU:HG3	2.17	0.43
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.96	0.43
2:B:1001:PHE:HD2	3:C:34:ARG:NH2	2.15	0.43
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.88	0.43
3:C:256:ALA:O	3:C:259:LEU:N	2.51	0.43
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.48	0.43
9:I:59:VAL:C	9:I:61:ASP:N	2.76	0.43
1:A:57:ARG:O	1:A:68:GLN:CG	2.64	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.43
1:A:463:ILE:HB	1:A:464:PRO:CD	2.46	0.43
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.00	0.43
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.33	0.43
1:A:1344:GLY:O	1:A:1345:ARG:C	2.60	0.43
2:B:360:PHE:O	2:B:361:LEU:C	2.60	0.43
2:B:428:ILE:O	2:B:432:MET:HE2	2.17	0.43
2:B:469:GLN:HB2	2:B:470:LYS:H	1.41	0.43
2:B:984:HIS:O	2:B:985:GLY:C	2.60	0.43
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.82	0.43
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.83	0.43
3:C:166:GLU:C	11:K:6:ARG:HH11	2.26	0.43
9:I:85:PHE:HD2	9:I:85:PHE:N	1.99	0.43
11:K:82:ASP:O	11:K:85:ASP:HB2	2.18	0.43
1:A:35:ILE:HB	1:A:83:HIS:O	2.18	0.43
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.76	0.43
1:A:329:LEU:O	1:A:330:LYS:C	2.61	0.43
1:A:358:ASN:HD22	11:K:66:PRO:HD2	1.83	0.43
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.45	0.43
1:A:569:LYS:O	1:A:571:LEU:HD13	2.17	0.43
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.99	0.43
1:A:874:ASP:O	1:A:876:ALA:N	2.52	0.43
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.99	0.43
1:A:1329:THR:CG2	1:A:1331:SER:HB3	2.48	0.43
2:B:376:PHE:O	2:B:586:TRP:HZ3	2.00	0.43
2:B:1151:LEU:N	2:B:1151:LEU:HD12	2.33	0.43
3:C:45:ALA:O	3:C:159:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLY:HA2	10:J:16:ASP:HB3	2.00	0.43
4:D:64:VAL:C	4:D:66:ARG:N	2.76	0.43
12:L:55:ILE:H	12:L:55:ILE:HG12	1.35	0.43
1:A:2:VAL:HG13	2:B:1195:HIS:CE1	2.53	0.43
1:A:68:GLN:C	1:A:70:CYS:N	2.65	0.43
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.01	0.43
1:A:188:ASP:OD1	1:A:189:ARG:N	2.51	0.43
1:A:283:GLY:O	1:A:285:PRO:CD	2.66	0.43
1:A:332:LYS:C	1:A:334:GLY:N	2.74	0.43
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.43
1:A:755:PHE:O	1:A:756:ILE:C	2.61	0.43
1:A:894:GLU:C	1:A:896:ARG:H	2.26	0.43
1:A:964:ILE:O	1:A:965:GLN:C	2.61	0.43
1:A:967:ALA:O	1:A:968:GLN:O	2.37	0.43
1:A:1007:ILE:C	1:A:1009:ASN:N	2.75	0.43
1:A:1244:ARG:NH2	1:A:1259:MET:HE1	2.33	0.43
2:B:434:ARG:HA	2:B:437:GLU:OE2	2.18	0.43
2:B:582:VAL:HA	2:B:626:ILE:O	2.18	0.43
2:B:644:GLU:C	2:B:646:LEU:N	2.76	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.18	0.43
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.01	0.43
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.32	0.43
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.95	0.43
5:E:168:TYR:C	5:E:169:ARG:HG3	2.43	0.43
6:F:89:GLU:HB3	6:F:134:ILE:HD13	2.01	0.43
7:G:13:LEU:HD22	7:G:14:HIS:O	2.18	0.43
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.43
9:I:34:TYR:C	9:I:35:VAL:HG23	2.44	0.43
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.48	0.43
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.48	0.43
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.19	0.43
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.99	0.43
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.18	0.43
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.43
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.76	0.43
2:B:1099:VAL:C	2:B:1101:ASP:N	2.77	0.43
3:C:70:ILE:O	3:C:70:ILE:HG22	2.18	0.43
4:D:134:THR:CG2	4:D:135:GLY:H	2.30	0.43
5:E:23:VAL:HG13	5:E:78:LEU:HD13	2.00	0.43
8:H:98:TYR:C	8:H:118:PHE:HD2	2.25	0.43
1:A:34:LYS:HD3	1:A:34:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:O	1:A:66:LYS:C	2.62	0.43
1:A:478:TYR:O	1:A:479:ASN:HB3	2.19	0.43
1:A:543:LEU:O	1:A:544:ASP:C	2.61	0.43
1:A:709:THR:HG21	9:I:93:LYS:O	2.18	0.43
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.69	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.48	0.43
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.67	0.43
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.49	0.43
2:B:911:ILE:CD1	2:B:941:LEU:HD13	2.40	0.43
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.82	0.43
3:C:74:SER:HB2	3:C:77:ILE:CG1	2.48	0.43
3:C:80:LEU:O	3:C:80:LEU:HG	2.17	0.43
4:D:119:ARG:HG2	4:D:120:GLU:N	2.33	0.43
7:G:62:LEU:HD23	7:G:62:LEU:HA	1.83	0.43
7:G:106:MET:CG	7:G:107:LYS:N	2.80	0.43
8:H:95:TYR:CE2	8:H:97:MET:CG	3.02	0.43
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.86	0.43
14:T:25:DT:H2''	14:T:26:DC:C5'	2.48	0.43
1:A:885:THR:O	1:A:885:THR:HG22	2.18	0.43
1:A:1209:MET:O	1:A:1210:GLY:C	2.61	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.18	0.43
2:B:400:HIS:O	2:B:402:GLY:N	2.52	0.43
2:B:560:GLU:O	2:B:561:TRP:CD1	2.72	0.43
2:B:604:ARG:NH2	2:B:613:VAL:O	2.52	0.43
2:B:839:MET:HB3	2:B:1012:ILE:HG22	2.00	0.43
2:B:871:THR:HG22	2:B:872:GLU:N	2.32	0.43
2:B:1162:ILE:HG23	2:B:1168:LEU:O	2.18	0.43
3:C:179:GLU:O	3:C:180:TYR:HB3	2.19	0.43
3:C:238:ILE:HG22	3:C:243:VAL:HG23	2.01	0.43
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.49	0.43
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.43
5:E:153:HIS:O	5:E:154:ILE:CG1	2.67	0.43
7:G:51:TYR:C	7:G:51:TYR:HD2	2.25	0.43
7:G:126:ASN:HD22	7:G:126:ASN:HA	1.64	0.43
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.33	0.43
1:A:47:ARG:O	1:A:48:ALA:HB2	2.19	0.43
1:A:381:THR:HG22	1:A:383:TYR:H	1.83	0.43
1:A:470:LEU:HD13	1:A:487:MET:HE1	2.00	0.43
1:A:590:ARG:NH2	1:A:620:LYS:CB	2.73	0.43
1:A:815:PHE:O	1:A:816:HIS:C	2.60	0.43
1:A:889:SER:C	1:A:891:ALA:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.16	0.43
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.49	0.43
2:B:95:ILE:HG13	2:B:130:VAL:HG22	2.01	0.43
2:B:129:PHE:HA	2:B:165:VAL:O	2.19	0.43
2:B:593:PRO:O	2:B:594:ALA:C	2.61	0.43
2:B:1002:THR:O	2:B:1003:ALA:C	2.61	0.43
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.45	0.43
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.99	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.73	0.43
4:D:35:LEU:HD13	4:D:174:PRO:HD2	2.01	0.43
4:D:122:GLU:HA	4:D:125:SER:OG	2.18	0.43
4:D:135:GLY:C	4:D:137:ASN:H	2.26	0.43
6:F:140:ASP:C	6:F:140:ASP:OD1	2.62	0.43
6:F:147:SER:O	6:F:148:VAL:C	2.60	0.43
7:G:25:TYR:CD2	7:G:25:TYR:C	2.96	0.43
11:K:31:VAL:O	11:K:74:ARG:HA	2.19	0.43
12:L:30:ILE:HG22	12:L:31:CYS:N	2.33	0.43
13:P:9:G:C2	14:T:21:DC:O2	2.72	0.43
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.17	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.43
1:A:600:PRO:C	1:A:602:ASP:H	2.27	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.99	0.43
2:B:175:ARG:HG2	2:B:175:ARG:NH1	2.31	0.43
2:B:337:ARG:HA	2:B:337:ARG:HD2	1.80	0.43
2:B:343:ILE:CG2	2:B:348:ARG:H	2.32	0.43
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.17	0.43
2:B:957:ASN:O	2:B:958:GLN:C	2.61	0.43
2:B:1134:GLU:CD	2:B:1134:GLU:N	2.75	0.43
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.54	0.43
3:C:124:LEU:CD2	3:C:129:ILE:HG22	2.48	0.43
3:C:166:GLU:C	11:K:6:ARG:NH1	2.76	0.43
3:C:229:TYR:CD1	3:C:229:TYR:N	2.86	0.43
4:D:23:ASN:O	7:G:83:LYS:HB2	2.19	0.43
4:D:141:LEU:HD12	4:D:141:LEU:HA	1.76	0.43
7:G:26:LEU:O	7:G:29:LYS:N	2.52	0.43
7:G:132:SER:OG	7:G:133:SER:N	2.51	0.43
1:A:106:VAL:HG13	1:A:112:LYS:C	2.44	0.43
1:A:353:ILE:HD12	1:A:487:MET:HE2	1.99	0.43
1:A:715:GLU:O	1:A:716:ASP:C	2.62	0.43
1:A:1142:THR:O	1:A:1143:LEU:C	2.62	0.43
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:LEU:O	1:A:1450:LEU:CG	2.65	0.43
2:B:550:ASP:OD1	2:B:552:MET:HE3	2.19	0.43
2:B:642:ASP:HB3	2:B:649:LYS:HE3	2.00	0.43
2:B:758:PHE:C	2:B:760:ASP:N	2.77	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.34	0.43
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.99	0.43
3:C:18:VAL:O	3:C:19:ASP:C	2.62	0.43
6:F:82:THR:HA	6:F:83:PRO:HD3	1.80	0.43
9:I:58:VAL:O	9:I:58:VAL:HG12	2.18	0.43
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.34	0.42
1:A:452:LYS:HE2	1:A:452:LYS:HB3	1.77	0.42
1:A:685:GLU:HG3	1:A:686:ALA:N	2.33	0.42
1:A:867:ILE:HD12	1:A:867:ILE:N	2.34	0.42
1:A:901:LEU:HD22	1:A:919:ILE:HG22	2.01	0.42
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.25	0.42
1:A:1225:PHE:HE2	1:A:1227:ILE:HD11	1.84	0.42
1:A:1323:ASP:O	1:A:1325:THR:N	2.52	0.42
2:B:644:GLU:C	2:B:646:LEU:H	2.26	0.42
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.49	0.42
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.83	0.42
2:B:1060:ARG:C	2:B:1062:HIS:N	2.77	0.42
3:C:3:GLU:O	3:C:4:GLU:CG	2.67	0.42
3:C:75:MET:HE2	3:C:239:PRO:CG	2.49	0.42
4:D:52:LEU:O	4:D:53:SER:OG	2.36	0.42
7:G:80:LYS:O	7:G:82:PHE:CE1	2.72	0.42
12:L:27:LEU:HD23	12:L:27:LEU:N	2.34	0.42
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.42
1:A:826:ASP:HB2	1:A:830:LYS:HD3	2.00	0.42
2:B:234:ILE:O	2:B:261:ARG:CZ	2.67	0.42
2:B:446:LEU:N	2:B:446:LEU:HD23	2.34	0.42
3:C:146:LYS:C	3:C:147:LEU:HD23	2.43	0.42
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.27	0.42
5:E:14:ARG:O	5:E:17:ARG:HB3	2.19	0.42
7:G:4:ILE:O	7:G:4:ILE:HG22	2.20	0.42
7:G:66:GLY:O	7:G:67:SER:C	2.60	0.42
8:H:11:GLN:O	8:H:28:ALA:HB1	2.18	0.42
10:J:36:LEU:HA	10:J:39:LEU:HD12	2.01	0.42
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.53	0.42
1:A:381:THR:HG22	1:A:383:TYR:N	2.34	0.42
1:A:603:ASN:O	1:A:604:GLY:O	2.37	0.42
1:A:639:PRO:CG	1:A:640:GLN:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:O	1:A:868:TYR:C	2.62	0.42
1:A:932:GLU:O	1:A:935:GLN:HB3	2.19	0.42
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.19	0.42
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.01	0.42
1:A:1277:GLU:C	1:A:1279:ILE:H	2.26	0.42
2:B:426:LYS:O	2:B:426:LYS:HG3	2.18	0.42
2:B:498:THR:HG23	2:B:499:ASN:N	2.33	0.42
2:B:999:MET:HA	2:B:999:MET:CE	2.47	0.42
2:B:1068:GLY:O	2:B:1069:PHE:C	2.63	0.42
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.32	0.42
2:B:1197:PRO:O	2:B:1200:ALA:N	2.52	0.42
2:B:1216:LEU:N	2:B:1216:LEU:HD23	2.34	0.42
3:C:74:SER:HB2	3:C:77:ILE:HG12	2.00	0.42
3:C:256:ALA:C	3:C:258:ILE:N	2.77	0.42
5:E:35:VAL:C	5:E:37:LEU:N	2.77	0.42
9:I:100:PHE:N	9:I:100:PHE:CD1	2.86	0.42
13:P:5:C:O2'	13:P:6:C:H5'	2.19	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.53	0.42
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.54	0.42
1:A:299:HIS:C	1:A:301:ALA:N	2.75	0.42
1:A:325:ILE:HG21	2:B:1210:MET:CG	2.45	0.42
1:A:388:LEU:HD22	1:A:432:VAL:HB	2.01	0.42
1:A:665:GLY:O	1:A:666:ILE:C	2.63	0.42
1:A:682:THR:HG23	1:A:728:LYS:HE3	2.00	0.42
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.48	0.42
1:A:913:LEU:HG	1:A:915:SER:N	2.34	0.42
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.19	0.42
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.49	0.42
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.99	0.42
2:B:331:LEU:HD12	2:B:331:LEU:N	2.35	0.42
2:B:683:SER:C	2:B:685:LEU:H	2.26	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.50	0.42
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.34	0.42
3:C:99:LEU:HD12	3:C:118:LEU:HD13	2.01	0.42
7:G:15:PRO:HG3	7:G:66:GLY:C	2.44	0.42
9:I:7:CYS:SG	9:I:8:ARG:O	2.77	0.42
11:K:36:GLU:O	11:K:37:LYS:C	2.63	0.42
1:A:61:ILE:CG2	1:A:62:ASP:H	2.24	0.42
1:A:77:CYS:C	1:A:78:PRO:O	2.59	0.42
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.39	0.42
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:MET:SD	2:B:1210:MET:HA	2.60	0.42
1:A:683:ILE:O	1:A:686:ALA:N	2.52	0.42
1:A:889:SER:O	1:A:890:ASP:C	2.62	0.42
1:A:901:LEU:N	1:A:926:GLN:NE2	2.57	0.42
1:A:1007:ILE:C	1:A:1009:ASN:H	2.27	0.42
1:A:1385:THR:O	1:A:1388:GLY:N	2.51	0.42
2:B:449:ASN:C	2:B:451:LYS:N	2.78	0.42
2:B:595:ARG:O	2:B:596:LEU:C	2.62	0.42
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.50	0.42
6:F:88:TYR:O	6:F:89:GLU:C	2.63	0.42
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.54	0.42
8:H:143:LEU:N	8:H:143:LEU:CD1	2.81	0.42
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.85	0.42
1:A:442:VAL:HG21	1:A:460:VAL:HG23	2.02	0.42
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.79	0.42
1:A:516:SER:O	1:A:518:LYS:N	2.53	0.42
1:A:901:LEU:HA	1:A:907:THR:OG1	2.20	0.42
1:A:964:ILE:O	1:A:967:ALA:N	2.53	0.42
1:A:1349:TYR:O	1:A:1350:LYS:C	2.61	0.42
1:A:1443:VAL:O	1:A:1444:MET:HG3	2.20	0.42
2:B:371:GLU:N	2:B:371:GLU:CD	2.78	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.42
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.07	0.42
3:C:236:GLY:O	3:C:238:ILE:N	2.52	0.42
8:H:84:ALA:C	8:H:87:ARG:H	2.28	0.42
11:K:2:ASN:O	11:K:3:ALA:C	2.62	0.42
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.54	0.42
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.72	0.42
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.35	0.42
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.53	0.42
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.02	0.42
2:B:43:LEU:HD13	2:B:812:LEU:HD23	2.02	0.42
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.55	0.42
2:B:820:GLY:N	2:B:1091:TYR:OH	2.52	0.42
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.33	0.42
2:B:895:ASP:C	2:B:897:GLY:H	2.27	0.42
2:B:1167:GLY:H	2:B:1217:TYR:HE1	1.68	0.42
3:C:193:TYR:C	3:C:193:TYR:CD1	2.97	0.42
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.02	0.42
4:D:7:THR:HB	7:G:42:PHE:CZ	2.55	0.42
5:E:136:ASN:OD1	5:E:137:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:CG	7:G:85:GLU:CD	2.93	0.42
8:H:4:THR:HG22	8:H:5:LEU:H	1.85	0.42
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.85	0.42
1:A:606:LEU:CD2	1:A:614:PHE:HE2	2.32	0.42
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.55	0.42
1:A:1009:ASN:O	1:A:1013:ASP:OD2	2.38	0.42
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.42
2:B:37:PHE:CD2	2:B:542:MET:SD	3.12	0.42
2:B:763:GLN:O	2:B:766:ARG:N	2.51	0.42
2:B:885:MET:HB3	2:B:886:LYS:H	1.67	0.42
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.01	0.42
2:B:1124:ARG:C	2:B:1126:GLY:N	2.74	0.42
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.73	0.42
3:C:88:CYS:SG	3:C:91:HIS:CA	3.07	0.42
5:E:88:VAL:HG12	5:E:89:GLY:N	2.34	0.42
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.54	0.42
1:A:516:SER:O	1:A:517:ASN:C	2.62	0.42
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	2.01	0.42
1:A:966:ASN:C	1:A:968:GLN:N	2.75	0.42
1:A:1125:ALA:C	1:A:1127:ASP:H	2.28	0.42
2:B:281:PRO:C	2:B:283:VAL:N	2.77	0.42
2:B:945:GLU:O	2:B:946:ASN:HB3	2.19	0.42
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.03	0.42
3:C:204:SER:C	3:C:206:ASN:N	2.76	0.42
4:D:118:THR:HG22	4:D:118:THR:O	2.20	0.42
5:E:35:VAL:O	5:E:37:LEU:N	2.52	0.42
5:E:168:TYR:HB3	5:E:170:LEU:HG	2.00	0.42
5:E:207:ARG:NH1	5:E:207:ARG:HB2	2.34	0.42
1:A:35:ILE:HD12	1:A:241:VAL:HG21	2.01	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.55	0.42
1:A:416:ARG:O	1:A:417:TYR:CD2	2.69	0.42
1:A:456:MET:HE3	1:A:478:TYR:CE1	2.55	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:761:MET:HA	1:A:804:TYR:HB2	2.01	0.42
1:A:791:ASP:OD1	1:A:791:ASP:C	2.63	0.42
1:A:1059:HIS:O	1:A:1060:PRO:C	2.59	0.42
1:A:1134:ILE:HB	1:A:1306:LEU:HD11	2.01	0.42
1:A:1385:THR:O	1:A:1386:ARG:C	2.63	0.42
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.50	0.42
2:B:230:ALA:N	2:B:231:PRO:HD2	2.34	0.42
2:B:482:VAL:O	2:B:483:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.89	0.42
2:B:765:PRO:O	2:B:768:THR:N	2.53	0.42
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.01	0.42
2:B:1024:ALA:O	2:B:1025:HIS:C	2.62	0.42
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.01	0.42
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.53	0.42
3:C:131:HIS:O	3:C:132:PRO:C	2.62	0.42
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.85	0.42
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.55	0.42
1:A:42:ASP:OD1	1:A:45:GLN:O	2.38	0.41
1:A:103:CYS:SG	1:A:108:MET:HE1	2.59	0.41
1:A:250:ILE:O	1:A:250:ILE:HG22	2.19	0.41
1:A:464:PRO:O	1:A:465:TYR:O	2.38	0.41
1:A:494:SER:O	1:A:495:GLU:C	2.63	0.41
1:A:816:HIS:CD2	2:B:764:SER:H	2.37	0.41
1:A:925:LEU:C	1:A:927:VAL:H	2.27	0.41
2:B:27:ALA:C	2:B:29:ASP:H	2.28	0.41
2:B:223:VAL:HG12	2:B:381:MET:HG2	2.02	0.41
2:B:1027:ILE:O	2:B:1028:GLU:C	2.62	0.41
3:C:84:ARG:NE	11:K:11:LEU:HD11	2.35	0.41
3:C:193:TYR:C	3:C:193:TYR:HD1	2.28	0.41
4:D:190:GLU:O	4:D:194:LEU:HG	2.21	0.41
6:F:90:ARG:HD3	6:F:155:LEU:HD12	2.02	0.41
7:G:73:LYS:HE2	7:G:74:TYR:O	2.20	0.41
8:H:99:GLY:HA3	8:H:117:SER:O	2.20	0.41
14:T:19:DT:H2'	14:T:20:DC:H6	1.81	0.41
1:A:33:ALA:HA	1:A:57:ARG:HH21	1.85	0.41
1:A:209:ASN:O	1:A:210:ILE:C	2.62	0.41
1:A:351:THR:O	1:A:486:GLU:HA	2.21	0.41
1:A:358:ASN:ND2	11:K:66:PRO:HD2	2.35	0.41
1:A:391:LEU:O	1:A:394:ASN:HB2	2.19	0.41
1:A:469:ARG:NH2	2:B:991:GLY:O	2.53	0.41
1:A:526:ASP:O	1:A:527:THR:C	2.63	0.41
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.84	0.41
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.45	0.41
2:B:283:VAL:O	2:B:286:PHE:N	2.54	0.41
2:B:352:ALA:O	2:B:353:LYS:C	2.64	0.41
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.54	0.41
2:B:641:GLU:OE1	2:B:641:GLU:HA	2.20	0.41
2:B:859:TYR:CD1	2:B:859:TYR:N	2.89	0.41
2:B:889:THR:HG22	2:B:891:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.01	0.41
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.41
4:D:63:LEU:HD22	4:D:63:LEU:HA	1.77	0.41
5:E:20:LYS:O	5:E:21:GLU:C	2.62	0.41
6:F:88:TYR:CD1	6:F:88:TYR:N	2.88	0.41
6:F:147:SER:OG	6:F:150:GLU:HG3	2.20	0.41
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.28	0.41
12:L:43:THR:HG22	12:L:43:THR:O	2.20	0.41
1:A:23:SER:HB2	1:A:233:TRP:HE1	1.85	0.41
1:A:119:ASN:O	1:A:122:MET:HB3	2.19	0.41
1:A:525:GLN:O	1:A:526:ASP:C	2.63	0.41
1:A:1096:SER:O	1:A:1100:ARG:CB	2.68	0.41
1:A:1260:LEU:O	1:A:1260:LEU:HG	2.20	0.41
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.50	0.41
1:A:1347:ALA:O	1:A:1348:LEU:C	2.63	0.41
2:B:336:ARG:CD	2:B:348:ARG:HD3	2.50	0.41
2:B:552:MET:O	2:B:554:ILE:N	2.53	0.41
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.41
2:B:1197:PRO:O	2:B:1198:TYR:C	2.62	0.41
2:B:1202:LEU:HD23	2:B:1206:GLU:HG3	2.02	0.41
5:E:58:MET:O	5:E:59:SER:O	2.38	0.41
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.66	0.41
11:K:7:PHE:CD1	11:K:7:PHE:C	2.98	0.41
14:T:21:DC:C5	14:T:22:BRU:BR	3.28	0.41
1:A:244:PRO:C	1:A:246:VAL:N	2.79	0.41
1:A:719:VAL:C	1:A:721:PHE:H	2.28	0.41
1:A:1409:LEU:HD23	1:A:1409:LEU:HA	1.93	0.41
2:B:294:ASP:OD2	2:B:294:ASP:N	2.51	0.41
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.50	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.21	0.41
3:C:75:MET:HE3	3:C:75:MET:HB2	1.99	0.41
5:E:58:MET:O	5:E:59:SER:C	2.64	0.41
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.55	0.41
7:G:87:VAL:HG23	7:G:103:VAL:HG21	2.02	0.41
7:G:88:ASP:HB3	7:G:144:ARG:HA	2.03	0.41
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.45	0.41
1:A:98:LYS:C	1:A:100:LYS:N	2.76	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.02	0.41
1:A:683:ILE:O	1:A:686:ALA:HB3	2.20	0.41
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.53	0.41
1:A:711:ARG:HA	9:I:97:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:O	1:A:842:VAL:HB	2.19	0.41
1:A:935:GLN:O	1:A:936:LEU:C	2.64	0.41
1:A:1053:PHE:C	1:A:1055:ARG:N	2.79	0.41
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.80	0.41
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.41
2:B:978:ASP:OD2	2:B:1098:MET:HG2	2.20	0.41
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.51	0.41
4:D:29:LEU:O	4:D:30:GLY:C	2.64	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.36	0.41
4:D:68:ARG:C	4:D:70:PHE:N	2.78	0.41
4:D:191:ALA:O	4:D:193:THR:N	2.54	0.41
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.35	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.41
7:G:25:TYR:O	7:G:26:LEU:C	2.63	0.41
10:J:36:LEU:O	10:J:37:SER:C	2.62	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.56	0.41
1:A:266:LEU:O	1:A:267:ALA:C	2.63	0.41
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.89	0.41
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.79	0.41
1:A:1115:SER:OG	1:A:1116:LEU:N	2.52	0.41
1:A:1243:VAL:CG1	1:A:1244:ARG:N	2.82	0.41
1:A:1323:ASP:C	1:A:1325:THR:N	2.77	0.41
2:B:95:ILE:HB	2:B:130:VAL:HG22	2.02	0.41
2:B:221:ASN:N	2:B:241:ARG:O	2.35	0.41
2:B:222:ILE:O	2:B:240:ILE:HA	2.20	0.41
2:B:382:ILE:HG13	2:B:382:ILE:H	1.67	0.41
2:B:700:SER:C	2:B:701:ILE:CG2	2.94	0.41
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.56	0.41
3:C:31:ASN:O	3:C:34:ARG:N	2.53	0.41
3:C:67:LEU:HD21	3:C:144:ILE:HD13	2.03	0.41
3:C:115:SER:HB3	3:C:142:VAL:HB	2.01	0.41
4:D:4:SER:O	4:D:5:THR:CB	2.68	0.41
4:D:40:HIS:C	4:D:42:GLY:N	2.77	0.41
8:H:12:VAL:HA	8:H:28:ALA:HB2	2.03	0.41
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.55	0.41
11:K:39:ASP:O	11:K:40:HIS:C	2.64	0.41
1:A:146:MET:HA	1:A:171:GLN:HB2	2.02	0.41
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.41
1:A:310:GLY:O	1:A:312:PRO:HD2	2.21	0.41
1:A:699:ALA:HB2	9:I:114:GLN:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:710:LEU:N	2.35	0.41
1:A:842:VAL:HG12	1:A:843:LYS:N	2.34	0.41
1:A:877:HIS:C	1:A:878:ILE:CG1	2.94	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.85	0.41
1:A:942:PHE:CD2	1:A:942:PHE:C	2.98	0.41
1:A:1010:ALA:O	1:A:1011:GLN:C	2.64	0.41
1:A:1317:MET:C	1:A:1319:VAL:H	2.28	0.41
1:A:1437:GLY:CA	6:F:88:TYR:CD2	3.03	0.41
2:B:185:THR:O	2:B:188:ASP:CB	2.68	0.41
2:B:254:LEU:HD23	2:B:381:MET:CE	2.28	0.41
2:B:467:GLY:CA	2:B:475:SER:HB3	2.49	0.41
2:B:604:ARG:O	2:B:606:LYS:N	2.53	0.41
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.51	0.41
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	2.02	0.41
2:B:1031:LEU:O	2:B:1034:VAL:HB	2.20	0.41
2:B:1182:CYS:C	2:B:1183:LYS:O	2.63	0.41
4:D:210:ILE:O	4:D:214:LEU:HG	2.20	0.41
6:F:128:LYS:HD3	6:F:149:GLU:O	2.20	0.41
7:G:110:VAL:HG22	7:G:161:GLY:O	2.20	0.41
11:K:69:ALA:O	11:K:70:ARG:CB	2.63	0.41
1:A:270:LEU:O	1:A:273:ASN:HB3	2.20	0.41
1:A:403:LYS:O	1:A:404:TYR:CD2	2.74	0.41
1:A:710:LEU:H	1:A:710:LEU:HD12	1.86	0.41
1:A:711:ARG:O	1:A:714:PHE:N	2.50	0.41
1:A:925:LEU:C	1:A:927:VAL:N	2.79	0.41
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.86	0.41
2:B:122:LEU:C	2:B:123:THR:HG1	2.26	0.41
2:B:751:VAL:HG13	2:B:812:LEU:HD22	2.03	0.41
2:B:764:SER:HB3	2:B:765:PRO:CD	2.50	0.41
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.21	0.41
3:C:258:ILE:N	3:C:258:ILE:HD12	2.36	0.41
4:D:146:GLN:O	4:D:149:THR:HG22	2.20	0.41
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.35	0.41
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.85	0.41
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.50	0.41
1:A:58:LEU:CD1	1:A:80:HIS:HB2	2.50	0.41
1:A:354:SER:HA	1:A:482:PHE:CD2	2.55	0.41
1:A:356:ASP:CB	1:A:469:ARG:NH1	2.80	0.41
1:A:714:PHE:CG	9:I:97:MET:HE1	2.55	0.41
1:A:719:VAL:O	1:A:721:PHE:N	2.54	0.41
1:A:897:TYR:N	1:A:897:TYR:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.61	0.41
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.21	0.41
1:A:1244:ARG:O	1:A:1245:PRO:O	2.39	0.41
1:A:1265:ASN:O	1:A:1268:LEU:N	2.51	0.41
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.51	0.41
2:B:100:PRO:HD3	2:B:172:ILE:HD12	2.03	0.41
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.08	0.41
2:B:314:LEU:O	2:B:317:CYS:HB3	2.20	0.41
2:B:681:TRP:O	2:B:682:SER:C	2.63	0.41
2:B:814:PHE:O	2:B:816:GLU:N	2.54	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.51	0.41
2:B:908:GLU:O	2:B:909:ASP:C	2.64	0.41
2:B:948:ILE:HG22	2:B:949:VAL:O	2.20	0.41
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.02	0.41
2:B:1121:GLY:O	2:B:1122:ARG:C	2.63	0.41
3:C:31:ASN:O	3:C:35:ARG:HG3	2.20	0.41
3:C:265:MET:HG2	3:C:265:MET:O	2.20	0.41
4:D:24:ALA:C	4:D:26:THR:N	2.79	0.41
4:D:191:ALA:C	4:D:193:THR:N	2.79	0.41
5:E:92:THR:HG22	5:E:92:THR:O	2.20	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.64	0.41
5:E:153:HIS:O	5:E:154:ILE:HG13	2.20	0.41
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.72	0.41
6:F:77:ASP:O	6:F:78:GLN:HB2	2.19	0.41
7:G:80:LYS:N	7:G:80:LYS:CD	2.72	0.41
7:G:88:ASP:HA	7:G:144:ARG:HA	2.02	0.41
8:H:80:ARG:HA	8:H:81:PRO:HD3	1.68	0.41
9:I:61:ASP:O	9:I:63:GLY:N	2.54	0.41
11:K:18:LYS:NZ	11:K:37:LYS:O	2.54	0.41
11:K:63:VAL:O	11:K:63:VAL:CG2	2.68	0.41
14:T:19:DT:H2''	14:T:20:DC:C5'	2.51	0.41
1:A:122:MET:O	1:A:123:ARG:C	2.62	0.41
1:A:282:ASN:HB3	1:A:283:GLY:H	1.78	0.41
1:A:535:THR:HG22	1:A:536:LEU:N	2.34	0.41
1:A:535:THR:HG23	1:A:575:LYS:HE2	2.03	0.41
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.56	0.41
1:A:874:ASP:O	1:A:875:ALA:C	2.64	0.41
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.54	0.41
1:A:935:GLN:C	1:A:937:VAL:N	2.76	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.21	0.41
1:A:1377:THR:O	1:A:1378:GLN:C	2.63	0.41
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.82	0.41
2:B:48:LEU:O	2:B:49:ASP:C	2.62	0.41
2:B:96:TYR:HE1	2:B:131:ASP:OD2	2.03	0.41
2:B:213:ILE:HD12	2:B:497:ARG:HB3	2.03	0.41
2:B:410:GLY:C	2:B:412:LEU:N	2.78	0.41
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.03	0.41
5:E:16:PHE:O	5:E:17:ARG:C	2.64	0.41
8:H:6:PHE:O	8:H:58:THR:HA	2.20	0.41
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.48	0.41
8:H:56:THR:HG21	8:H:145:ARG:HE	1.85	0.41
9:I:69:PRO:O	9:I:84:VAL:HA	2.21	0.41
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.60	0.41
10:J:13:VAL:O	10:J:14:VAL:CG2	2.69	0.41
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.50	0.41
1:A:73:GLY:O	1:A:74:MET:C	2.64	0.40
1:A:406:ILE:HG13	1:A:431:LYS:CB	2.51	0.40
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.56	0.40
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.40
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.36	0.40
1:A:1375:MET:HE2	1:A:1375:MET:HB3	2.00	0.40
2:B:39:ARG:NH2	2:B:665:GLU:CD	2.77	0.40
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.51	0.40
2:B:820:GLY:C	2:B:1091:TYR:CE1	2.99	0.40
2:B:1040:ASN:O	2:B:1042:GLY:N	2.54	0.40
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.86	0.40
3:C:208:GLU:C	3:C:210:GLU:N	2.77	0.40
4:D:27:LEU:HG	4:D:197:SER:HB2	2.03	0.40
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.40
7:G:20:PRO:HG2	7:G:21:ARG:N	2.36	0.40
9:I:87:GLN:O	9:I:88:SER:C	2.64	0.40
9:I:90:GLN:HE21	9:I:92:ARG:HD2	1.86	0.40
1:A:70:CYS:O	1:A:70:CYS:SG	2.80	0.40
1:A:73:GLY:O	1:A:75:ASN:N	2.54	0.40
1:A:103:CYS:O	1:A:106:VAL:O	2.39	0.40
1:A:208:LEU:HD23	1:A:208:LEU:C	2.46	0.40
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.57	0.40
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.88	0.40
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.81	0.40
1:A:1111:MET:HE2	1:A:1114:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:C	1:A:1315:GLU:H	2.30	0.40
2:B:419:THR:O	2:B:419:THR:HG22	2.21	0.40
2:B:707:PRO:HG2	2:B:708:GLU:H	1.84	0.40
2:B:911:ILE:O	2:B:912:ILE:CG1	2.68	0.40
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.55	0.40
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.76	0.40
5:E:173:SER:C	5:E:175:LEU:H	2.29	0.40
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.40
7:G:9:LEU:HD23	7:G:30:LEU:HD12	2.03	0.40
1:A:23:SER:CA	1:A:233:TRP:NE1	2.84	0.40
1:A:33:ALA:O	1:A:83:HIS:CD2	2.71	0.40
1:A:50:ILE:HG22	1:A:51:GLY:N	2.36	0.40
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.85	0.40
1:A:491:VAL:O	1:A:493:GLN:NE2	2.55	0.40
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.51	0.40
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.87	0.40
1:A:695:LYS:C	1:A:697:ALA:N	2.78	0.40
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.57	0.40
1:A:909:ASP:C	1:A:911:SER:N	2.78	0.40
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.86	0.40
1:A:1048:ASN:O	1:A:1049:ILE:C	2.64	0.40
1:A:1213:GLY:O	1:A:1216:ILE:N	2.55	0.40
1:A:1315:GLU:C	1:A:1317:MET:H	2.29	0.40
2:B:368:GLU:O	2:B:370:PHE:N	2.52	0.40
2:B:376:PHE:CE2	2:B:569:TYR:CD2	3.07	0.40
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.51	0.40
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.56	0.40
3:C:168:ALA:C	3:C:170:TRP:H	2.29	0.40
4:D:160:VAL:O	4:D:164:ILE:HG13	2.20	0.40
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.51	0.40
7:G:1:MET:CE	7:G:80:LYS:O	2.70	0.40
7:G:39:THR:CG2	7:G:40:GLY:N	2.82	0.40
8:H:83:GLN:O	8:H:85:GLY:N	2.53	0.40
10:J:56:LEU:O	10:J:57:ILE:C	2.63	0.40
11:K:18:LYS:HZ2	11:K:38:GLU:CD	2.27	0.40
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.52	0.40
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.42	0.40
1:A:24:PRO:HD2	1:A:233:TRP:NE1	2.37	0.40
1:A:263:THR:O	1:A:263:THR:HG22	2.20	0.40
1:A:284:ALA:C	1:A:286:HIS:N	2.78	0.40
1:A:362:ASP:HB3	1:A:508:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:O	1:A:498:ARG:C	2.63	0.40
1:A:1004:ASN:OD1	1:A:1004:ASN:C	2.64	0.40
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.46	0.40
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	2.04	0.40
1:A:1213:GLY:C	1:A:1215:ARG:N	2.77	0.40
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.21	0.40
1:A:1260:LEU:O	1:A:1260:LEU:CG	2.70	0.40
2:B:603:LEU:HD12	2:B:609:ILE:CG1	2.47	0.40
2:B:806:THR:HG22	2:B:808:ALA:CB	2.51	0.40
2:B:936:ASP:CG	2:B:938:SER:H	2.29	0.40
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.55	0.40
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.88	0.40
5:E:177:ARG:HG2	5:E:213:ILE:CG2	2.51	0.40
6:F:89:GLU:O	6:F:93:ILE:HG13	2.21	0.40
7:G:56:ILE:C	7:G:57:GLN:O	2.62	0.40
8:H:55:LEU:HD22	8:H:144:ILE:HG21	2.01	0.40
8:H:99:GLY:N	8:H:118:PHE:CD2	2.90	0.40
9:I:13:MET:O	9:I:14:LEU:HD23	2.21	0.40
11:K:65:HIS:NE2	11:K:67:PHE:CD2	2.85	0.40
1:A:31:SER:OG	1:A:82:GLY:HA2	2.21	0.40
1:A:41:MET:HB2	1:A:42:ASP:H	1.49	0.40
1:A:167:CYS:SG	1:A:167:CYS:O	2.78	0.40
1:A:244:PRO:C	1:A:246:VAL:H	2.29	0.40
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.21	0.40
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.52	0.40
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.03	0.40
1:A:598:LEU:O	1:A:599:SER:C	2.64	0.40
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.53	0.40
1:A:1315:GLU:C	1:A:1317:MET:N	2.77	0.40
2:B:60:GLN:CD	2:B:95:ILE:HG22	2.46	0.40
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.37	0.40
2:B:552:MET:HA	2:B:555:ILE:HB	2.03	0.40
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.56	0.40
2:B:744:HIS:CD2	2:B:746:SER:OG	2.69	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.86	0.40
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.50	0.40
3:C:254:LYS:O	3:C:258:ILE:HD13	2.22	0.40
4:D:40:HIS:C	4:D:42:GLY:H	2.29	0.40
6:F:93:ILE:HD13	6:F:148:VAL:CG1	2.50	0.40
7:G:35:GLU:OE2	7:G:47:CYS:HA	2.21	0.40
9:I:34:TYR:O	9:I:35:VAL:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1410/1733 (81%)	975 (69%)	289 (20%)	146 (10%)	0	6
2	B	1096/1224 (90%)	781 (71%)	200 (18%)	115 (10%)	0	6
3	C	264/318 (83%)	171 (65%)	65 (25%)	28 (11%)	0	6
4	D	173/221 (78%)	124 (72%)	31 (18%)	18 (10%)	0	6
5	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	13
6	F	84/155 (54%)	69 (82%)	11 (13%)	4 (5%)	2	17
7	G	169/171 (99%)	131 (78%)	28 (17%)	10 (6%)	1	15
8	H	131/146 (90%)	82 (63%)	32 (24%)	17 (13%)	0	3
9	I	114/122 (93%)	80 (70%)	23 (20%)	11 (10%)	0	7
10	J	63/70 (90%)	37 (59%)	12 (19%)	14 (22%)	0	1
11	K	112/120 (93%)	85 (76%)	16 (14%)	11 (10%)	0	7
12	L	44/70 (63%)	18 (41%)	17 (39%)	9 (20%)	0	1
All	All	3872/4565 (85%)	2707 (70%)	768 (20%)	397 (10%)	0	6

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	93	VAL
1	A	167	CYS
1	A	223	GLY

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Mol	Chain	Res	Type
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	322	VAL
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	517	ASN
1	A	536	LEU
1	A	567	LYS
1	A	597	LEU
1	A	666	ILE
1	A	789	LYS
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1014	ALA
1	A	1036	ARG
1	A	1096	SER
1	A	1115	SER
1	A	1122	PRO
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1378	GLN
1	A	1405	THR
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	258	LEU
2	B	282	ILE
2	B	367	LEU
2	B	450	ALA
2	B	466	TRP
2	B	467	GLY
2	B	474	SER

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Mol	Chain	Res	Type
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	831	SER
2	B	881	ASN
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
3	C	6	PRO
3	C	78	GLU
3	C	87	PHE
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	177	VAL
4	D	199	ASN

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Mol	Chain	Res	Type
5	E	3	GLN
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	106	GLN
5	E	130	ALA
5	E	206	GLY
7	G	63	PRO
7	G	139	ILE
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR
9	I	9	ASP
9	I	11	ASN
9	I	57	GLY
9	I	79	HIS
9	I	106	CYS
10	J	2	ILE
10	J	6	ARG
10	J	27	GLU
10	J	28	ASP
10	J	29	GLU
10	J	32	GLU
10	J	55	ASP
10	J	64	ASN
11	K	7	PHE
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	76	GLU
1	A	154	SER

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Mol	Chain	Res	Type
1	A	219	PHE
1	A	244	PRO
1	A	250	ILE
1	A	253	ASN
1	A	263	THR
1	A	283	GLY
1	A	336	ILE
1	A	394	ASN
1	A	465	TYR
1	A	543	LEU
1	A	604	GLY
1	A	626	ASN
1	A	649	ILE
1	A	661	GLY
1	A	753	GLY
1	A	780	VAL
1	A	825	ILE
1	A	847	ASP
1	A	875	ALA
1	A	1054	LEU
1	A	1114	PRO
1	A	1116	LEU
1	A	1212	VAL
1	A	1335	ILE
1	A	1366	ARG
1	A	1377	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1397	LEU
2	B	28	GLU
2	B	48	LEU
2	B	115	GLN
2	B	186	GLU
2	B	260	GLY
2	B	266	ALA
2	B	322	PHE
2	B	345	LYS
2	B	369	GLY
2	B	387	LEU
2	B	401	PHE
2	B	513	GLN
2	B	591	ARG

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Mol	Chain	Res	Type
2	B	605	ARG
2	B	619	ILE
2	B	641	GLU
2	B	655	LYS
2	B	764	SER
2	B	792	MET
2	B	869	SER
2	B	907	GLY
2	B	909	ASP
2	B	1017	ILE
2	B	1018	PRO
2	B	1065	GLN
2	B	1100	ASP
2	B	1108	ARG
2	B	1155	SER
3	C	4	GLU
3	C	81	GLU
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
4	D	21	GLU
4	D	53	SER
4	D	131	GLU
4	D	192	LYS
5	E	36	GLU
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	77	ARG
8	H	84	ALA
9	I	47	GLU
9	I	113	ASP
10	J	14	VAL
10	J	17	LYS
10	J	33	GLY
11	K	15	GLY
11	K	53	ASP
11	K	70	ARG
11	K	112	GLN
12	L	26	THR

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Mol	Chain	Res	Type
12	L	53	HIS
12	L	55	ILE
1	A	69	THR
1	A	111	GLY
1	A	135	PHE
1	A	245	PRO
1	A	317	LYS
1	A	386	ASP
1	A	399	HIS
1	A	409	SER
1	A	418	SER
1	A	483	ASP
1	A	492	PRO
1	A	525	GLN
1	A	544	ASP
1	A	619	LYS
1	A	648	ASN
1	A	731	ARG
1	A	846	GLU
1	A	871	ASP
1	A	979	SER
1	A	1120	LEU
1	A	1124	HIS
1	A	1221	LYS
1	A	1280	GLU
2	B	56	ASP
2	B	65	GLU
2	B	94	LYS
2	B	229	ALA
2	B	259	TYR
2	B	264	SER
2	B	283	VAL
2	B	559	SER
2	B	613	VAL
2	B	711	GLU
2	B	746	SER
2	B	884	ARG
2	B	891	ASP
2	B	945	GLU
2	B	1003	ALA
2	B	1041	GLU
2	B	1143	ALA

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Mol	Chain	Res	Type
3	C	60	ASP
3	C	148	ARG
3	C	240	VAL
4	D	12	ARG
4	D	47	LEU
4	D	65	GLU
5	E	44	ALA
5	E	45	LYS
5	E	115	ASN
5	E	192	ARG
6	F	154	ASP
8	H	44	VAL
8	H	90	ALA
8	H	92	ASP
8	H	140	ALA
9	I	34	TYR
9	I	78	CYS
11	K	88	LYS
11	K	90	ALA
11	K	104	ASN
1	A	113	LEU
1	A	148	CYS
1	A	272	ALA
1	A	331	GLY
1	A	332	LYS
1	A	333	GLU
1	A	526	ASP
1	A	609	ASP
1	A	636	GLU
1	A	759	ALA
1	A	817	ALA
1	A	1165	GLU
1	A	1233	ASP
1	A	1402	PHE
2	B	61	ASP
2	B	206	ASN
2	B	328	GLU
2	B	365	THR
2	B	389	ALA
2	B	531	GLN
2	B	540	SER
2	B	598	GLU

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Mol	Chain	Res	Type
2	B	629	ASP
2	B	752	ALA
2	B	758	PHE
2	B	818	PRO
2	B	951	GLN
2	B	982	SER
2	B	1011	ILE
3	C	56	THR
3	C	167	HIS
4	D	9	GLN
4	D	30	GLY
6	F	112	GLU
6	F	150	GLU
7	G	17	PHE
7	G	154	VAL
8	H	52	GLN
10	J	8	PHE
10	J	63	TYR
11	K	29	ASN
11	K	41	THR
1	A	55	ASP
1	A	86	LEU
1	A	99	ILE
1	A	108	MET
1	A	169	ASN
1	A	400	PRO
1	A	419	LYS
1	A	424	ILE
1	A	516	SER
1	A	605	MET
1	A	854	ASN
1	A	895	LYS
1	A	958	VAL
1	A	975	HIS
1	A	1127	ASP
1	A	1454	MET
2	B	58	THR
2	B	114	PRO
2	B	124	TYR
2	B	571	PRO
2	B	867	GLY
2	B	878	GLN

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Mol	Chain	Res	Type
2	B	894	ASP
2	B	901	PRO
3	C	117	ASP
3	C	142	VAL
3	C	164	ALA
3	C	212	PRO
4	D	119	ARG
5	E	43	LYS
6	F	81	THR
7	G	20	PRO
8	H	43	ASN
10	J	24	LEU
12	L	39	SER
12	L	57	LEU
1	A	362	ASP
1	A	720	ARG
1	A	1098	VAL
1	A	1318	THR
1	A	1324	PRO
2	B	470	LYS
2	B	728	ARG
2	B	734	HIS
2	B	797	TYR
2	B	880	THR
4	D	6	SER
7	G	26	LEU
7	G	115	MET
1	A	84	ILE
1	A	673	GLY
1	A	1158	PRO
2	B	712	PRO
2	B	1214	PRO
5	E	76	GLY
7	G	62	LEU
1	A	196	GLU
1	A	1437	GLY
2	B	364	ILE
2	B	759	PRO
9	I	62	ILE
1	A	842	VAL
1	A	1164	PRO
3	C	5	GLY

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Mol	Chain	Res	Type
3	C	126	GLY
7	G	19	GLY
7	G	34	VAL
1	A	35	ILE
1	A	357	PRO
1	A	775	ILE
2	B	231	PRO
2	B	411	PRO
2	B	1103	ILE
2	B	824	ILE

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	1244/1520 (82%)	1116 (90%)	128 (10%)	7	27
2	B	967/1061 (91%)	881 (91%)	86 (9%)	9	32
3	C	235/274 (86%)	212 (90%)	23 (10%)	7	29
4	D	159/200 (80%)	133 (84%)	26 (16%)	2	14
5	E	196/197 (100%)	191 (97%)	5 (3%)	40	60
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	32
7	G	152/152 (100%)	140 (92%)	12 (8%)	11	36
8	H	119/128 (93%)	113 (95%)	6 (5%)	22	47
9	I	110/116 (95%)	97 (88%)	13 (12%)	5	22
10	J	60/65 (92%)	55 (92%)	5 (8%)	10	34
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	27
12	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3458/4009 (86%)	3134 (91%)	324 (9%)	8	30

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	GLN
1	A	11	LEU
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	62	ASP
1	A	67	CYS
1	A	70	CYS
1	A	93	VAL
1	A	100	LYS
1	A	108	MET
1	A	130	ASP
1	A	142	CYS
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	245	PRO
1	A	270	LEU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	326	ARG
1	A	335	ARG
1	A	345	VAL
1	A	350	ARG
1	A	354	SER
1	A	379	VAL
1	A	381	THR
1	A	385	ILE
1	A	388	LEU
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	418	SER
1	A	425	GLN
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	450	LEU

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Mol	Chain	Res	Type
1	A	451	HIS
1	A	460	VAL
1	A	461	LYS
1	A	462	VAL
1	A	466	SER
1	A	481	ASP
1	A	493	GLN
1	A	497	THR
1	A	498	ARG
1	A	512	VAL
1	A	515	GLN
1	A	524	VAL
1	A	535	THR
1	A	560	ILE
1	A	562	THR
1	A	565	ILE
1	A	577	ILE
1	A	590	ARG
1	A	629	LEU
1	A	635	ARG
1	A	657	LEU
1	A	663	SER
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	741	ASN
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	827	THR
1	A	834	THR
1	A	845	LEU
1	A	854	ASN
1	A	858	ASN
1	A	859	SER
1	A	886	ILE
1	A	890	ASP
1	A	902	LEU
1	A	907	THR
1	A	929	LEU
1	A	937	VAL
1	A	940	ARG

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Mol	Chain	Res	Type
1	A	941	LYS
1	A	969	GLN
1	A	983	ILE
1	A	992	ASP
1	A	1006	ILE
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1152	ILE
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1267	MET
1	A	1271	ILE
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1325	THR
1	A	1329	THR
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1371	LEU
1	A	1372	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1405	THR
1	A	1425	SER
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE

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Mol	Chain	Res	Type
1	A	1447	GLU
2	B	30	SER
2	B	35	SER
2	B	57	TYR
2	B	104	GLU
2	B	106	ASP
2	B	128	LEU
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	223	VAL
2	B	258	LEU
2	B	268	THR
2	B	294	ASP
2	B	298	LEU
2	B	323	VAL
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	427	ASP
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	485	ARG
2	B	498	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	628	THR
2	B	635	ARG
2	B	644	GLU
2	B	649	LYS
2	B	682	SER

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Mol	Chain	Res	Type
2	B	684	LEU
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	755	ILE
2	B	790	ASP
2	B	830	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	844	SER
2	B	858	SER
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	935	ARG
2	B	939	THR
2	B	953	LEU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1018	PRO
2	B	1022	THR
2	B	1047	PHE
2	B	1069	PHE
2	B	1084	GLN
2	B	1085	ILE
2	B	1095	LEU
2	B	1099	VAL
2	B	1103	ILE
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1133	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1169	MET
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	8	VAL
3	C	22	LEU
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	77	ILE
3	C	93	ASP
3	C	99	LEU
3	C	108	GLU
3	C	129	ILE
3	C	140	ASN
3	C	147	LEU
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	172	PRO
3	C	193	TYR
3	C	214	ASN
3	C	233	GLU
3	C	240	VAL
3	C	245	VAL
3	C	259	LEU
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	32	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	126	ILE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	151	PHE
4	D	156	ASP

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Mol	Chain	Res	Type
4	D	159	THR
4	D	170	THR
4	D	174	PRO
4	D	182	SER
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	206	GLU
4	D	208	GLU
4	D	221	TYR
5	E	40	GLU
5	E	60	PHE
5	E	74	ASP
5	E	78	LEU
5	E	114	ASN
6	F	79	ARG
6	F	90	ARG
6	F	99	LEU
6	F	111	LEU
6	F	119	ARG
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	74	TYR
7	G	77	VAL
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	96	GLN
7	G	115	MET
7	G	126	ASN
7	G	171	ILE
8	H	42	ILE
8	H	86	ASP
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP

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Mol	Chain	Res	Type
9	I	13	MET
9	I	15	TYR
9	I	40	SER
9	I	59	VAL
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	99	LEU
9	I	101	PHE
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	44	TYR
10	J	46	CYS
11	K	10	PHE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	78	THR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
11	K	114	LEU
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	209	ASN
1	A	225	ASN
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	339	ASN
1	A	358	ASN
1	A	399	HIS
1	A	435	HIS
1	A	479	ASN
1	A	515	GLN
1	A	589	GLN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
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	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	1009	ASN
1	A	1040	GLN
1	A	1070	GLN
1	A	1140	HIS
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	47	GLN
2	B	53	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS

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Mol	Chain	Res	Type
2	B	538	ASN
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	794	ASN
2	B	821	GLN
2	B	834	ASN
2	B	842	ASN
2	B	843	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
4	D	39	ASN
4	D	40	HIS
4	D	132	GLN
4	D	137	ASN
4	D	150	ASN
4	D	157	GLN
4	D	179	GLN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	146	HIS
5	E	147	HIS
6	F	104	ASN
7	G	53	ASN
7	G	96	GLN
7	G	97	HIS
7	G	102	GLN

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Mol	Chain	Res	Type
7	G	122	ASN
7	G	126	ASN
7	G	158	HIS
8	H	139	ASN
9	I	12	ASN
9	I	51	ASN
9	I	60	GLN
9	I	90	GLN
10	J	64	ASN
11	K	29	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	BRU	T	22	13,14	18,21,22	0.62	0	25,30,33	1.24	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BRU	T	22	13,14	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	22	BRU	C6-C5-C4	-3.27	117.36	120.67
14	T	22	BRU	BR-C5-C4	2.72	121.15	118.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	22	BRU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	4.08
1	B	18:PHE	C	19:GLU	N	3.80
1	F	69:LEU	C	70:LYS	N	3.44
1	A	1175:SER	C	1176:LEU	N	3.41
1	B	337:ARG	C	338:GLY	N	2.62

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	1421/1733 (81%)	0.10	40 (2%)	55	38	12, 73, 146, 189	0
2	B	1115/1224 (91%)	0.33	63 (5%)	29	23	12, 83, 154, 191	0
3	C	267/318 (83%)	-0.02	4 (1%)	72	50	30, 69, 125, 150	0
4	D	177/221 (80%)	0.41	9 (5%)	33	25	53, 104, 144, 162	0
5	E	214/215 (99%)	0.38	3 (1%)	73	51	45, 126, 174, 178	0
6	F	87/155 (56%)	-0.25	2 (2%)	61	42	17, 49, 91, 119	0
7	G	171/171 (100%)	0.20	7 (4%)	41	30	53, 77, 115, 126	0
8	H	135/146 (92%)	0.86	15 (11%)	10	13	87, 128, 162, 171	0
9	I	116/122 (95%)	0.61	9 (7%)	19	17	68, 122, 151, 173	0
10	J	65/70 (92%)	-0.09	1 (1%)	72	50	35, 66, 109, 118	0
11	K	114/120 (95%)	0.01	4 (3%)	47	33	33, 73, 102, 140	0
12	L	46/70 (65%)	1.21	6 (13%)	7	11	69, 141, 161, 169	0
13	P	10/11 (90%)	0.86	2 (20%)	3	5	71, 85, 160, 163	0
14	T	10/25 (40%)	1.09	2 (20%)	3	5	72, 96, 137, 158	0
All	All	3948/4601 (85%)	0.24	167 (4%)	40	29	12, 82, 154, 191	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	8.5
11	K	113	THR	7.5
4	D	25	ALA	6.4
1	A	1081	LEU	6.1
8	H	90	ALA	5.7
11	K	114	LEU	5.5
2	B	879	ARG	5.4
10	J	65	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	4.7
2	B	471	LYS	4.5
1	A	1176	LEU	4.4
1	A	1254	ALA	4.3
8	H	65	LEU	4.3
4	D	18	VAL	4.2
1	A	1257	ASP	4.2
1	A	69	THR	4.1
2	B	230	ALA	4.1
2	B	732	SER	3.9
1	A	56	PRO	3.9
2	B	731	VAL	3.8
7	G	21	ARG	3.7
1	A	830	LYS	3.7
2	B	883	LEU	3.7
6	F	69	LEU	3.7
4	D	4	SER	3.6
1	A	171	GLN	3.6
1	A	144	THR	3.6
1	A	1245	PRO	3.6
2	B	571	PRO	3.6
2	B	733	HIS	3.6
2	B	884	ARG	3.5
5	E	88	VAL	3.5
1	A	1173	HIS	3.5
2	B	641	GLU	3.5
13	P	1	U	3.4
1	A	1125	ALA	3.4
2	B	734	HIS	3.3
8	H	139	ASN	3.3
7	G	124	GLY	3.3
9	I	64	SER	3.3
4	D	24	ALA	3.2
2	B	1224	PHE	3.2
2	B	937	ALA	3.2
2	B	468	GLU	3.1
9	I	117	LYS	3.1
2	B	110	HIS	3.1
2	B	90	ILE	3.1
2	B	282	ILE	3.1
2	B	709	ASP	3.1
11	K	111	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
13	P	2	C	3.1
4	D	8	PHE	3.0
1	A	1280	GLU	3.0
2	B	69	LEU	3.0
9	I	55	THR	3.0
2	B	461	LEU	2.9
7	G	19	GLY	2.9
12	L	32	ALA	2.9
3	C	130	GLY	2.9
8	H	78	SER	2.9
2	B	710	LEU	2.9
9	I	2	THR	2.8
8	H	130	ARG	2.8
4	D	17	LYS	2.8
2	B	70	ILE	2.8
8	H	135	LEU	2.8
7	G	148	GLU	2.8
1	A	705	LYS	2.8
1	A	50	ILE	2.8
4	D	20	GLU	2.8
7	G	85	GLU	2.8
12	L	50	ASP	2.8
7	G	20	PRO	2.8
14	T	28	DT	2.7
1	A	51	GLY	2.7
1	A	145	LYS	2.7
1	A	40	THR	2.7
4	D	13	ARG	2.7
1	A	1093	LYS	2.7
2	B	885	MET	2.7
1	A	2	VAL	2.7
12	L	27	LEU	2.7
12	L	25	ALA	2.7
2	B	115	GLN	2.6
2	B	104	GLU	2.6
2	B	448	ILE	2.6
3	C	2	SER	2.6
2	B	101	MET	2.6
2	B	476	ARG	2.6
8	H	81	PRO	2.6
2	B	860	MET	2.6
8	H	31	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	598	GLU	2.6
1	A	147	VAL	2.6
1	A	1110	ASN	2.6
8	H	86	ASP	2.5
1	A	251	SER	2.5
2	B	580	VAL	2.5
2	B	881	ASN	2.5
11	K	112	GLN	2.5
5	E	194	GLU	2.5
1	A	159	THR	2.5
2	B	728	ARG	2.5
2	B	730	ARG	2.5
12	L	46	VAL	2.5
1	A	252	PHE	2.4
8	H	105	GLU	2.4
2	B	102	VAL	2.4
1	A	1187	GLN	2.4
5	E	110	PHE	2.4
2	B	262	GLU	2.4
2	B	484	ASN	2.4
1	A	1281	ARG	2.4
2	B	601	ARG	2.4
8	H	137	GLN	2.3
9	I	23	ASN	2.3
2	B	469	GLN	2.3
2	B	615	MET	2.3
8	H	119	GLY	2.3
8	H	120	GLY	2.3
2	B	708	GLU	2.3
14	T	18	DT	2.3
2	B	870	ILE	2.3
2	B	958	GLN	2.3
1	A	1142	THR	2.2
1	A	587	HIS	2.2
1	A	33	ALA	2.2
1	A	1158	PRO	2.2
2	B	587	HIS	2.2
8	H	22	LYS	2.2
1	A	1165	GLU	2.2
2	B	132	VAL	2.2
2	B	428	ILE	2.2
2	B	487	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	610	ASN	2.2
2	B	486	TYR	2.2
9	I	44	TYR	2.2
2	B	239	GLU	2.2
2	B	887	HIS	2.2
2	B	896	ASP	2.2
2	B	250	PHE	2.2
2	B	963	PHE	2.2
1	A	292	ALA	2.1
1	A	49	LYS	2.1
1	A	1175	SER	2.1
3	C	6	PRO	2.1
2	B	1167	GLY	2.1
2	B	729	ILE	2.1
1	A	323	LYS	2.1
2	B	652	LYS	2.1
2	B	178	ASN	2.1
1	A	1124	HIS	2.1
3	C	108	GLU	2.1
9	I	52	ILE	2.0
9	I	93	LYS	2.0
12	L	59	ALA	2.0
7	G	113	HIS	2.0
8	H	136	LYS	2.0
4	D	118	THR	2.0
2	B	245	GLU	2.0
9	I	87	GLN	2.0
2	B	100	PRO	2.0
1	A	975	HIS	2.0
1	A	39	GLU	2.0
2	B	273	LEU	2.0
6	F	155	LEU	2.0
2	B	715	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	BRU	T	22	20/21	0.85	0.12	59,61,68,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
16	ZN	A	2461	1/1	0.97	0.09	163,163,163,163	0
16	ZN	A	2464	1/1	0.98	0.05	82,82,82,82	0
16	ZN	A	2459	1/1	0.99	0.03	115,115,115,115	0
16	ZN	A	2460	1/1	1.00	0.05	69,69,69,69	0
16	ZN	A	2458	1/1	1.00	0.04	51,51,51,51	0
16	ZN	A	2462	1/1	1.00	0.01	23,23,23,23	0
16	ZN	A	2463	1/1	1.00	0.01	42,42,42,42	0
15	MG	A	2457	1/1	1.00	0.02	21,21,21,21	0
16	ZN	A	2465	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.