



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

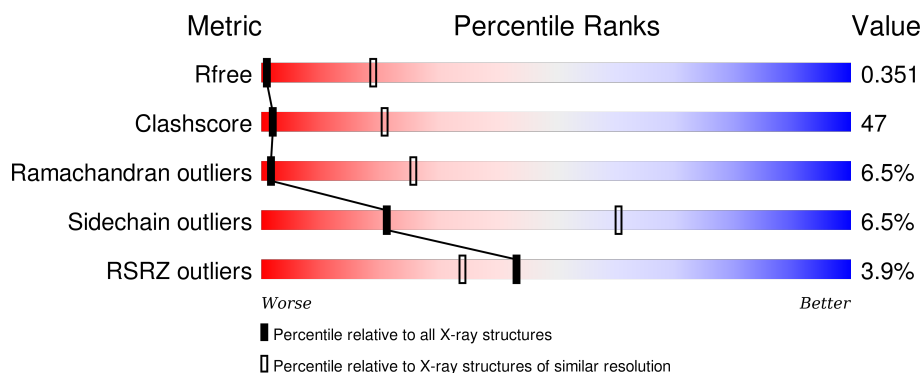
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>2%</div> <div>31% 41% 7% 20%</div> </div>
2	B	1224	<div> <div>4%</div> <div>32% 50% 7% 10%</div> </div>
3	C	318	<div> <div>%</div> <div>38% 39% 7% 16%</div> </div>
4	E	215	<div> <div>6%</div> <div>42% 54% .</div> </div>
5	F	155	<div> <div>%</div> <div>17% 34% . 46%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	86	

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

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

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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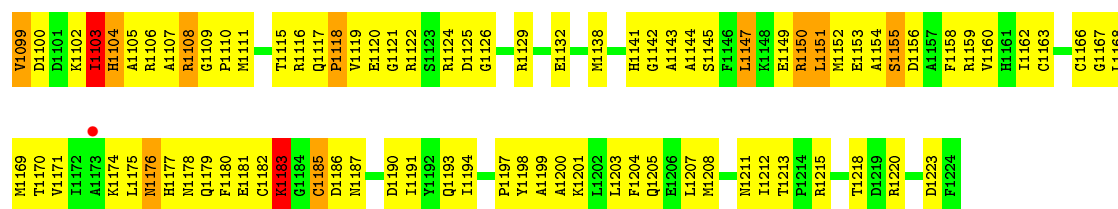
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0
12	M	1	Total 1	Zn 1	0	0

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

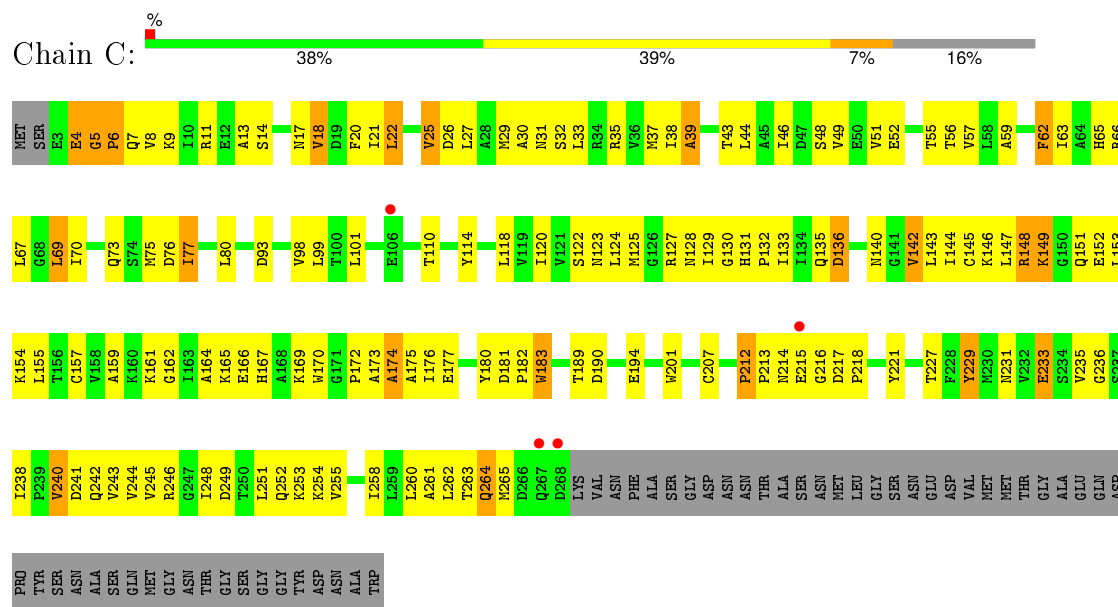
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Mg 1	0	0



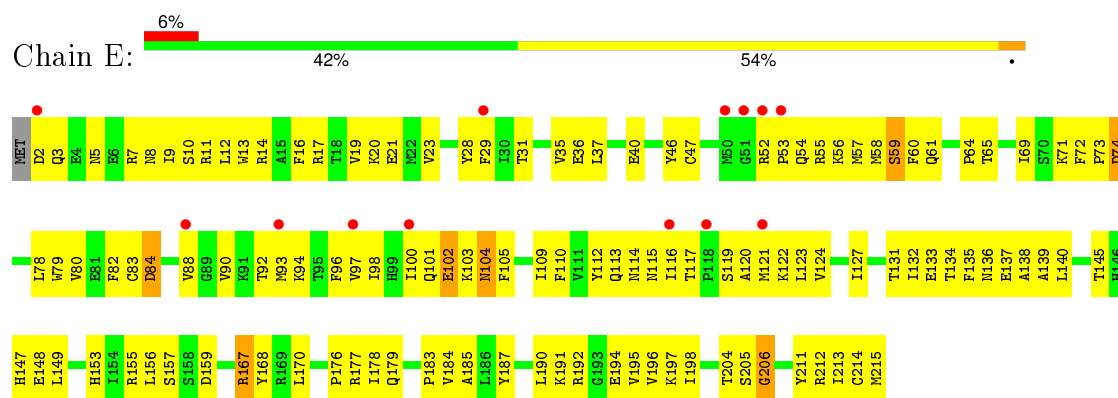
G980	L1030	G987	S831	P759	E699	A830	I555	R485	A409	ARG	T288	D198	V132	D66	MET
L961	L1033	L898	G832	D760	S700	G631	T586	Y486	G410	GLY	T289	M199	K133	L70	SER
A982	R1033	L899	Y833	E761	L701	R632	P557	T487	F417	THR	A271	G200	K134	LEU	ASP
F963	R1034	A900	N834	N762	L702	V633	L588	Y488	R418	ALA		G201	ARG	GLN	LEU
K965	A1035	P901	Q835	Q763	L703	R634	S559	S489	T419	LEU		F203	THR	GLN	ASN
V966			E836	S764	A704	R635	G562	I485	T419	GLY	P274	F202	TYR	LEU	SER
			D837	P765	N705	P836	N863	R496	L420	ILE		I204	ALA	ALA	GLU
			S838		Q706	L637	L566		F421	K345	T277	N205	ILE	GLN	LYS
R969	G1038	N839	N839	Q770	E708	F638	L566		R423	E346	Q278	G207	ASP	HIS	TYR
T970	N1040	L840	N841	M773	D709	V640			K423	K347	D279	S208	VAL	THR	THR
			N842	M778	L710	E641	Y569	P501	D426	R348	T280	E209	PRO	THR	ASP
D1043	D1043	N910	Q843	M778	E711	D642	V570		K427	K349	T281	K210	GLY	GLU	GLU
A1044	S1045	I911	S844	G779	F742	D643			I428	Q350	T282	V211	ARG	SER	ASP
Q975	P1046	I912	S845	V780	A713	E844	Q573	ARG	F429	Y351	V283	L212	GLU	ASP	PRO
			S846	L781	E714		S574	ASP	R430	A352	T284	L213	LEU	ASN	THR
G977		G913	D847	L782	A715		P575	GLY	Y431	I355	T285	A214	ILE	GLY	GLY
D1049	D1049	R914	R848	T783	ASN	G647	D576	LYS	N432		F286	Q215	TYR	PHE	PHE
K978	K978	T915	R849	N784	GLU	H648	A577	LEU	N431	K358	R287	E216	LEU	ARG	GLU
F980	T1051	T916	L550		GLU	K649	T578		T435	E359	A288	R217	LEU	LYS	D20
A981	V1052	P917	L550	V787	GLU	E650	T579	A509	V436	F360		N221	ILE	TYR	E21
S982	E1053	I918	P851	R787	ASN	L651	R579	P510	E437	F361	T291		ALA	GLU	S22
R983	G1054	PR0	F855	R788	ASP	K652	F580	P511	GLU	L361	T292		GLU	ALA	A23
H984	I1055	ASP	P856	M789	LEU	V653	F581	R512	ALA	P262	T293		GLU	S91	P24
G985	S1056	GLY	R857	D790	V722	R654	V582	Q513	HTS	H363	D294		SER	F92	T25
Q986	K1057	ASP	R857	T791	V723		N583	L514	ASP	I364	G295		GLU	G93	T26
K987	L1058	GLU	S858	M792	D724		N586	H515	PHE	T365	G296		ASP		A27
		GLU	T859	A793	F725		H587	H516	ASP	Q366	K228		ASP	Y96	E28
T990	L1059	LEU	R860	N794	A726	K660	H587	T517	ASN	T367	T297		SER	Y97	D29
G991	E1061	GLY	D861	L796	R727		G588	H518	MET	L367	L298		GLU	T98	S30
I1062	H1062	GLN	R728	T797	K728	A663	V589	W519	LYS	E368	E299		SER	X99	X31
T993	G1063	ARG	R798	T798	V729	T664	H590	A520	L446	G369	H300		GLY	P100	
Y994	Y1064	THR	K864	Y797	R730	E665	P593	L521	A447	F370		P233		M101	
R995	Y1066	ALA	K865	P799	V731	Q667		V522		E371	Y303		R164	V102	
R996	S1066	TYR	Q867	Q800	S732	Q677	R601	C523	A450	F376	D304		I167		S35
E997	R1067	HIS	N868	N801	H733	D668	L603	A525	L457	F377	Q309		G168	S105	A36
D998	G1068	ASP	S869	P802	A735	ILE	R604	A526		L378	N310		R169	D106	F37
K999	F1069	R934	T871	G804	T736	GLY	R605	T527	L461	G379	L311		F38	G187	F38
P1000	E1070	T805	E872	T805	T737	GLY			A462		E312		P171	T108	R39
F1001	Y1071	D936	T873	T806	F738	PHE			Q463	N381	N313		I172	Y109	L43
T1002	M1072	A937	T874	R807	T739	GLU	N610	Q530	Q464	N383	L314		M173	L112	Q46
A1003	Y1073	S938	E875	A808	H740	ASP	P611	Q531	N465	R384	K315		L174	Y113	Q47
E1004			E876	N809	G741	VAL	E612	L535	G467	L385	P316		R175	P114	
G1005	T1077	L941	P877		E742	GLU	V613	V536			G317			Q115	
I1006	K1078	T944	Q878	L812	L743	E678	S614	K537	GLU	L386	V318		N178		S50
V1007	K1079	E945	R879	K813	H744	Y679	S614	N537	GLN	L387	E319		C179	Q115	P51
P1008	K1080	N946	T880	F814	P745	T680	N615	N538	LYS	C388	D320		Y180	R118	N52
D1009	L1081	R815	N881	R815	S746	W681	I616	L539	LYS	A389	G321		L181	L119	Q53
I1010			T882		M747	S682	R617		ALA		F322		T185	R120	P54
T1011	Q1084		L883	P818	L748	S683	T618	N542	MET	D394	V323			M121	F54
I1012	F1085		N884		L749		I619	I545	SER	Q395	I324			L122	D56
F1086					G750	N686	K622	S546	SER	D396	I324		D188	L122	D56
F1087					G751	E687	V547	S546	ARG		T329		L189	Y124	T58
	Y1091		H887	N822	N822	E687	G548	V547	A477	H400			L189	S125	L59
				A823	A752	G688	E823	G548	F401	F401	L331		L192	S126	Q60
	R1094		Y890	N824	A753	L689	L624	T549	V478		D332		K193	S126	Q60
	L1095		T891	V825	S764	V690	K625	D550	S480	R405	F333		E194	K127	D61
S1019			K892	A826	L755	E891	I626	P551		L406	F333		E282	L128	I62
R1096			T893	I827	L756	P627	F627	M552	L483	D407	G335		G263	F129	I63
H1097					P757	I693	T628	P552					P196	V130	C64
M1098			D896	Y830	F758	D629		I554	N484	L408	ARG		F197	D131	E65



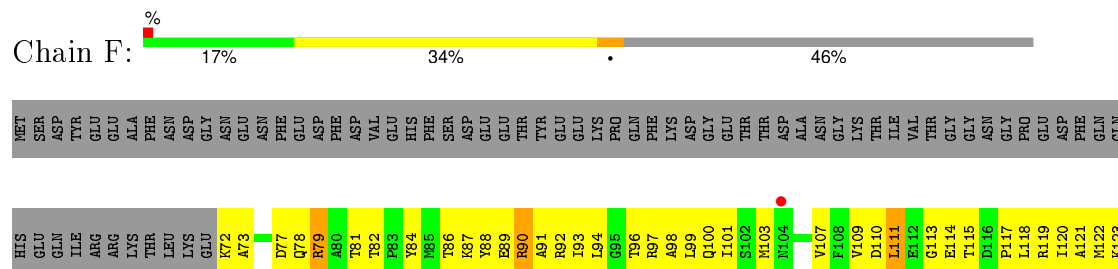
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

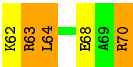


• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

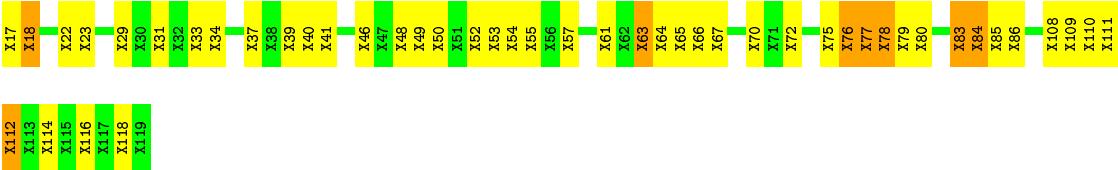


• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide





● Molecule 11: TRANSCRIPTION FACTOR II B (TFIIB)



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	212.44Å 217.18Å 422.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 51.23 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-4.50) 99.2 (51.23-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.345 , 0.373 0.330 , 0.351	Depositor DCC
R_{free} test set	1721 reflections (3.07%)	DCC
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	1.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 177.8	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	6 of 111208 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28300	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

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

All (5) bond length outliers are listed below:

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

All (21) bond angle outliers are listed below:

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

There are no chirality outliers.

All (35) planarity outliers are listed below:

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

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10850	0	10952	1129	3
2	B	8721	0	8747	936	1
3	C	2095	0	2052	164	0
4	E	1752	0	1776	129	1
5	F	679	0	701	63	0
6	H	1068	0	1040	129	0
7	I	967	0	929	139	2
8	J	532	0	544	77	0
9	K	919	0	929	87	0
10	L	364	0	388	54	0
11	M	343	0	19	34	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	2	0
12	J	1	0	0	1	0
12	L	1	0	0	0	0
12	M	1	0	0	0	0
13	A	1	0	0	0	0
All	All	28300	0	28077	2623	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 47.

All (2623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.11	0.80
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.62	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.11	0.80
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.63	0.80
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.63	0.80
6:H:5:LEU:HD11	6:H:135:LEU:HG	1.63	0.79
7:I:50:THR:CG2	7:I:52:ILE:HG23	2.11	0.79
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.28	0.79
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.12	0.79
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.17	0.79
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.64	0.79
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.63	0.79
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.12	0.79
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.63	0.79
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.12	0.79
2:B:842:ASN:ND2	2:B:845:SER:N	2.31	0.79
1:A:1152:ILE:O	7:I:43:VAL:CG1	2.31	0.79
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.64	0.79
1:A:1151:GLU:HA	7:I:44:TYR:CB	2.10	0.79
3:C:56:THR:HG22	3:C:57:VAL:N	1.97	0.79
2:B:487:THR:HG22	2:B:489:SER:H	1.48	0.79
2:B:121:ASN:HD22	2:B:121:ASN:N	1.79	0.79
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.64	0.79
2:B:855:PHE:HZ	2:B:857:ARG:NH1	1.81	0.79
1:A:298:PHE:O	1:A:302:THR:HB	1.83	0.79
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.11	0.78
1:A:825:ILE:HD11	2:B:512:ARG:O	1.83	0.78
1:A:58:LEU:HD22	1:A:80:HIS:O	1.83	0.78
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.48	0.78
1:A:313:GLN:HB2	1:A:322:VAL:CG2	2.14	0.78
1:A:32:VAL:HG21	1:A:68:GLN:NE2	1.97	0.78
1:A:913:LEU:HD12	1:A:914:GLU:N	1.99	0.78
11:M:63:UNK:N	11:M:63:UNK:C	2.46	0.78
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.64	0.78
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.14	0.78
1:A:353:ILE:HD13	1:A:487:MET:CE	2.14	0.78
1:A:666:ILE:HD13	2:B:1030:LEU:HD22	1.65	0.78
6:H:40:LEU:HD23	6:H:42:ILE:HD11	1.65	0.78
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.49	0.78
2:B:583:ASN:HD21	2:B:628:THR:HB	1.49	0.78
1:A:810:PRO:CB	2:B:519:TRP:CH2	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLU:CA	2:B:513:GLN:NE2	2.46	0.78
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	1.84	0.78
1:A:70:CYS:O	1:A:72:GLU:HG2	1.84	0.77
1:A:825:ILE:HG23	2:B:512:ARG:HD3	1.66	0.77
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	1.84	0.77
1:A:313:GLN:HB2	1:A:322:VAL:HG23	1.64	0.77
1:A:742:ASN:HA	1:A:745:GLN:HB2	1.63	0.77
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.13	0.77
1:A:901:LEU:H	1:A:926:GLN:NE2	1.82	0.77
1:A:1150:SER:C	7:I:44:TYR:HD2	1.88	0.77
2:B:1166:CYS:O	2:B:1168:LEU:N	2.18	0.77
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.47	0.77
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.49	0.77
2:B:707:PRO:HG2	2:B:708:GLU:H	1.49	0.77
1:A:1281:ARG:O	1:A:1282:VAL:HG23	1.83	0.77
8:J:12:LYS:O	8:J:14:VAL:HG23	1.85	0.77
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.66	0.77
1:A:813:PHE:CE2	2:B:524:PRO:HG3	2.20	0.77
1:A:399:HIS:O	1:A:401:GLY:N	2.17	0.77
2:B:1106:ARG:HE	2:B:1109:GLY:H	1.29	0.77
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.19	0.77
2:B:496:ARG:NH1	2:B:539:LEU:HB2	1.99	0.77
3:C:124:LEU:O	3:C:127:ARG:HG2	1.85	0.76
1:A:40:THR:HG22	1:A:41:MET:HG3	1.64	0.76
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.67	0.76
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.65	0.76
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.50	0.76
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.51	0.76
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.85	0.76
3:C:167:HIS:HD2	3:C:169:LYS:N	1.76	0.76
3:C:165:LYS:O	9:K:6:ARG:NH1	2.17	0.76
1:A:265:LYS:NZ	1:A:323:LYS:H	1.84	0.76
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.68	0.76
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.51	0.76
2:B:423:LYS:HA	2:B:426:LYS:HE2	1.68	0.76
1:A:223:GLY:O	1:A:1415:SER:HA	1.86	0.76
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.68	0.76
1:A:768:GLN:CG	1:A:816:HIS:HA	2.16	0.76
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.16	0.76
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.21	0.76
1:A:95:PHE:O	1:A:99:ILE:HG13	1.85	0.76

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:61:GLN:NE2	4:E:105:PHE:HE2	1.87	0.72
2:B:570:VAL:HB	2:B:573:GLN:CB	2.18	0.72
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.71	0.72
1:A:575:LYS:HB3	1:A:612:ILE:HG23	1.71	0.72
2:B:313:MET:CE	2:B:386:LEU:HD22	2.19	0.72
1:A:598:LEU:HD22	6:H:25:ARG:NH1	2.05	0.72
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.70	0.72
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.30	0.72
1:A:340:LEU:HD21	2:B:1200:ALA:HB2	1.72	0.72
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.72	0.72
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.69	0.72
2:B:636:PRO:O	2:B:637:LEU:HG	1.90	0.72
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.71	0.72
2:B:737:THR:HG23	7:I:66:PRO:CB	2.20	0.72
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.04	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.72
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.23	0.72
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.90	0.72
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.70	0.71
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.71	0.71
1:A:1390:ASN:ND2	1:A:1399:ARG:HA	2.05	0.71
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.72	0.71
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.38	0.71
1:A:1397:LEU:O	1:A:1400:CYS:HB2	1.89	0.71
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.25	0.71
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.54	0.71
10:L:47:ARG:HG2	10:L:52:GLY:HA2	1.72	0.71
1:A:337:ARG:NH1	1:A:839:ARG:NH1	2.37	0.71
2:B:555:ILE:HD13	2:B:587:HIS:CE1	2.26	0.71
9:K:55:LYS:HD3	9:K:78:THR:CB	2.20	0.71
1:A:900:ASP:OD2	1:A:903:ASN:HB2	1.90	0.71
1:A:44:THR:O	1:A:45:GLN:HB2	1.91	0.71
2:B:65:GLU:HG3	2:B:66:ASP:H	1.56	0.71
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.38	0.71
11:M:40:UNK:O	11:M:41:UNK:CA	2.36	0.71
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.73	0.71
1:A:675:THR:CB	1:A:736:ASN:HD21	2.04	0.71
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.06	0.71
1:A:1153:TYR:OH	7:I:42:LEU:CD1	2.39	0.70
10:L:60:ARG:CG	10:L:61:THR:H	1.94	0.70
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HB3	1:A:466:SER:HA	1.74	0.70
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.26	0.70
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.57	0.70
2:B:792:MET:HA	2:B:856:PHE:O	1.91	0.70
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.72	0.70
9:K:55:LYS:HD3	9:K:78:THR:HB	1.72	0.70
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.56	0.70
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.31	0.70
1:A:567:LYS:HE3	6:H:46:LEU:CD1	2.22	0.70
2:B:1066:SER:O	2:B:1067:ARG:HD3	1.90	0.70
1:A:351:THR:HG21	2:B:1103:ILE:HG23	1.71	0.70
1:A:418:SER:HA	11:M:46:UNK:O	1.91	0.70
2:B:637:LEU:CD1	2:B:693:ILE:HD12	2.20	0.70
4:E:56:LYS:HG3	4:E:84:ASP:HB2	1.73	0.70
2:B:130:VAL:HG12	2:B:131:ASP:N	2.07	0.70
1:A:343:LYS:HE3	2:B:1151:LEU:O	1.92	0.70
1:A:1153:TYR:HA	7:I:43:VAL:CG2	2.21	0.69
2:B:378:LEU:O	2:B:382:ILE:HG13	1.92	0.69
6:H:36:CYS:SG	6:H:130:ARG:NH2	2.65	0.69
1:A:775:ILE:CD1	1:A:815:PHE:CB	2.67	0.69
2:B:54:PHE:HA	2:B:58:THR:HB	1.74	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.69
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.74	0.69
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.74	0.69
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.08	0.69
2:B:463:THR:CG2	2:B:465:ASN:HD22	2.05	0.69
1:A:858:ASN:HD22	1:A:858:ASN:C	1.95	0.69
6:H:49:VAL:HG12	6:H:50:ALA:N	2.07	0.69
2:B:955:THR:HG23	10:L:54:ARG:O	1.91	0.69
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.93	0.69
2:B:108:VAL:HG12	2:B:109:THR:N	2.06	0.69
1:A:763:ALA:O	1:A:803:SER:HB3	1.92	0.69
4:E:168:TYR:HB3	4:E:170:LEU:HD21	1.72	0.69
2:B:542:MET:CE	2:B:747:MET:HG3	2.22	0.69
1:A:72:GLU:OE2	2:B:1175:LEU:HD12	1.92	0.69
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.74	0.69
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.74	0.69
1:A:391:LEU:HD22	1:A:400:PRO:O	1.93	0.69
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.74	0.69
2:B:314:LEU:O	2:B:317:CYS:HB2	1.92	0.69
1:A:225:ASN:O	1:A:227:VAL:N	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:CYS:SG	4:E:88:VAL:HG22	2.32	0.68
1:A:584:ASN:O	1:A:637:LYS:HE3	1.92	0.68
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.74	0.68
3:C:254:LYS:HB3	9:K:42:LEU:HD11	1.75	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
1:A:1152:ILE:O	7:I:43:VAL:CB	2.41	0.68
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.21	0.68
1:A:535:THR:HG21	1:A:616:VAL:HA	1.75	0.68
1:A:599:SER:HB2	1:A:603:ASN:H	1.58	0.68
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.08	0.68
2:B:882:THR:HG21	2:B:935:ARG:HA	1.75	0.68
2:B:884:ARG:O	2:B:936:ASP:HB3	1.93	0.68
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.76	0.68
2:B:46:GLN:HG3	2:B:47:GLN:H	1.58	0.68
1:A:535:THR:HG21	1:A:617:VAL:N	2.08	0.68
2:B:976:ILE:O	2:B:990:ILE:HB	1.94	0.68
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.75	0.68
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.23	0.68
8:J:1:MET:H2	8:J:56:LEU:HB2	1.59	0.68
5:F:81:THR:HG21	5:F:136:ARG:CD	2.20	0.68
2:B:954:VAL:O	10:L:55:ILE:O	2.11	0.68
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.76	0.68
2:B:842:ASN:ND2	2:B:844:SER:HB2	2.09	0.68
1:A:994:GLN:HE21	1:A:1019:CYS:HB3	1.59	0.68
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.59	0.68
2:B:711:GLU:N	2:B:712:PRO:CD	2.57	0.67
4:E:127:ILE:O	4:E:127:ILE:HG13	1.93	0.67
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.07	0.67
2:B:864:LYS:HB3	2:B:872:GLU:H	1.59	0.67
7:I:53:GLY:O	7:I:89:GLN:HB2	1.94	0.67
6:H:7:ASP:O	6:H:8:ASP:HB2	1.92	0.67
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.29	0.67
2:B:280:ILE:HG22	2:B:285:ILE:HG13	1.76	0.67
1:A:351:THR:CG2	2:B:1103:ILE:HG23	2.24	0.67
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.76	0.67
2:B:1039:GLY:HA2	8:J:51:LEU:HD21	1.77	0.67
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.77	0.67
2:B:986:GLN:HE22	2:B:1020:ARG:CZ	2.08	0.67
3:C:8:VAL:HG12	3:C:9:LYS:N	2.09	0.67
1:A:814:PHE:O	1:A:817:ALA:HB3	1.95	0.67
1:A:563:PRO:HB2	1:A:565:ILE:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.43	0.67
1:A:525:GLN:CB	2:B:835:GLN:HG2	2.25	0.67
2:B:514:LEU:HD12	2:B:515:HIS:N	2.09	0.67
2:B:22:SER:O	2:B:654:ARG:HD2	1.94	0.67
3:C:93:ASP:O	3:C:127:ARG:NH2	2.27	0.67
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.07	0.67
1:A:694:THR:O	1:A:698:GLN:HG3	1.94	0.67
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.10	0.67
3:C:8:VAL:HG12	3:C:9:LYS:H	1.60	0.67
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.77	0.67
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.76	0.67
2:B:957:ASN:O	2:B:959:ASP:N	2.29	0.67
3:C:80:LEU:HD22	3:C:129:ILE:CD1	2.21	0.67
1:A:914:GLU:HB2	1:A:979:SER:O	1.95	0.67
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.60	0.67
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.76	0.67
1:A:590:ARG:HB3	1:A:605:MET:N	2.10	0.66
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.28	0.66
5:F:109:VAL:HG12	5:F:110:ASP:N	2.10	0.66
1:A:305:ASP:HB3	1:A:308:ILE:HD11	1.77	0.66
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.76	0.66
2:B:709:ASP:O	2:B:710:LEU:HD23	1.94	0.66
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.76	0.66
9:K:47:ARG:NH1	9:K:47:ARG:HB3	2.09	0.66
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.30	0.66
4:E:93:MET:HE2	4:E:120:ALA:HB1	1.76	0.66
1:A:751:SER:O	1:A:752:LYS:HG2	1.96	0.66
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.43	0.66
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.76	0.66
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.29	0.66
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.30	0.66
3:C:56:THR:HG21	3:C:145:CYS:SG	2.35	0.66
10:L:45:ALA:O	10:L:46:VAL:HG23	1.95	0.66
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.28	0.66
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.77	0.66
2:B:751:VAL:O	2:B:754:SER:HB2	1.95	0.66
2:B:649:LYS:HE2	2:B:738:PHE:O	1.96	0.66
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.77	0.66
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.26	0.66
1:A:1333:ILE:O	1:A:1336:MET:HB3	1.96	0.66
3:C:98:VAL:C	3:C:99:LEU:HD23	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.77	0.66
3:C:260:LEU:O	3:C:264:GLN:HG3	1.95	0.66
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.78	0.66
7:I:32:CYS:SG	7:I:33:SER:N	2.69	0.66
2:B:711:GLU:H	2:B:712:PRO:HD3	1.60	0.66
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.31	0.66
3:C:5:GLY:O	3:C:7:GLN:HG3	1.95	0.66
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.30	0.66
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.31	0.65
7:I:111:THR:HG21	7:I:113:ASP:HB2	1.78	0.65
1:A:590:ARG:CG	1:A:590:ARG:HH11	2.06	0.65
4:E:176:PRO:O	4:E:212:ARG:HA	1.95	0.65
2:B:363:HIS:O	2:B:364:ILE:CB	2.44	0.65
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.77	0.65
1:A:810:PRO:HG2	2:B:705:MET:SD	2.36	0.65
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.77	0.65
1:A:1115:SER:HA	1:A:1308:THR:HG22	1.77	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.28	0.65
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.35	0.65
5:F:96:THR:O	5:F:100:GLN:HG3	1.97	0.65
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.62	0.65
4:E:124:VAL:HG22	4:E:132:ILE:HG21	1.79	0.65
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.79	0.65
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.31	0.65
1:A:741:ASN:HD22	1:A:741:ASN:C	1.99	0.65
1:A:715:GLU:O	1:A:719:VAL:HG23	1.96	0.65
1:A:1153:TYR:CE2	7:I:42:LEU:CA	2.69	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.65
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.27	0.65
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.78	0.65
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.31	0.65
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.78	0.65
1:A:329:LEU:HD23	1:A:335:ARG:HG3	1.78	0.65
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.62	0.65
2:B:128:LEU:HB3	2:B:167:ILE:O	1.95	0.65
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.65
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.97	0.65
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
6:H:107:VAL:HG21	6:H:126:GLU:HG3	1.79	0.64
2:B:1116:ARG:HD2	2:B:1198:TYR:CG	2.32	0.64
10:L:51:CYS:O	10:L:53:HIS:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.27	0.64
1:A:1035:TYR:O	1:A:1037:LEU:N	2.30	0.64
2:B:349:ILE:O	2:B:352:ALA:HB3	1.96	0.64
2:B:805:THR:HG21	2:B:815:ARG:HE	1.62	0.64
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.27	0.64
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.12	0.64
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.26	0.64
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.31	0.64
2:B:1051:THR:CG2	2:B:1053:GLU:H	1.93	0.64
1:A:306:ASN:HD21	1:A:324:SER:H	1.43	0.64
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.28	0.64
2:B:1201:LYS:O	2:B:1205:GLN:HG3	1.98	0.64
1:A:994:GLN:HE22	1:A:1023:ARG:NE	1.95	0.64
1:A:381:THR:HG22	1:A:383:TYR:N	2.09	0.64
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.79	0.64
2:B:604:ARG:HG2	2:B:604:ARG:O	1.98	0.64
6:H:49:VAL:HG12	6:H:50:ALA:H	1.62	0.64
1:A:901:LEU:HA	1:A:907:THR:HG23	1.80	0.64
2:B:247:GLY:H	2:B:418:LYS:NZ	1.96	0.64
1:A:579:SER:OG	1:A:612:ILE:HG22	1.97	0.64
5:F:111:LEU:H	5:F:111:LEU:HD12	1.61	0.64
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.32	0.64
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.64
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.32	0.64
11:M:31:UNK:CA	11:M:114:UNK:O	2.45	0.64
2:B:1170:THR:O	2:B:1170:THR:HG22	1.97	0.64
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.79	0.64
6:H:12:VAL:HA	6:H:28:ALA:CB	2.28	0.64
5:F:86:THR:OG1	5:F:89:GLU:HG3	1.98	0.64
10:L:40:LEU:HD13	10:L:44:ASP:CG	2.19	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.81	0.63
2:B:525:ALA:O	2:B:527:THR:HG22	1.99	0.63
11:M:52:UNK:C	11:M:53:UNK:O	2.46	0.63
2:B:25:ILE:HG22	2:B:29:ASP:HB2	1.79	0.63
2:B:708:GLU:CG	2:B:709:ASP:H	1.97	0.63
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.63
1:A:73:GLY:O	1:A:75:ASN:N	2.32	0.63
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.79	0.63
7:I:7:CYS:HB2	7:I:29:CYS:HB2	1.81	0.63
1:A:475:THR:HG22	1:A:476:SER:N	2.12	0.63
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:LYS:HB3	2:B:937:ALA:O	1.99	0.63
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.62	0.63
4:E:96:PHE:O	4:E:100:ILE:HG13	1.99	0.63
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
1:A:354:SER:HA	1:A:482:PHE:CD2	2.34	0.63
1:A:337:ARG:NE	1:A:839:ARG:HH22	1.97	0.63
1:A:1150:SER:OG	7:I:44:TYR:CE2	2.51	0.63
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.29	0.63
1:A:33:ALA:O	1:A:83:HIS:HB3	1.99	0.63
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.79	0.63
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.80	0.63
10:L:48:CYS:SG	10:L:49:LYS:N	2.70	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HG3	2.33	0.63
7:I:29:CYS:HG	7:I:32:CYS:HG	1.44	0.63
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.80	0.63
2:B:1034:VAL:HG23	2:B:1059:LEU:HB2	1.80	0.63
7:I:106:CYS:HG	12:I:204:ZN:ZN	1.12	0.63
10:L:55:ILE:HG13	10:L:56:LEU:H	1.63	0.63
8:J:9:SER:OG	8:J:48:ARG:NH2	2.30	0.63
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.80	0.63
3:C:22:LEU:HD22	3:C:25:VAL:CG2	2.25	0.63
1:A:328:ARG:O	1:A:335:ARG:HG2	1.99	0.63
6:H:31:THR:O	6:H:32:THR:CB	2.47	0.63
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.79	0.63
5:F:97:ARG:O	5:F:101:ILE:HG13	1.99	0.63
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.34	0.63
2:B:247:GLY:N	2:B:418:LYS:NZ	2.47	0.63
2:B:1106:ARG:HD2	2:B:1126:GLY:O	1.99	0.63
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.29	0.63
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.14	0.63
2:B:221:ASN:OD1	2:B:242:SER:HA	1.98	0.63
2:B:824:ILE:CG1	8:J:48:ARG:HH12	2.08	0.62
11:M:80:UNK:CA	11:M:83:UNK:O	2.47	0.62
1:A:108:MET:O	1:A:109:HIS:HB2	1.99	0.62
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.34	0.62
2:B:512:ARG:NH2	2:B:535:LEU:HD11	2.02	0.62
1:A:706:HIS:CG	1:A:1135:ARG:NH2	2.67	0.62
1:A:871:ASP:OD2	4:E:204:THR:HG23	1.99	0.62
1:A:418:SER:O	1:A:420:ARG:N	2.32	0.62
5:F:111:LEU:H	5:F:111:LEU:CD1	2.12	0.62
4:E:78:LEU:C	4:E:78:LEU:HD23	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ARG:HA	2:B:631:GLY:O	1.99	0.62
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.33	0.62
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.80	0.62
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	1.99	0.62
1:A:915:SER:O	1:A:919:ILE:HG13	2.00	0.62
1:A:590:ARG:HB3	1:A:605:MET:H	1.64	0.62
3:C:166:GLU:HA	9:K:6:ARG:HB3	1.82	0.62
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.81	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.80	0.62
4:E:156:LEU:HD12	4:E:195:VAL:HG12	1.81	0.62
1:A:825:ILE:HG23	2:B:512:ARG:CD	2.28	0.62
1:A:381:THR:CG2	1:A:383:TYR:H	2.09	0.62
4:E:178:ILE:HG23	4:E:214:CYS:HA	1.81	0.62
1:A:814:PHE:CE1	2:B:519:TRP:CA	2.83	0.62
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.00	0.62
2:B:549:THR:HB	2:B:628:THR:CG2	2.30	0.62
1:A:225:ASN:O	1:A:226:GLU:HG2	1.99	0.62
1:A:1054:LEU:O	1:A:1057:VAL:HG23	1.99	0.62
1:A:783:THR:HG22	1:A:815:PHE:CE2	2.21	0.62
2:B:542:MET:CG	2:B:747:MET:HE3	2.29	0.62
1:A:689:LYS:O	1:A:693:VAL:HG23	2.00	0.62
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.79	0.62
3:C:46:ILE:HA	3:C:159:ALA:HA	1.82	0.62
1:A:982:THR:HG22	1:A:984:LYS:H	1.64	0.62
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.20	0.62
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.30	0.61
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.82	0.61
2:B:1072:MET:HE3	2:B:1085:ILE:HD12	1.82	0.61
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.34	0.61
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.65	0.61
2:B:616:ILE:N	2:B:616:ILE:HD12	2.15	0.61
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.81	0.61
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.63	0.61
1:A:961:ARG:O	1:A:965:GLN:HG3	2.00	0.61
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.00	0.61
2:B:1116:ARG:NH1	2:B:1198:TYR:CD1	2.67	0.61
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.66	0.61
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.82	0.61
3:C:173:ALA:O	3:C:174:ALA:HB3	2.00	0.61
9:K:63:VAL:O	9:K:63:VAL:CG2	2.48	0.61
2:B:208:SER:OG	2:B:210:LYS:HD3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.30	0.61
1:A:1212:VAL:O	1:A:1216:ILE:HG13	1.99	0.61
2:B:1187:ASN:OD1	2:B:1190:ASP:HB3	1.99	0.61
1:A:709:THR:HB	1:A:712:GLU:H	1.64	0.61
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.82	0.61
1:A:789:LYS:HG3	7:I:67:THR:HB	1.83	0.61
8:J:48:ARG:HE	8:J:49:MET:HE2	1.66	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.01	0.61
1:A:445:ASN:HB2	1:A:454:SER:O	2.00	0.61
2:B:787:VAL:HG12	2:B:787:VAL:O	2.00	0.61
2:B:446:LEU:O	2:B:447:ALA:CB	2.48	0.61
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.29	0.61
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.82	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
2:B:1169:MET:HE1	2:B:1201:LYS:O	2.01	0.61
3:C:49:VAL:HG21	3:C:67:LEU:HD12	1.83	0.61
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.65	0.61
10:L:51:CYS:HB2	10:L:53:HIS:CD2	2.35	0.61
4:E:93:MET:O	4:E:97:VAL:HG23	2.00	0.61
2:B:686:ASN:C	2:B:688:GLY:H	2.04	0.61
1:A:148:CYS:O	1:A:168:GLY:HA2	2.00	0.61
2:B:120:ARG:CG	2:B:955:THR:HG21	2.23	0.61
2:B:114:PRO:HB3	2:B:174:LEU:HD11	1.82	0.61
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.30	0.61
1:A:1192:LEU:HD22	1:A:1239:ARG:NH2	2.16	0.61
1:A:672:ASP:OD1	1:A:674:PRO:HD2	2.00	0.61
4:E:47:CYS:HA	4:E:53:PRO:HA	1.83	0.61
2:B:25:ILE:HG22	2:B:26:THR:H	1.65	0.61
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.83	0.61
5:F:101:ILE:HD12	5:F:121:ALA:HB2	1.82	0.61
10:L:26:THR:O	10:L:27:LEU:HB3	2.01	0.61
2:B:1102:LYS:O	2:B:1104:HIS:N	2.32	0.60
2:B:995:ARG:NH1	2:B:995:ARG:HB2	2.16	0.60
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.01	0.60
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.27	0.60
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.81	0.60
7:I:5:ARG:HD3	7:I:36:GLU:OE2	2.01	0.60
1:A:1152:ILE:O	7:I:43:VAL:HB	2.01	0.60
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.84	0.60
2:B:1039:GLY:HA2	8:J:51:LEU:CD2	2.31	0.60
1:A:306:ASN:OD1	1:A:324:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.01	0.60
1:A:824:LEU:O	1:A:827:THR:HB	2.00	0.60
1:A:418:SER:O	1:A:419:LYS:C	2.39	0.60
2:B:839:MET:HE3	2:B:1010:LEU:CD1	2.31	0.60
1:A:663:SER:OG	1:A:664:THR:N	2.34	0.60
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.81	0.60
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.60
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.31	0.60
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.83	0.60
1:A:736:ASN:O	1:A:737:LEU:C	2.38	0.60
1:A:1158:PRO:HB3	1:A:1241:ARG:NH1	2.17	0.60
6:H:106:GLU:C	6:H:108:SER:H	2.02	0.60
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.31	0.60
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.04	0.60
1:A:704:ALA:HB2	1:A:710:LEU:CG	2.23	0.60
7:I:8:ARG:HG3	7:I:9:ASP:N	2.15	0.60
2:B:803:LEU:H	2:B:822:ASN:HD21	1.48	0.60
2:B:975:GLN:HG2	2:B:976:ILE:H	1.67	0.60
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.02	0.60
1:A:567:LYS:O	1:A:569:LYS:N	2.35	0.60
2:B:394:ASP:OD2	7:I:91:ARG:CG	2.45	0.60
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.66	0.60
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.02	0.60
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.01	0.60
1:A:567:LYS:CB	1:A:568:PRO:CD	2.67	0.60
1:A:549:MET:SD	1:A:577:ILE:CD1	2.87	0.60
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.32	0.60
2:B:121:ASN:ND2	2:B:121:ASN:N	2.50	0.60
1:A:219:PHE:O	1:A:222:LEU:N	2.33	0.60
8:J:1:MET:N	8:J:56:LEU:HB2	2.17	0.60
2:B:1106:ARG:HH12	2:B:1118:PRO:HB3	1.67	0.60
1:A:231:PRO:HA	1:A:234:MET:HE2	1.83	0.60
2:B:429:PHE:HA	2:B:432:MET:HE2	1.84	0.60
6:H:89:LEU:C	6:H:91:ASP:N	2.55	0.59
1:A:44:THR:HG22	1:A:44:THR:O	2.02	0.59
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.83	0.59
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.83	0.59
3:C:166:GLU:CG	9:K:10:PHE:HZ	2.14	0.59
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.32	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.02	0.59
2:B:90:ILE:HD12	2:B:432:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:90:ALA:O	9:K:94:ILE:HG13	2.01	0.59
1:A:322:VAL:O	1:A:323:LYS:HG3	2.01	0.59
4:E:78:LEU:HD23	4:E:79:TRP:N	2.16	0.59
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.84	0.59
1:A:166:GLY:O	1:A:167:CYS:HB3	2.02	0.59
6:H:84:ALA:HA	6:H:87:ARG:CG	2.32	0.59
1:A:469:ARG:NH2	2:B:976:ILE:HD13	2.18	0.59
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.68	0.59
7:I:15:TYR:O	7:I:27:PHE:HA	2.02	0.59
1:A:68:GLN:HE22	1:A:80:HIS:CB	2.15	0.59
2:B:913:GLY:HA2	2:B:938:SER:CB	2.32	0.59
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.01	0.59
4:E:29:PHE:HB2	4:E:65:THR:HG22	1.83	0.59
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.33	0.59
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.56	0.59
5:F:81:THR:HG22	5:F:82:THR:N	2.18	0.59
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.00	0.59
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.38	0.59
1:A:779:PHE:CZ	2:B:517:THR:HA	2.37	0.59
7:I:111:THR:CG2	7:I:113:ASP:HB2	2.33	0.59
1:A:1390:ASN:HD22	1:A:1399:ARG:HA	1.67	0.59
1:A:742:ASN:CA	1:A:745:GLN:HB2	2.33	0.59
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.83	0.59
6:H:109:LYS:NZ	6:H:109:LYS:HB2	2.18	0.59
1:A:783:THR:HG21	1:A:815:PHE:CE1	2.27	0.59
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.85	0.59
1:A:1153:TYR:CZ	7:I:42:LEU:CA	2.72	0.59
1:A:93:VAL:HG11	1:A:308:ILE:CD1	2.33	0.59
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.59
1:A:68:GLN:HE22	1:A:80:HIS:HB3	1.68	0.59
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.33	0.59
2:B:806:THR:HB	2:B:809:MET:HG3	1.85	0.59
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.37	0.59
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.03	0.59
2:B:642:ASP:O	2:B:644:GLU:N	2.36	0.59
1:A:1150:SER:OG	7:I:44:TYR:HE2	1.85	0.59
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.59
6:H:81:PRO:CB	6:H:82:PRO:CD	2.81	0.59
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.18	0.59
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.43	0.59
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.17	0.58
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.15	0.58
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.03	0.58
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.58
1:A:756:ILE:HG22	1:A:757:ASN:N	2.17	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.85	0.58
1:A:76:GLU:O	1:A:76:GLU:HG3	2.02	0.58
1:A:385:ILE:HG22	1:A:386:ASP:N	2.18	0.58
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.49	0.58
3:C:148:ARG:HG3	8:J:61:LEU:O	2.03	0.58
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.33	0.58
2:B:463:THR:HG22	2:B:465:ASN:HD22	1.66	0.58
1:A:225:ASN:HD22	1:A:227:VAL:HB	1.68	0.58
5:F:127:GLU:O	5:F:129:LYS:HG3	2.03	0.58
7:I:16:PRO:HB3	7:I:27:PHE:CE2	2.38	0.58
1:A:97:ALA:HA	1:A:100:LYS:HE3	1.84	0.58
7:I:85:PHE:CD1	7:I:99:LEU:HD22	2.37	0.58
2:B:955:THR:OG1	10:L:55:ILE:HA	2.04	0.58
1:A:31:SER:OG	1:A:83:HIS:HB2	2.02	0.58
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.33	0.58
6:H:123:MET:HE3	6:H:142:LEU:CD2	2.31	0.58
4:E:5:ASN:ND2	4:E:52:ARG:HG2	2.12	0.58
1:A:840:ARG:HB3	1:A:1384:VAL:HG12	1.85	0.58
1:A:414:ASP:O	1:A:417:TYR:O	2.22	0.58
2:B:479:VAL:HG12	2:B:480:SER:N	2.17	0.58
1:A:783:THR:HG22	1:A:815:PHE:HZ	1.44	0.58
1:A:1115:SER:O	1:A:1329:THR:HG23	2.02	0.58
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.85	0.58
2:B:46:GLN:O	2:B:408:LEU:HD23	2.03	0.58
4:E:156:LEU:HD12	4:E:195:VAL:CG1	2.33	0.58
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.35	0.58
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.86	0.58
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.04	0.58
2:B:287:ARG:NH1	2:B:324:ILE:O	2.37	0.58
1:A:399:HIS:O	1:A:435:HIS:HD2	1.87	0.58
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.36	0.58
1:A:151:ASP:HA	1:A:162:VAL:O	2.02	0.58
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.33	0.58
2:B:1171:VAL:CG1	2:B:1191:ILE:HD13	2.32	0.58
2:B:519:TRP:C	2:B:519:TRP:CD1	2.76	0.58
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.86	0.58
2:B:806:THR:OG1	2:B:809:MET:HE3	2.04	0.58
1:A:101:LYS:O	1:A:105:CYS:HB2	2.04	0.58
2:B:666:TYR:C	2:B:668:ASP:H	2.06	0.58
3:C:244:VAL:O	3:C:248:ILE:HG13	2.03	0.58
1:A:1315:GLU:O	1:A:1318:THR:HG23	2.04	0.58
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.67	0.58
1:A:225:ASN:ND2	1:A:227:VAL:HB	2.18	0.58
2:B:589:VAL:HG12	2:B:590:HIS:N	2.18	0.58
1:A:810:PRO:HB2	2:B:519:TRP:HH2	1.67	0.58
2:B:512:ARG:NH2	2:B:535:LEU:CD1	2.62	0.58
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.86	0.58
2:B:1116:ARG:CZ	2:B:1198:TYR:CE1	2.87	0.58
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.18	0.58
2:B:756:ILE:O	2:B:759:PRO:HD3	2.04	0.58
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.68	0.58
6:H:97:MET:HE2	6:H:142:LEU:HD23	1.86	0.58
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.69	0.58
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.84	0.58
1:A:524:VAL:HG12	1:A:525:GLN:H	1.69	0.58
3:C:258:ILE:O	3:C:261:ALA:HB3	2.04	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.19	0.58
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.86	0.58
2:B:25:ILE:HG22	2:B:29:ASP:CB	2.34	0.57
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.04	0.57
1:A:1399:ARG:CB	1:A:1408:ILE:HD13	2.28	0.57
2:B:130:VAL:HG12	2:B:131:ASP:H	1.67	0.57
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.69	0.57
1:A:814:PHE:CZ	2:B:519:TRP:N	2.72	0.57
1:A:41:MET:HB3	1:A:48:ALA:O	2.04	0.57
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.37	0.57
2:B:860:MET:HG2	2:B:861:ASP:N	2.18	0.57
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.52	0.57
1:A:1325:THR:O	4:E:148:GLU:HB2	2.04	0.57
1:A:511:ILE:HA	1:A:521:MET:HE3	1.85	0.57
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.31	0.57
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.84	0.57
4:E:157:SER:C	4:E:159:ASP:H	2.07	0.57
1:A:825:ILE:HD12	2:B:513:GLN:NE2	2.19	0.57
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.86	0.57
6:H:97:MET:CE	6:H:142:LEU:HD23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:N	5:F:111:LEU:CD1	2.67	0.57
4:E:46:TYR:HA	4:E:57:MET:SD	2.43	0.57
5:F:111:LEU:C	5:F:113:GLY:H	2.07	0.57
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.44	0.57
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.20	0.57
1:A:882:SER:HA	1:A:952:ALA:O	2.04	0.57
10:L:70:ARG:HG2	10:L:70:ARG:HH11	1.66	0.57
3:C:55:THR:HB	3:C:152:GLU:H	1.70	0.57
1:A:710:LEU:N	1:A:710:LEU:HD12	2.20	0.57
8:J:48:ARG:HE	8:J:49:MET:CE	2.16	0.57
2:B:803:LEU:N	2:B:822:ASN:HD21	2.02	0.57
9:K:65:HIS:HD2	9:K:67:PHE:N	2.02	0.57
1:A:443:LEU:HD13	1:A:455:MET:HE1	1.87	0.57
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.45	0.57
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.38	0.57
4:E:213:ILE:O	4:E:213:ILE:HG23	2.04	0.57
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.86	0.57
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.86	0.57
1:A:57:ARG:O	1:A:68:GLN:HG3	2.03	0.57
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.39	0.57
1:A:1074:GLU:O	1:A:1076:ALA:N	2.37	0.57
5:F:87:LYS:HE2	5:F:88:TYR:CZ	2.39	0.57
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.04	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:HB2	2.34	0.57
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.39	0.57
1:A:537:ARG:HB2	6:H:20:TYR:CE2	2.39	0.57
6:H:82:PRO:O	6:H:83:GLN:HB2	2.04	0.57
9:K:47:ARG:HD3	9:K:59:ALA:O	2.03	0.57
1:A:401:GLY:C	1:A:435:HIS:CD2	2.79	0.57
6:H:89:LEU:HD22	6:H:91:ASP:OD2	2.05	0.57
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.39	0.57
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.85	0.57
2:B:1022:THR:HG23	2:B:1022:THR:O	2.05	0.57
1:A:1365:TYR:O	1:A:1366:ARG:C	2.43	0.57
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.35	0.57
1:A:76:GLU:O	1:A:76:GLU:CG	2.53	0.57
3:C:56:THR:CG2	3:C:57:VAL:H	2.09	0.57
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.85	0.57
1:A:260:ASP:OD1	1:A:261:ASP:N	2.37	0.57
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.86	0.57
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.53	0.57
1:A:901:LEU:H	1:A:926:GLN:HE21	1.50	0.57
2:B:287:ARG:CG	2:B:292:ILE:HA	2.26	0.57
1:A:577:ILE:O	1:A:580:VAL:HG23	2.04	0.57
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.70	0.57
2:B:243:ALA:HA	2:B:250:PHE:O	2.05	0.57
1:A:1300:LYS:NZ	1:A:1300:LYS:HB3	2.20	0.56
3:C:248:ILE:CD1	9:K:101:LEU:HD22	2.35	0.56
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.05	0.56
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.86	0.56
10:L:32:ALA:HB3	10:L:55:ILE:CD1	2.26	0.56
2:B:57:TYR:HD1	2:B:57:TYR:N	2.03	0.56
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.56
4:E:46:TYR:CE2	4:E:58:MET:HA	2.40	0.56
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.40	0.56
1:A:1444:MET:HE1	5:F:135:ARG:NE	2.20	0.56
2:B:704:ALA:HB1	2:B:710:LEU:HD12	1.87	0.56
2:B:958:GLN:O	2:B:960:GLY:N	2.33	0.56
1:A:1389:PHE:O	1:A:1392:SER:HB3	2.06	0.56
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.02	0.56
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.06	0.56
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.20	0.56
3:C:229:TYR:N	3:C:229:TYR:CD1	2.74	0.56
1:A:401:GLY:O	1:A:435:HIS:CD2	2.58	0.56
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.85	0.56
10:L:49:LYS:O	10:L:50:ASP:HB2	2.03	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.04	0.56
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.41	0.56
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.72	0.56
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.05	0.56
2:B:1180:PHE:O	2:B:1181:GLU:HB2	2.05	0.56
2:B:101:MET:HB2	2:B:169:ARG:HH12	1.69	0.56
7:I:111:THR:HG22	7:I:112:SER:N	2.19	0.56
7:I:7:CYS:C	7:I:8:ARG:O	2.43	0.56
6:H:89:LEU:HD22	6:H:91:ASP:CG	2.25	0.56
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.05	0.56
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.40	0.56
3:C:145:CYS:SG	3:C:146:LYS:N	2.79	0.56
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.87	0.56
1:A:665:GLY:HA3	2:B:1086:PHE:CD1	2.41	0.56
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.40	0.56
1:A:838:GLN:O	1:A:842:VAL:HG23	2.06	0.56
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.48	0.56
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.13	0.56
2:B:566:LEU:HD22	2:B:586:TRP:O	2.06	0.56
9:K:50:LEU:CD1	9:K:73:LEU:HD21	2.35	0.56
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.41	0.56
1:A:35:ILE:HG12	1:A:52:GLY:O	2.06	0.56
5:F:99:LEU:HD12	5:F:99:LEU:O	2.06	0.56
1:A:567:LYS:NZ	6:H:46:LEU:CB	2.67	0.56
2:B:848:ARG:NH1	8:J:8:PHE:O	2.36	0.56
2:B:744:HIS:CD2	2:B:746:SER:H	2.14	0.56
1:A:885:THR:O	1:A:885:THR:HG22	2.05	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
4:E:195:VAL:HG22	4:E:213:ILE:HB	1.88	0.56
6:H:106:GLU:C	6:H:108:SER:N	2.57	0.56
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.87	0.56
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.06	0.56
2:B:23:ALA:O	2:B:654:ARG:HB3	2.04	0.56
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.88	0.56
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.05	0.56
6:H:84:ALA:HA	6:H:87:ARG:HG3	1.88	0.56
2:B:34:ILE:O	2:B:37:PHE:HB3	2.06	0.56
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.54	0.56
1:A:1328:TYR:CG	1:A:1329:THR:N	2.74	0.56
1:A:1017:LEU:HD23	4:E:204:THR:O	2.06	0.56
6:H:89:LEU:O	6:H:91:ASP:N	2.37	0.56
2:B:429:PHE:HA	2:B:432:MET:CE	2.35	0.56
1:A:50:ILE:C	1:A:52:GLY:H	2.09	0.56
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.55
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.88	0.55
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.88	0.55
6:H:59:ILE:HG22	6:H:60:ALA:N	2.20	0.55
10:L:63:ARG:O	10:L:64:LEU:O	2.25	0.55
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.86	0.55
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.36	0.55
1:A:710:LEU:H	1:A:710:LEU:CD1	2.19	0.55
2:B:120:ARG:NH1	10:L:54:ARG:NH1	2.54	0.55
4:E:168:TYR:HB3	4:E:170:LEU:CD2	2.36	0.55
4:E:195:VAL:HG22	4:E:213:ILE:CB	2.36	0.55
2:B:794:ASN:C	2:B:795:ILE:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.55
1:A:1329:THR:HG22	1:A:1331:SER:N	2.01	0.55
2:B:120:ARG:HE	2:B:955:THR:CG2	2.20	0.55
2:B:864:LYS:HG3	2:B:865:LYS:N	2.21	0.55
1:A:511:ILE:HG12	1:A:521:MET:HE3	1.89	0.55
2:B:566:LEU:HD13	2:B:588:GLY:CA	2.36	0.55
1:A:775:ILE:HD12	1:A:815:PHE:CG	2.41	0.55
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.41	0.55
1:A:672:ASP:HB3	1:A:675:THR:OG1	2.05	0.55
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.89	0.55
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.37	0.55
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.55
5:F:94:LEU:HD21	5:F:122:MET:HA	1.89	0.55
8:J:21:TYR:HA	8:J:39:LEU:HD11	1.89	0.55
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.47	0.55
1:A:15:LYS:HD2	2:B:1220:ARG:HE	1.72	0.55
1:A:399:HIS:O	1:A:435:HIS:CD2	2.60	0.55
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.60	0.55
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.47	0.55
10:L:26:THR:HG22	10:L:27:LEU:N	2.21	0.55
2:B:556:THR:HG22	2:B:557:PHE:N	2.20	0.55
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.37	0.55
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.89	0.55
2:B:361:LEU:N	2:B:362:PRO:CD	2.69	0.55
1:A:92:HIS:HD2	1:A:94:GLY:H	1.53	0.55
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.89	0.55
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.89	0.55
7:I:7:CYS:O	7:I:8:ARG:O	2.24	0.55
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.07	0.55
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.41	0.55
1:A:122:MET:O	1:A:126:LEU:HG	2.07	0.55
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.70	0.55
3:C:37:MET:HG2	3:C:243:VAL:CG1	2.34	0.55
3:C:99:LEU:HD23	3:C:99:LEU:N	2.20	0.55
1:A:216:VAL:O	1:A:219:PHE:HB2	2.06	0.55
9:K:61:TYR:HA	9:K:72:LYS:O	2.06	0.55
1:A:845:LEU:N	1:A:845:LEU:HD23	2.22	0.55
2:B:542:MET:HE1	2:B:743:ILE:CG2	2.37	0.55
2:B:783:THR:HA	8:J:60:PHE:HE1	1.72	0.55
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.07	0.55
1:A:741:ASN:ND2	1:A:743:VAL:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:THR:HG22	2:B:681:TRP:H	1.72	0.55
1:A:515:GLN:HG3	1:A:516:SER:N	2.22	0.55
1:A:89:PRO:O	1:A:204:THR:HG21	2.07	0.54
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.89	0.54
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.91	0.54
2:B:1171:VAL:HG11	2:B:1191:ILE:HD13	1.88	0.54
1:A:867:ILE:HG22	1:A:872:GLY:N	2.22	0.54
3:C:13:ALA:O	9:K:114:LEU:HD13	2.08	0.54
4:E:176:PRO:HD2	4:E:211:TYR:O	2.07	0.54
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.67	0.54
2:B:479:VAL:HG12	2:B:480:SER:H	1.72	0.54
2:B:864:LYS:N	2:B:872:GLU:OE1	2.39	0.54
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.42	0.54
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.07	0.54
1:A:821:ARG:O	1:A:822:GLU:C	2.46	0.54
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.89	0.54
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.31	0.54
4:E:61:GLN:NE2	4:E:105:PHE:CE2	2.71	0.54
2:B:756:ILE:HG21	2:B:759:PRO:HB3	1.90	0.54
10:L:70:ARG:HG2	10:L:70:ARG:NH1	2.22	0.54
2:B:758:PHE:C	2:B:760:ASP:H	2.11	0.54
1:A:885:THR:O	1:A:940:ARG:HG3	2.07	0.54
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.23	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.42	0.54
1:A:646:PHE:O	1:A:650:GLN:HG3	2.08	0.54
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.38	0.54
2:B:292:ILE:H	2:B:293:PRO:HD2	1.73	0.54
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.54	0.54
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.89	0.54
1:A:533:LYS:O	1:A:535:THR:N	2.40	0.54
6:H:6:PHE:HE1	6:H:130:ARG:HE	1.53	0.54
1:A:1299:VAL:CG1	1:A:1300:LYS:H	2.20	0.54
5:F:72:LYS:N	5:F:142:SER:HA	2.22	0.54
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.67	0.54
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.88	0.54
7:I:29:CYS:O	7:I:29:CYS:SG	2.66	0.54
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.88	0.54
6:H:38:LEU:CD1	6:H:125:LEU:HD13	2.38	0.54
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.71	0.54
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.23	0.54
3:C:248:ILE:HD13	9:K:101:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.42	0.54
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.89	0.54
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.38	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.88	0.54
1:A:852:TYR:CE2	5:F:136:ARG:HG2	2.43	0.54
2:B:93:GLY:N	2:B:131:ASP:O	2.37	0.54
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.42	0.54
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.37	0.54
1:A:226:GLU:HG2	1:A:227:VAL:HG23	1.90	0.54
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.38	0.54
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.08	0.54
8:J:32:GLU:O	8:J:36:LEU:HG	2.07	0.54
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.10	0.54
1:A:1116:LEU:O	1:A:1308:THR:HB	2.07	0.54
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.42	0.54
1:A:1375:MET:HG2	1:A:1382:THR:O	2.08	0.54
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.43	0.54
3:C:241:ASP:O	3:C:245:VAL:HG23	2.08	0.54
5:F:118:LEU:O	5:F:122:MET:HG3	2.08	0.54
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.38	0.54
5:F:114:GLU:OE1	5:F:119:ARG:HG3	2.08	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
1:A:1151:GLU:CB	7:I:44:TYR:O	2.52	0.54
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.42	0.54
1:A:902:LEU:HD21	1:A:923:LEU:HD23	1.90	0.54
6:H:5:LEU:CD1	6:H:135:LEU:HG	2.34	0.54
2:B:549:THR:HB	2:B:628:THR:HG23	1.89	0.54
1:A:1205:LYS:O	1:A:1207:LEU:N	2.41	0.54
2:B:405:ARG:HB3	2:B:631:GLY:O	2.07	0.54
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.43	0.54
7:I:111:THR:CG2	7:I:112:SER:N	2.69	0.53
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.09	0.53
11:M:53:UNK:C	11:M:55:UNK:N	2.63	0.53
10:L:27:LEU:HD13	10:L:37:LYS:HB3	1.90	0.53
1:A:38:PRO:N	1:A:270:LEU:HD23	2.22	0.53
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.08	0.53
7:I:2:THR:HG22	7:I:2:THR:O	2.07	0.53
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.37	0.53
1:A:367:PRO:HB3	1:A:465:TYR:O	2.08	0.53
6:H:32:THR:HG22	6:H:33:GLN:HG3	1.90	0.53
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CD2	1:A:94:GLY:H	2.26	0.53
2:B:484:ASN:ND2	2:B:486:TYR:CD1	2.76	0.53
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.43	0.53
1:A:814:PHE:CZ	2:B:514:LEU:HD11	2.43	0.53
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.24	0.53
2:B:801:LYS:O	8:J:52:THR:CG2	2.52	0.53
2:B:108:VAL:CG1	2:B:109:THR:H	2.18	0.53
4:E:78:LEU:HD21	4:E:109:ILE:HD12	1.90	0.53
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.53
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.23	0.53
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.28	0.53
3:C:189:THR:HG22	3:C:190:ASP:N	2.24	0.53
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.88	0.53
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.90	0.53
6:H:6:PHE:O	6:H:58:THR:HA	2.08	0.53
1:A:683:ILE:HD11	1:A:764:CYS:CB	2.35	0.53
1:A:225:ASN:O	1:A:227:VAL:HG23	2.09	0.53
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.90	0.53
2:B:755:ILE:CG2	2:B:755:ILE:O	2.55	0.53
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.72	0.53
1:A:384:ASN:OD1	1:A:385:ILE:N	2.42	0.53
1:A:590:ARG:O	1:A:591:PHE:HB2	2.08	0.53
1:A:529:CYS:HB2	2:B:1015:HIS:CE1	2.43	0.53
1:A:233:TRP:C	1:A:235:ILE:N	2.60	0.53
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.89	0.53
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.74	0.53
5:F:107:VAL:HG12	5:F:109:VAL:H	1.72	0.53
2:B:916:THR:HG22	2:B:918:ILE:HG13	1.90	0.53
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.53
1:A:1366:ARG:O	1:A:1369:ALA:HB3	2.08	0.53
7:I:75:CYS:C	7:I:77:LYS:N	2.59	0.53
10:L:47:ARG:HG2	10:L:52:GLY:CA	2.39	0.53
2:B:287:ARG:HA	2:B:291:ILE:O	2.09	0.53
2:B:899:ILE:HD11	2:B:910:VAL:O	2.09	0.53
10:L:51:CYS:C	10:L:53:HIS:H	2.12	0.53
1:A:387:ARG:O	1:A:391:LEU:HG	2.09	0.53
1:A:399:HIS:C	1:A:401:GLY:H	2.10	0.53
1:A:339:ASN:O	1:A:343:LYS:HG2	2.07	0.53
7:I:62:ILE:HG23	7:I:63:GLY:N	2.22	0.53
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.77	0.53
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:HG21	2:B:257:LYS:HB3	1.91	0.53
1:A:898:ARG:HD2	1:A:899:VAL:H	1.73	0.53
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.41	0.53
9:K:63:VAL:HG23	9:K:63:VAL:O	2.08	0.53
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.24	0.53
2:B:90:ILE:CD1	2:B:432:MET:SD	2.97	0.53
1:A:696:GLU:OE2	1:A:702:LEU:HD23	2.08	0.53
3:C:131:HIS:O	3:C:132:PRO:C	2.43	0.53
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.74	0.53
1:A:817:ALA:CB	2:B:514:LEU:HD23	2.39	0.53
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.53
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.91	0.53
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.11	0.53
2:B:875:GLU:O	2:B:877:PRO:HD3	2.09	0.53
1:A:825:ILE:CG2	2:B:512:ARG:CD	2.87	0.53
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.73	0.53
1:A:13:THR:HG23	1:A:1432:GLN:NE2	2.24	0.53
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.39	0.53
5:F:77:ASP:O	5:F:78:GLN:HB2	2.09	0.53
2:B:515:HIS:H	2:B:518:HIS:HD2	1.55	0.53
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.73	0.53
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.24	0.53
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.09	0.53
1:A:741:ASN:ND2	1:A:741:ASN:C	2.62	0.53
2:B:43:LEU:HD13	2:B:812:LEU:CD2	2.38	0.53
4:E:35:VAL:C	4:E:37:LEU:H	2.12	0.53
2:B:235:SER:OG	2:B:236:HIS:HD2	1.91	0.53
1:A:619:LYS:O	1:A:623:GLY:N	2.38	0.53
2:B:552:MET:N	2:B:553:PRO:HD2	2.24	0.53
2:B:25:ILE:HG22	2:B:26:THR:N	2.24	0.52
1:A:1365:TYR:O	1:A:1367:HIS:N	2.42	0.52
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.24	0.52
7:I:29:CYS:C	7:I:31:THR:H	2.13	0.52
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.68	0.52
1:A:1436:ILE:CG2	1:A:1437:GLY:H	2.22	0.52
2:B:806:THR:C	2:B:808:ALA:H	2.12	0.52
10:L:62:LYS:C	10:L:64:LEU:H	2.13	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.10	0.52
8:J:52:THR:O	8:J:52:THR:HG22	2.08	0.52
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.34	0.52
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:457:ALA:HA	2.09	0.52
8:J:36:LEU:HD12	8:J:47:ARG:NH1	2.23	0.52
2:B:842:ASN:HD22	2:B:845:SER:CB	2.21	0.52
1:A:1220:PHE:O	1:A:1222:ASN:N	2.42	0.52
1:A:1436:ILE:CG2	1:A:1437:GLY:N	2.72	0.52
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.91	0.52
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.90	0.52
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.74	0.52
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.91	0.52
2:B:240:ILE:HG23	2:B:240:ILE:O	2.10	0.52
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.57	0.52
1:A:852:TYR:CZ	5:F:136:ARG:HG2	2.44	0.52
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.52
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.91	0.52
10:L:38:LEU:HG	10:L:39:SER:N	2.24	0.52
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.92	0.52
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.74	0.52
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.90	0.52
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.77	0.52
7:I:46:HIS:CD2	7:I:48:LEU:HD21	2.44	0.52
7:I:50:THR:HG22	7:I:52:ILE:H	1.75	0.52
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.71	0.52
2:B:271:ALA:HB3	2:B:285:ILE:CD1	2.40	0.52
2:B:844:SER:OG	2:B:996:ARG:N	2.33	0.52
4:E:28:TYR:CE1	4:E:78:LEU:HD12	2.44	0.52
4:E:17:ARG:O	4:E:21:GLU:HG3	2.09	0.52
1:A:61:ILE:HG22	1:A:62:ASP:N	2.16	0.52
8:J:9:SER:CB	8:J:45:CYS:HB2	2.40	0.52
1:A:261:ASP:OD2	1:A:323:LYS:HD2	2.10	0.52
2:B:405:ARG:CA	2:B:631:GLY:O	2.58	0.52
1:A:219:PHE:O	1:A:222:LEU:O	2.28	0.52
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.52
2:B:428:ILE:O	2:B:431:TYR:HB3	2.10	0.52
5:F:132:LEU:O	5:F:148:VAL:HG23	2.09	0.52
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.52
1:A:907:THR:HG22	1:A:908:LEU:N	2.25	0.52
1:A:1438:THR:HG23	5:F:92:ARG:HD2	1.92	0.52
1:A:596:THR:O	1:A:597:LEU:C	2.47	0.52
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.92	0.52
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.92	0.52
1:A:928:LEU:O	1:A:931:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:109:VAL:CG1	5:F:110:ASP:N	2.73	0.52
2:B:846:ILE:HD13	2:B:974:PRO:HG2	1.91	0.52
2:B:98:THR:OG1	2:B:127:GLY:HA3	2.09	0.52
1:A:134:ARG:NH1	1:A:220:THR:O	2.42	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.24	0.52
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.91	0.52
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.52
1:A:27:VAL:HG13	1:A:240:PRO:HB3	1.91	0.52
2:B:547:VAL:H	2:B:612:GLU:CD	2.12	0.52
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.91	0.52
2:B:234:ILE:H	2:B:234:ILE:CD1	2.16	0.52
2:B:864:LYS:HD3	2:B:871:THR:HA	1.91	0.52
1:A:91:PHE:HB2	1:A:297:GLN:OE1	2.09	0.52
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.10	0.52
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.75	0.52
1:A:50:ILE:HG22	1:A:51:GLY:N	2.24	0.52
1:A:134:ARG:HH12	1:A:220:THR:HG22	1.74	0.52
1:A:1359:ASP:C	1:A:1361:SER:H	2.13	0.52
2:B:25:ILE:CG2	2:B:29:ASP:HB3	2.40	0.52
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.75	0.52
1:A:1392:SER:O	1:A:1393:ASN:CB	2.58	0.52
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.52
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.44	0.52
4:E:23:VAL:HG13	4:E:28:TYR:CD1	2.45	0.52
1:A:507:VAL:N	1:A:508:PRO:CD	2.72	0.52
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.50	0.52
1:A:929:LEU:H	1:A:929:LEU:CD2	2.23	0.52
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.38	0.52
4:E:155:ARG:HD2	4:E:194:GLU:OE2	2.09	0.52
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.10	0.52
4:E:12:LEU:HD22	4:E:55:ARG:CZ	2.39	0.52
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.92	0.51
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.91	0.51
8:J:7:CYS:SG	8:J:9:SER:HB2	2.50	0.51
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.92	0.51
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.40	0.51
6:H:84:ALA:C	6:H:86:ASP:H	2.13	0.51
1:A:817:ALA:HB1	2:B:514:LEU:HD23	1.92	0.51
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.78	0.51
2:B:707:PRO:CG	2:B:708:GLU:H	2.21	0.51
1:A:1149:ALA:CB	7:I:46:HIS:H	2.00	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HG2	1:A:49:LYS:HG2	1.92	0.51
1:A:306:ASN:HD21	1:A:324:SER:N	2.09	0.51
2:B:614:SER:OG	2:B:627:PHE:HB2	2.10	0.51
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.10	0.51
2:B:1163:CYS:SG	2:B:1182:CYS:SG	3.08	0.51
9:K:49:GLU:OE2	9:K:97:LYS:HE3	2.10	0.51
9:K:46:ILE:O	9:K:50:LEU:HB2	2.09	0.51
1:A:357:PRO:HG2	2:B:833:TYR:CE1	2.45	0.51
4:E:124:VAL:HG22	4:E:132:ILE:CG2	2.40	0.51
2:B:130:VAL:CG1	2:B:131:ASP:N	2.74	0.51
2:B:559:SER:HA	2:B:563:MET:HB3	1.91	0.51
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.91	0.51
1:A:96:ILE:O	1:A:100:LYS:HG3	2.10	0.51
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.11	0.51
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.90	0.51
10:L:62:LYS:O	10:L:64:LEU:N	2.37	0.51
2:B:292:ILE:N	2:B:293:PRO:HD2	2.25	0.51
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.45	0.51
1:A:326:ARG:HG2	1:A:1406:VAL:CG2	2.39	0.51
2:B:248:SER:O	2:B:249:ARG:HB2	2.09	0.51
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.92	0.51
7:I:73:ARG:O	7:I:81:ARG:HA	2.09	0.51
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.45	0.51
7:I:78:CYS:SG	7:I:106:CYS:SG	3.02	0.51
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.11	0.51
6:H:83:GLN:C	6:H:85:GLY:H	2.14	0.51
8:J:14:VAL:HG12	8:J:50:ILE:HD11	1.92	0.51
1:A:341:MET:CE	1:A:1401:SER:HB2	2.41	0.51
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.92	0.51
2:B:463:THR:HG21	2:B:465:ASN:HD22	1.74	0.51
6:H:84:ALA:C	6:H:86:ASP:N	2.64	0.51
1:A:808:LEU:O	2:B:728:ARG:NH1	2.43	0.51
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.09	0.51
8:J:48:ARG:NE	8:J:49:MET:HE2	2.26	0.51
8:J:54:VAL:O	8:J:56:LEU:N	2.43	0.51
2:B:247:GLY:N	2:B:418:LYS:HZ3	2.06	0.51
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.93	0.51
10:L:38:LEU:O	10:L:39:SER:CB	2.56	0.51
1:A:675:THR:CG2	1:A:736:ASN:HD21	2.22	0.51
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.92	0.51
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.40	0.51
1:A:822:GLU:HA	2:B:513:GLN:HE21	1.63	0.51
1:A:1153:TYR:OH	7:I:42:LEU:HA	2.09	0.51
1:A:15:LYS:CB	2:B:1220:ARG:HG2	2.33	0.51
1:A:1410:PHE:CE2	2:B:1212:ILE:HD11	2.45	0.51
7:I:55:THR:HG21	7:I:109:ILE:HD13	1.93	0.51
10:L:40:LEU:HD13	10:L:44:ASP:OD1	2.11	0.51
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.41	0.51
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.45	0.51
4:E:121:MET:C	4:E:123:LEU:H	2.13	0.51
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.41	0.51
1:A:1150:SER:HB2	1:A:1195:LEU:HD23	1.93	0.51
1:A:1376:THR:HG23	4:E:212:ARG:NH2	2.26	0.51
1:A:115:LEU:HB2	1:A:122:MET:CE	2.41	0.51
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.93	0.51
2:B:283:VAL:HG13	2:B:297:ILE:CD1	2.41	0.51
3:C:66:ARG:NH2	8:J:2:ILE:CG2	2.74	0.51
1:A:898:ARG:HD2	1:A:899:VAL:N	2.26	0.51
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.26	0.51
2:B:283:VAL:O	2:B:286:PHE:HB2	2.11	0.51
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.93	0.51
1:A:233:TRP:C	1:A:235:ILE:H	2.13	0.51
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.25	0.51
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.40	0.51
2:B:405:ARG:O	2:B:406:LEU:HD23	2.11	0.51
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.84	0.51
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	2.10	0.51
2:B:737:THR:CG2	7:I:66:PRO:HB2	2.40	0.50
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.92	0.50
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.39	0.50
1:A:418:SER:C	1:A:420:ARG:N	2.63	0.50
1:A:500:GLU:OE1	2:B:1143:ALA:HB1	2.11	0.50
1:A:649:ILE:O	1:A:653:VAL:HG23	2.11	0.50
6:H:31:THR:O	6:H:32:THR:HB	2.11	0.50
2:B:185:THR:O	2:B:189:LEU:HG	2.11	0.50
9:K:101:LEU:HD23	9:K:101:LEU:O	2.11	0.50
8:J:36:LEU:HD13	8:J:47:ARG:HG2	1.92	0.50
1:A:814:PHE:HZ	2:B:518:HIS:HB2	1.75	0.50
1:A:1384:VAL:HG12	1:A:1384:VAL:O	2.11	0.50
2:B:858:SER:HA	2:B:966:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:GLY:O	1:A:940:ARG:NH2	2.44	0.50
4:E:54:GLN:O	4:E:57:MET:HB3	2.11	0.50
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.76	0.50
2:B:563:MET:HG3	2:B:563:MET:O	2.10	0.50
7:I:25:LEU:HD12	7:I:26:LEU:H	1.76	0.50
1:A:100:LYS:NZ	1:A:176:LYS:HD2	2.27	0.50
1:A:587:HIS:HA	1:A:607:ILE:O	2.11	0.50
1:A:810:PRO:O	1:A:813:PHE:HB3	2.11	0.50
2:B:514:LEU:HD12	2:B:515:HIS:H	1.74	0.50
1:A:771:GLU:H	1:A:822:GLU:CD	2.14	0.50
2:B:271:ALA:O	2:B:279:ASP:HA	2.11	0.50
8:J:7:CYS:O	8:J:8:PHE:C	2.50	0.50
1:A:332:LYS:H	1:A:337:ARG:HD2	1.76	0.50
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.76	0.50
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.14	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.11	0.50
2:B:271:ALA:HB3	2:B:285:ILE:HD11	1.93	0.50
1:A:706:HIS:CG	1:A:1135:ARG:CZ	2.94	0.50
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.50
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.93	0.50
6:H:44:VAL:O	6:H:44:VAL:HG12	2.12	0.50
1:A:167:CYS:O	1:A:169:ASN:N	2.45	0.50
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.26	0.50
6:H:128:ASN:O	6:H:131:ASN:ND2	2.45	0.50
2:B:839:MET:HE2	2:B:980:PHE:CD1	2.47	0.50
1:A:994:GLN:NE2	1:A:1019:CYS:HB3	2.27	0.50
2:B:756:ILE:CG2	2:B:759:PRO:HB3	2.42	0.50
4:E:157:SER:C	4:E:159:ASP:N	2.64	0.50
10:L:62:LYS:O	10:L:64:LEU:HG	2.11	0.50
1:A:821:ARG:CG	1:A:825:ILE:HD11	2.41	0.50
1:A:1362:TYR:OH	1:A:1364:ASN:HA	2.11	0.50
1:A:517:ASN:HB2	1:A:875:ALA:O	2.11	0.50
7:I:99:LEU:HB2	7:I:112:SER:HB3	1.94	0.50
1:A:340:LEU:HD21	2:B:1200:ALA:CB	2.40	0.50
1:A:329:LEU:HD22	2:B:1203:LEU:CD1	2.41	0.50
4:E:168:TYR:HB3	4:E:170:LEU:CG	2.41	0.50
9:K:97:LYS:O	9:K:100:ALA:HB3	2.12	0.50
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.52	0.50
1:A:814:PHE:HB2	2:B:519:TRP:HE3	1.75	0.50
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.94	0.50
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.94	0.50
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.50
2:B:751:VAL:HG12	2:B:752:ALA:N	2.26	0.50
2:B:737:THR:CG2	7:I:66:PRO:CB	2.89	0.50
7:I:75:CYS:O	7:I:77:LYS:N	2.44	0.50
2:B:800:GLN:OE1	2:B:822:ASN:HB2	2.12	0.50
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.27	0.50
1:A:69:THR:HG22	1:A:69:THR:O	2.12	0.50
4:E:98:ILE:O	4:E:102:GLU:HG3	2.12	0.50
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.93	0.50
1:A:573:SER:O	1:A:576:GLN:HB2	2.11	0.50
1:A:775:ILE:HD11	1:A:815:PHE:HB3	1.90	0.50
1:A:709:THR:CB	1:A:712:GLU:HG3	2.41	0.50
1:A:107:CYS:HB2	1:A:114:LEU:HD23	1.93	0.50
6:H:76:THR:HG22	6:H:76:THR:O	2.11	0.50
2:B:1208:MET:HA	2:B:1212:ILE:O	2.12	0.49
2:B:1106:ARG:HH12	2:B:1118:PRO:CB	2.24	0.49
2:B:269:ILE:CD1	2:B:386:LEU:HD21	2.39	0.49
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.24	0.49
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.27	0.49
1:A:1326:ARG:O	1:A:1327:ILE:C	2.49	0.49
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.24	0.49
2:B:240:ILE:O	2:B:253:THR:HG23	2.11	0.49
1:A:1351:GLU:O	1:A:1352:VAL:C	2.49	0.49
2:B:648:HIS:NE2	2:B:650:GLU:OE1	2.43	0.49
1:A:706:HIS:HD2	1:A:1135:ARG:NH2	2.05	0.49
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.47	0.49
1:A:893:PHE:CE1	1:A:940:ARG:HD2	2.46	0.49
8:J:57:ILE:HG12	8:J:61:LEU:HD11	1.94	0.49
2:B:975:GLN:O	2:B:990:ILE:HD12	2.12	0.49
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.51	0.49
11:M:17:UNK:O	11:M:18:UNK:O	2.30	0.49
1:A:834:THR:HG21	1:A:1077:THR:CA	2.43	0.49
1:A:810:PRO:HG2	2:B:705:MET:CG	2.42	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.44	0.49
6:H:40:LEU:CD2	6:H:42:ILE:HD11	2.39	0.49
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.12	0.49
7:I:29:CYS:SG	7:I:31:THR:HG22	2.52	0.49
4:E:5:ASN:O	4:E:9:ILE:HG13	2.11	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.49
2:B:911:ILE:HD11	2:B:941:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:46:TYR:HE2	4:E:58:MET:HA	1.76	0.49
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.76	0.49
2:B:781:PHE:O	2:B:782:LEU:HG	2.12	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.12	0.49
1:A:819:GLY:O	1:A:820:GLY:C	2.49	0.49
2:B:25:ILE:CG2	2:B:29:ASP:CB	2.91	0.49
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.95	0.49
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.76	0.49
1:A:412:ARG:O	11:M:50:UNK:C	2.60	0.49
1:A:1376:THR:HG23	1:A:1376:THR:O	2.12	0.49
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.94	0.49
1:A:511:ILE:HG12	1:A:521:MET:CE	2.42	0.49
1:A:1142:THR:O	1:A:1273:LEU:HD22	2.12	0.49
2:B:660:LYS:O	2:B:663:ALA:HB3	2.13	0.49
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.94	0.49
8:J:16:ASP:OD1	8:J:17:LYS:HE3	2.12	0.49
2:B:35:SER:O	2:B:36:ALA:C	2.50	0.49
7:I:7:CYS:CB	7:I:14:LEU:HD21	2.32	0.49
2:B:1077:THR:HG22	2:B:1079:LYS:HB2	1.94	0.49
5:F:133:VAL:HG22	5:F:147:SER:HA	1.95	0.49
1:A:418:SER:HB3	1:A:421:ALA:HB2	1.94	0.49
4:E:177:ARG:O	4:E:212:ARG:HD3	2.11	0.49
4:E:102:GLU:O	4:E:104:ASN:N	2.46	0.49
1:A:829:VAL:C	1:A:831:THR:H	2.15	0.49
1:A:612:ILE:HG23	1:A:612:ILE:O	2.12	0.49
1:A:751:SER:O	1:A:752:LYS:CG	2.59	0.49
3:C:33:LEU:HG	3:C:37:MET:CE	2.41	0.49
1:A:394:ASN:OD1	1:A:398:GLU:OE1	2.30	0.49
6:H:88:SER:O	6:H:89:LEU:HG	2.12	0.49
7:I:101:PHE:O	7:I:109:ILE:HA	2.12	0.49
4:E:191:LYS:O	4:E:192:ARG:C	2.50	0.49
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.42	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
5:F:82:THR:HG22	5:F:84:TYR:H	1.77	0.49
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.93	0.49
7:I:15:TYR:CD1	7:I:15:TYR:N	2.79	0.49
1:A:821:ARG:NE	2:B:512:ARG:O	2.44	0.49
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.43	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.75	0.49
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.43	0.49
10:L:31:CYS:SG	10:L:34:CYS:SG	3.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:C	1:A:227:VAL:H	2.10	0.49
6:H:84:ALA:HB1	6:H:87:ARG:HB2	1.94	0.49
5:F:87:LYS:HE2	5:F:88:TYR:CE1	2.48	0.49
1:A:754:SER:O	1:A:755:PHE:C	2.48	0.49
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.48	0.49
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.77	0.49
1:A:1100:ARG:NH2	1:A:1330:ASN:HB2	2.28	0.49
7:I:85:PHE:O	7:I:86:PHE:HB3	2.13	0.49
3:C:80:LEU:CD2	3:C:129:ILE:HD11	2.29	0.49
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.47	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
1:A:381:THR:O	1:A:384:ASN:N	2.41	0.49
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.95	0.49
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.95	0.49
2:B:55:VAL:HG12	2:B:56:ASP:N	2.28	0.49
1:A:89:PRO:C	1:A:204:THR:HG21	2.33	0.49
1:A:475:THR:CG2	1:A:476:SER:N	2.76	0.49
1:A:679:ILE:HG23	1:A:729:ALA:CB	2.39	0.49
1:A:1300:LYS:HB3	1:A:1300:LYS:HZ2	1.77	0.49
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.72	0.49
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.94	0.49
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.53	0.49
2:B:405:ARG:CB	2:B:631:GLY:O	2.61	0.49
3:C:254:LYS:HE2	9:K:42:LEU:HD13	1.94	0.49
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.13	0.49
2:B:825:VAL:CG1	2:B:826:ALA:N	2.76	0.49
1:A:178:GLY:O	1:A:179:LEU:HD23	2.13	0.49
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.43	0.49
2:B:365:THR:HG23	2:B:367:LEU:HG	1.93	0.49
1:A:918:GLU:O	1:A:918:GLU:HG3	2.12	0.49
2:B:708:GLU:C	2:B:710:LEU:H	2.16	0.49
2:B:1053:GLU:O	2:B:1054:GLY:C	2.50	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.95	0.49
6:H:36:CYS:HA	6:H:126:GLU:O	2.13	0.49
6:H:6:PHE:HE1	6:H:130:ARG:NE	2.10	0.49
2:B:906:SER:O	2:B:907:GLY:C	2.50	0.49
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.39	0.49
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.78	0.49
2:B:1043:ASP:O	2:B:1050:ILE:HD12	2.13	0.49
1:A:567:LYS:NZ	6:H:95:TYR:CD1	2.80	0.48
1:A:61:ILE:HA	1:A:74:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:OE1	1:A:591:PHE:HE1	1.96	0.48
6:H:125:LEU:HG	6:H:130:ARG:CZ	2.43	0.48
6:H:93:TYR:HA	6:H:145:ARG:CB	2.41	0.48
4:E:100:ILE:CG2	4:E:105:PHE:HB2	2.42	0.48
4:E:78:LEU:HD21	4:E:80:VAL:HG22	1.95	0.48
1:A:466:SER:HB3	9:K:2:ASN:ND2	2.28	0.48
3:C:142:VAL:H	8:J:16:ASP:CB	2.26	0.48
1:A:538:ASP:OD1	6:H:22:LYS:HB2	2.12	0.48
2:B:260:GLY:O	2:B:267:ARG:HD3	2.12	0.48
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.45	0.48
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.77	0.48
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.73	0.48
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.46	0.48
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.48
1:A:674:PRO:O	1:A:677:ARG:HB3	2.14	0.48
6:H:33:GLN:OE1	6:H:129:TYR:CE2	2.67	0.48
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.13	0.48
1:A:1066:VAL:O	1:A:1068:ALA:N	2.46	0.48
7:I:50:THR:HG22	7:I:51:ASN:N	2.28	0.48
2:B:1054:GLY:O	2:B:1058:LEU:HG	2.13	0.48
5:F:82:THR:HG22	5:F:84:TYR:N	2.27	0.48
1:A:74:MET:O	1:A:75:ASN:HB2	2.13	0.48
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.61	0.48
3:C:75:MET:HG3	3:C:246:ARG:NH2	2.28	0.48
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.48	0.48
9:K:55:LYS:CD	9:K:78:THR:HB	2.42	0.48
1:A:226:GLU:CG	1:A:227:VAL:N	2.75	0.48
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.41	0.48
3:C:4:GLU:O	3:C:5:GLY:O	2.31	0.48
4:E:102:GLU:C	4:E:104:ASN:N	2.67	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.48
9:K:43:GLY:HA2	9:K:71:PHE:CZ	2.49	0.48
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.13	0.48
2:B:890:TYR:O	2:B:892:LYS:N	2.46	0.48
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.14	0.48
1:A:491:VAL:O	1:A:493:GLN:NE2	2.46	0.48
1:A:1149:ALA:CA	7:I:46:HIS:HB3	2.32	0.48
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.43	0.48
5:F:81:THR:HG22	5:F:82:THR:H	1.78	0.48
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.43	0.48
2:B:351:TYR:O	2:B:355:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:MET:HG3	3:C:246:ARG:HH22	1.77	0.48
2:B:46:GLN:HE21	2:B:496:ARG:HG2	1.78	0.48
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.78	0.48
3:C:254:LYS:O	3:C:258:ILE:HD13	2.13	0.48
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.95	0.48
1:A:474:VAL:HG13	1:A:478:TYR:CE1	2.48	0.48
10:L:52:GLY:O	10:L:54:ARG:HG3	2.12	0.48
2:B:873:THR:O	2:B:914:LYS:HA	2.12	0.48
1:A:391:LEU:O	1:A:394:ASN:N	2.46	0.48
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.48
1:A:226:GLU:HG2	1:A:227:VAL:N	2.29	0.48
1:A:294:SER:HA	1:A:297:GLN:HB3	1.96	0.48
1:A:1386:ARG:HE	1:A:1387:HIS:CE1	2.32	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.94	0.48
9:K:27:ALA:HB1	9:K:28:PRO:HD2	1.96	0.48
3:C:35:ARG:O	3:C:38:ILE:N	2.47	0.48
2:B:1053:GLU:O	2:B:1055:ILE:N	2.46	0.48
6:H:39:THR:O	6:H:123:MET:HA	2.14	0.48
2:B:570:VAL:HG11	2:B:573:GLN:OE1	2.13	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CB	2.76	0.48
2:B:1104:HIS:HB2	2:B:1122:ARG:CD	2.44	0.48
1:A:1406:VAL:CG1	1:A:1410:PHE:HE1	2.26	0.48
2:B:864:LYS:HB3	2:B:871:THR:HA	1.96	0.48
3:C:142:VAL:H	8:J:16:ASP:HB3	1.77	0.48
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.54	0.48
1:A:810:PRO:HB2	2:B:705:MET:SD	2.53	0.48
2:B:1065:GLN:HE22	2:B:1067:ARG:HG2	1.78	0.48
2:B:1106:ARG:NH2	2:B:1109:GLY:C	2.67	0.48
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.48
1:A:18:GLN:O	2:B:1215:ARG:CG	2.62	0.48
2:B:300:HIS:ND1	2:B:376:PHE:CD2	2.81	0.48
4:E:7:ARG:C	4:E:9:ILE:H	2.17	0.48
1:A:1392:SER:O	1:A:1393:ASN:CG	2.52	0.48
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.68	0.48
1:A:741:ASN:ND2	1:A:743:VAL:N	2.60	0.48
2:B:806:THR:HG22	2:B:808:ALA:H	1.79	0.48
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.49	0.48
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.78	0.48
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.95	0.48
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.60	0.48
1:A:1116:LEU:HD12	1:A:1329:THR:HG1	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASP:C	2:B:334:ILE:H	2.17	0.48
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.37	0.48
2:B:1106:ARG:HH21	2:B:1109:GLY:C	2.16	0.48
1:A:332:LYS:N	1:A:337:ARG:HD2	2.28	0.48
2:B:763:GLN:CG	2:B:765:PRO:HD2	2.40	0.48
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.91	0.48
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.96	0.48
2:B:1182:CYS:O	2:B:1183:LYS:O	2.31	0.48
2:B:225:VAL:HG11	2:B:388:CYS:HB3	1.95	0.48
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.95	0.48
1:A:67:CYS:SG	1:A:77:CYS:SG	3.11	0.48
2:B:653:VAL:HG12	2:B:654:ARG:N	2.28	0.48
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.29	0.48
2:B:230:ALA:C	2:B:232:SER:H	2.17	0.48
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.48
9:K:83:PRO:HA	9:K:86:ALA:HB3	1.95	0.48
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.14	0.48
1:A:1410:PHE:C	1:A:1412:ALA:N	2.67	0.47
1:A:531:ILE:CD1	1:A:617:VAL:HG11	2.44	0.47
1:A:535:THR:HG21	1:A:616:VAL:CA	2.43	0.47
2:B:487:THR:HG22	2:B:489:SER:N	2.24	0.47
2:B:871:THR:HG22	2:B:872:GLU:O	2.14	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.47
2:B:321:GLY:C	2:B:323:VAL:H	2.17	0.47
1:A:954:TRP:O	1:A:956:LEU:HG	2.14	0.47
1:A:116:ASP:HB2	1:A:118:HIS:CD2	2.49	0.47
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.79	0.47
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.96	0.47
2:B:800:GLN:CB	8:J:52:THR:CG2	2.89	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.47
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.79	0.47
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.14	0.47
2:B:773:MET:SD	2:B:987:LYS:HD2	2.55	0.47
1:A:770:VAL:HG13	1:A:822:GLU:OE1	2.15	0.47
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.86	0.47
3:C:66:ARG:CZ	8:J:2:ILE:HG21	2.44	0.47
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.14	0.47
1:A:816:HIS:CE1	2:B:764:SER:CB	2.89	0.47
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.96	0.47
6:H:138:GLU:O	6:H:139:ASN:C	2.53	0.47
2:B:210:LYS:HE2	2:B:461:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HG2	1:A:113:LEU:H	1.79	0.47
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.49	0.47
1:A:20:GLY:HA2	1:A:1413:GLY:O	2.14	0.47
6:H:47:PHE:CD1	6:H:95:TYR:HB2	2.49	0.47
1:A:89:PRO:HG3	1:A:208:LEU:CD1	2.44	0.47
1:A:352:VAL:HG12	1:A:353:ILE:N	2.29	0.47
9:K:59:ALA:HA	9:K:74:ARG:O	2.15	0.47
4:E:96:PHE:CE1	4:E:100:ILE:HD11	2.50	0.47
2:B:100:PRO:O	2:B:180:TYR:OH	2.31	0.47
2:B:303:TYR:HH	2:B:586:TRP:HZ3	1.62	0.47
7:I:62:ILE:CG2	7:I:63:GLY:N	2.77	0.47
5:F:79:ARG:HG2	5:F:146:TRP:CZ2	2.49	0.47
2:B:956:THR:HG21	2:B:960:GLY:HA2	1.96	0.47
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.47
9:K:47:ARG:CB	9:K:47:ARG:HH11	2.23	0.47
1:A:90:VAL:HG21	1:A:296:LEU:HG	1.95	0.47
1:A:1074:GLU:C	1:A:1076:ALA:N	2.67	0.47
1:A:376:TYR:CD2	1:A:376:TYR:C	2.87	0.47
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.50	0.47
3:C:258:ILE:N	3:C:258:ILE:HD12	2.30	0.47
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.45	0.47
1:A:843:LYS:HG3	1:A:1402:PHE:HD1	1.79	0.47
2:B:217:ARG:HD2	2:B:241:ARG:NH2	2.29	0.47
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.35	0.47
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.46	0.47
6:H:49:VAL:CG1	6:H:50:ALA:N	2.74	0.47
1:A:923:LEU:O	1:A:927:VAL:HG23	2.14	0.47
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.95	0.47
2:B:294:ASP:H	7:I:12:ASN:ND2	2.13	0.47
2:B:324:ILE:HG23	2:B:329:THR:HB	1.96	0.47
2:B:1098:MET:O	2:B:1099:VAL:C	2.53	0.47
8:J:48:ARG:HH21	8:J:49:MET:CE	2.24	0.47
2:B:201:GLY:H	2:B:202:TYR:HD2	1.63	0.47
1:A:869:GLY:O	4:E:204:THR:HG21	2.14	0.47
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.62	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:742:ASN:O	1:A:745:GLN:HB2	2.13	0.47
1:A:83:HIS:CE1	1:A:238:CYS:SG	3.08	0.47
2:B:123:THR:O	2:B:125:SER:N	2.47	0.47
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.50	0.47
1:A:443:LEU:CD2	1:A:455:MET:HB3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:MET:SD	2:B:1201:LYS:HG2	2.54	0.47
2:B:65:GLU:HG3	2:B:66:ASP:N	2.27	0.47
1:A:804:TYR:HE1	2:B:1021:MET:CE	2.27	0.47
5:F:98:ALA:O	5:F:117:PRO:HB2	2.14	0.47
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.14	0.47
1:A:1074:GLU:C	1:A:1076:ALA:H	2.18	0.47
1:A:167:CYS:C	1:A:169:ASN:H	2.18	0.47
2:B:821:GLN:HB2	2:B:851:PHE:CE2	2.49	0.47
1:A:1134:ILE:HD11	1:A:1321:GLY:HA3	1.96	0.47
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.15	0.47
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.45	0.47
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.50	0.47
1:A:666:ILE:HD11	2:B:1030:LEU:CD1	2.20	0.47
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.80	0.47
1:A:1392:SER:O	1:A:1393:ASN:ND2	2.48	0.47
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.79	0.47
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.49	0.47
2:B:1072:MET:HE3	2:B:1085:ILE:CD1	2.44	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.46	0.47
1:A:12:ARG:HD3	2:B:1218:THR:HB	1.97	0.47
2:B:1060:ARG:O	2:B:1063:GLY:N	2.45	0.47
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.30	0.47
2:B:640:VAL:HG12	2:B:640:VAL:O	2.15	0.47
2:B:780:VAL:HG21	8:J:56:LEU:HD11	1.97	0.47
7:I:54:GLU:O	7:I:89:GLN:HG2	2.15	0.47
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.30	0.47
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.98	0.47
1:A:53:LEU:HD13	1:A:263:THR:HG23	1.97	0.47
1:A:848:ILE:CD1	1:A:1374:VAL:HG21	2.45	0.47
1:A:573:SER:OG	1:A:576:GLN:HG3	2.15	0.47
1:A:829:VAL:O	1:A:831:THR:N	2.48	0.47
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.45	0.47
3:C:263:THR:C	3:C:265:MET:H	2.18	0.47
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.41	0.47
1:A:1194:ARG:HH22	1:A:1237:ILE:HD13	1.73	0.47
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.45	0.47
2:B:1198:TYR:HE1	2:B:1201:LYS:HZ2	1.63	0.47
1:A:87:ALA:HB3	1:A:276:LEU:CD2	2.45	0.47
2:B:96:TYR:CD1	2:B:96:TYR:N	2.83	0.47
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.49	0.46
8:J:1:MET:O	8:J:2:ILE:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:CB	2:B:946:ASN:HB2	2.45	0.46
2:B:298:LEU:HD23	2:B:298:LEU:N	2.29	0.46
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.45	0.46
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.45	0.46
3:C:43:THR:HG22	3:C:44:LEU:N	2.29	0.46
1:A:1017:LEU:O	1:A:1018:PHE:C	2.53	0.46
2:B:1106:ARG:NH1	2:B:1118:PRO:CB	2.72	0.46
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.15	0.46
5:F:101:ILE:HD11	5:F:124:GLU:OE1	2.15	0.46
2:B:851:PHE:O	2:B:974:PRO:HD3	2.15	0.46
3:C:262:LEU:O	3:C:265:MET:HB3	2.15	0.46
1:A:813:PHE:HE2	2:B:524:PRO:CG	2.15	0.46
2:B:167:ILE:HG22	2:B:167:ILE:O	2.14	0.46
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.80	0.46
1:A:329:LEU:HA	1:A:335:ARG:HB2	1.98	0.46
2:B:864:LYS:H	2:B:872:GLU:CG	2.28	0.46
2:B:1182:CYS:O	2:B:1183:LYS:HD2	2.15	0.46
2:B:890:TYR:C	2:B:892:LYS:H	2.19	0.46
10:L:30:ILE:CD1	10:L:59:ALA:HA	2.44	0.46
3:C:180:TYR:O	3:C:181:ASP:HB3	2.15	0.46
11:M:76:UNK:O	11:M:77:UNK:O	2.33	0.46
2:B:332:ASP:C	2:B:334:ILE:N	2.68	0.46
1:A:418:SER:O	1:A:421:ALA:N	2.49	0.46
1:A:658:LEU:HD13	2:B:831:SER:HA	1.98	0.46
1:A:1209:MET:CG	1:A:1236:LEU:HD22	2.45	0.46
2:B:574:SER:HB3	2:B:577:ALA:HB2	1.98	0.46
1:A:964:ILE:HD13	1:A:1035:TYR:CZ	2.50	0.46
2:B:805:THR:HA	2:B:809:MET:HE1	1.98	0.46
9:K:83:PRO:O	9:K:87:LEU:N	2.46	0.46
1:A:50:ILE:HG22	1:A:51:GLY:H	1.81	0.46
1:A:890:ASP:N	1:A:1296:GLY:HA3	2.30	0.46
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.97	0.46
1:A:530:GLY:O	1:A:531:ILE:C	2.54	0.46
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.46
1:A:893:PHE:CD1	1:A:940:ARG:HD2	2.51	0.46
2:B:1117:GLN:HG3	2:B:1156:ASP:OD1	2.16	0.46
1:A:1394:THR:CG2	1:A:1395:GLY:N	2.78	0.46
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.98	0.46
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.98	0.46
2:B:322:PHE:O	2:B:322:PHE:CG	2.69	0.46
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.97	0.46
1:A:666:ILE:O	1:A:667:GLY:C	2.53	0.46
2:B:300:HIS:ND1	2:B:376:PHE:CE2	2.83	0.46
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.78	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.29	0.46
1:A:1405:THR:O	1:A:1406:VAL:C	2.54	0.46
4:E:56:LYS:HG3	4:E:84:ASP:CB	2.42	0.46
3:C:5:GLY:O	3:C:6:PRO:C	2.54	0.46
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.49	0.46
2:B:758:PHE:C	2:B:760:ASP:N	2.68	0.46
7:I:100:PHE:HZ	7:I:118:ARG:HH12	1.62	0.46
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.98	0.46
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.50	0.46
2:B:515:HIS:O	2:B:516:ASN:C	2.54	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CH2	2.48	0.46
3:C:236:GLY:C	3:C:238:ILE:N	2.69	0.46
2:B:230:ALA:N	2:B:231:PRO:HD2	2.31	0.46
1:A:418:SER:HA	11:M:46:UNK:C	2.45	0.46
2:B:1177:HIS:C	2:B:1179:GLN:N	2.68	0.46
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.46
1:A:849:MET:HB2	1:A:1063:MET:SD	2.55	0.46
2:B:680:THR:O	2:B:683:SER:OG	2.34	0.46
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.81	0.46
2:B:1051:THR:HG21	2:B:1053:GLU:HB2	1.97	0.46
6:H:40:LEU:HG	6:H:42:ILE:HG13	1.98	0.46
1:A:517:ASN:OD1	1:A:517:ASN:O	2.34	0.46
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.19	0.46
1:A:592:ASP:N	1:A:595:THR:OG1	2.48	0.46
2:B:914:LYS:H	2:B:938:SER:HB3	1.81	0.46
5:F:117:PRO:O	5:F:120:ILE:HB	2.16	0.46
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.96	0.46
1:A:1394:THR:HG23	1:A:1398:MET:CE	2.46	0.46
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.16	0.46
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.37	0.46
3:C:62:PHE:C	3:C:62:PHE:CD2	2.89	0.46
4:E:58:MET:O	4:E:59:SER:C	2.53	0.46
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.78	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.46
1:A:645:LEU:O	1:A:649:ILE:HG13	2.15	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
9:K:91:CYS:O	9:K:94:ILE:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:GLN:CG	9:K:95:ILE:HG23	2.46	0.46
2:B:282:ILE:HG13	2:B:283:VAL:N	2.31	0.46
1:A:573:SER:H	1:A:576:GLN:HG3	1.81	0.46
2:B:893:LEU:HD22	2:B:897:GLY:O	2.16	0.46
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.16	0.46
4:E:10:SER:O	4:E:14:ARG:HG3	2.16	0.46
2:B:704:ALA:HB2	2:B:738:PHE:CE1	2.51	0.46
1:A:1153:TYR:CD2	7:I:41:PRO:HB2	2.51	0.46
9:K:113:THR:O	9:K:114:LEU:CB	2.47	0.46
1:A:47:ARG:O	1:A:48:ALA:HB2	2.16	0.46
3:C:173:ALA:O	3:C:174:ALA:CB	2.64	0.46
1:A:709:THR:C	1:A:711:ARG:N	2.67	0.46
9:K:73:LEU:CD2	9:K:75:ILE:HD11	2.46	0.46
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.51	0.46
2:B:50:SER:O	2:B:53:GLN:HB3	2.16	0.46
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.97	0.46
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.31	0.46
1:A:814:PHE:CE1	2:B:519:TRP:N	2.83	0.45
7:I:75:CYS:O	7:I:76:PRO:C	2.52	0.45
1:A:420:ARG:O	1:A:424:ILE:HG13	2.16	0.45
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.97	0.45
2:B:361:LEU:N	2:B:362:PRO:HD2	2.31	0.45
2:B:1158:PHE:HE2	2:B:1201:LYS:HE3	1.80	0.45
6:H:101:ALA:HB2	6:H:116:TYR:CD2	2.51	0.45
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.97	0.45
1:A:112:LYS:HG2	1:A:113:LEU:N	2.31	0.45
2:B:25:ILE:HD11	2:B:653:VAL:CB	2.46	0.45
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.98	0.45
2:B:345:LYS:O	2:B:347:LYS:N	2.49	0.45
1:A:542:GLU:C	1:A:546:VAL:HG23	2.36	0.45
8:J:5:VAL:O	8:J:6:ARG:HB2	2.15	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.44	0.45
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.78	0.45
4:E:94:LYS:O	4:E:98:ILE:HG13	2.16	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.45
6:H:98:TYR:O	6:H:118:PHE:HD2	1.99	0.45
4:E:190:LEU:HD11	4:E:196:VAL:HG11	1.98	0.45
2:B:887:HIS:CD2	11:M:37:UNK:O	2.39	0.45
1:A:1147:THR:HB	7:I:48:LEU:HD11	1.98	0.45
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.46	0.45
1:A:666:ILE:H	1:A:666:ILE:HG13	1.33	0.45
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.46	0.45
7:I:29:CYS:O	7:I:31:THR:N	2.49	0.45
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.36	0.45
2:B:1154:ALA:O	2:B:1155:SER:CB	2.63	0.45
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.15	0.45
2:B:589:VAL:HG12	2:B:590:HIS:H	1.81	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.51	0.45
6:H:116:TYR:HE2	6:H:140:ALA:CB	2.30	0.45
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.98	0.45
1:A:50:ILE:C	1:A:52:GLY:N	2.69	0.45
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.47	0.45
2:B:260:GLY:HA3	2:B:267:ARG:HG2	1.98	0.45
3:C:120:ILE:HD11	3:C:130:GLY:O	2.17	0.45
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.45
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.82	0.45
9:K:12:LEU:CD1	9:K:12:LEU:H	2.23	0.45
1:A:337:ARG:CD	1:A:839:ARG:HH22	2.29	0.45
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.31	0.45
2:B:100:PRO:HA	2:B:125:SER:O	2.17	0.45
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.31	0.45
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	1.98	0.45
7:I:34:TYR:O	7:I:35:VAL:CG2	2.65	0.45
2:B:542:MET:HG3	2:B:747:MET:CE	2.39	0.45
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.99	0.45
1:A:545:GLN:O	1:A:546:VAL:C	2.55	0.45
7:I:99:LEU:HB2	7:I:112:SER:CB	2.46	0.45
2:B:977:GLY:C	2:B:1099:VAL:HG23	2.37	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:CG1	2.46	0.45
1:A:388:LEU:O	1:A:392:VAL:HG23	2.17	0.45
1:A:337:ARG:CZ	1:A:839:ARG:HH12	2.26	0.45
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.81	0.45
1:A:994:GLN:HE21	1:A:1019:CYS:CB	2.26	0.45
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.49	0.45
1:A:738:LYS:NZ	3:C:194:GLU:CA	2.79	0.45
1:A:701:LEU:HA	7:I:115:LYS:HE3	1.98	0.45
2:B:370:PHE:N	2:B:371:GLU:OE1	2.50	0.45
4:E:179:GLN:OE1	4:E:179:GLN:HA	2.16	0.45
2:B:745:PRO:C	2:B:747:MET:N	2.70	0.45
11:M:40:UNK:C	11:M:41:UNK:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HD13	2:B:334:ILE:CG2	2.47	0.45
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.45	0.45
1:A:540:PHE:C	1:A:541:ILE:HD12	2.35	0.45
1:A:223:GLY:HA3	1:A:1415:SER:HB3	1.98	0.45
2:B:405:ARG:HD2	2:B:631:GLY:O	2.17	0.45
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.32	0.45
1:A:1336:MET:SD	1:A:1381:LEU:HG	2.56	0.45
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.98	0.45
2:B:295:GLY:O	2:B:299:GLU:HG3	2.16	0.45
1:A:210:ILE:O	1:A:214:ILE:HG13	2.17	0.45
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.45
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.64	0.45
1:A:1114:PRO:O	1:A:1330:ASN:OD1	2.35	0.45
2:B:276:ILE:HD13	2:B:334:ILE:HG23	1.99	0.45
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.98	0.45
1:A:336:ILE:CD1	1:A:1405:THR:HG21	2.44	0.45
1:A:960:ILE:HD12	1:A:1021:LEU:HD21	1.99	0.45
2:B:316:PRO:HA	2:B:319:GLU:HG2	1.98	0.45
1:A:233:TRP:O	1:A:235:ILE:N	2.50	0.45
6:H:111:LEU:HA	6:H:127:GLY:O	2.17	0.45
3:C:18:VAL:O	3:C:18:VAL:HG12	2.15	0.45
9:K:61:TYR:CD1	9:K:61:TYR:C	2.89	0.45
2:B:653:VAL:C	2:B:654:ARG:HG2	2.36	0.45
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.17	0.45
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.45
4:E:147:HIS:CD2	4:E:149:LEU:H	2.35	0.45
7:I:34:TYR:O	7:I:35:VAL:HG23	2.16	0.45
2:B:1149:GLU:HG3	2:B:1153:GLU:OE1	2.17	0.45
4:E:112:TYR:CE2	4:E:134:THR:HB	2.51	0.45
1:A:1144:LYS:O	7:I:48:LEU:HD13	2.17	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.45
2:B:957:ASN:O	2:B:958:GLN:C	2.55	0.45
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.45
2:B:332:ASP:O	2:B:334:ILE:N	2.50	0.45
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.16	0.45
2:B:168:GLY:H	2:B:450:ALA:HB1	1.82	0.45
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.98	0.45
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.99	0.45
2:B:1200:ALA:O	2:B:1201:LYS:C	2.54	0.45
3:C:8:VAL:CG1	3:C:9:LYS:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.99	0.45
1:A:1153:TYR:CZ	7:I:42:LEU:HD12	2.51	0.45
1:A:55:ASP:HB3	1:A:56:PRO:HD3	1.98	0.45
1:A:541:ILE:HG12	1:A:549:MET:HE3	1.99	0.45
4:E:205:SER:O	4:E:206:GLY:C	2.54	0.45
2:B:130:VAL:CG1	2:B:131:ASP:H	2.29	0.45
3:C:148:ARG:HD3	3:C:149:LYS:H	1.83	0.45
6:H:114:VAL:O	6:H:124:ARG:HA	2.16	0.45
1:A:84:ILE:HG23	1:A:84:ILE:O	2.17	0.45
4:E:102:GLU:C	4:E:104:ASN:H	2.20	0.45
2:B:365:THR:CG2	2:B:367:LEU:H	2.30	0.45
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.47	0.45
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.98	0.45
2:B:1060:ARG:C	2:B:1062:HIS:N	2.69	0.45
2:B:519:TRP:HE1	2:B:635:ARG:HH22	1.64	0.44
1:A:821:ARG:HG2	2:B:512:ARG:O	2.17	0.44
7:I:8:ARG:HG3	7:I:9:ASP:CG	2.37	0.44
1:A:1410:PHE:C	1:A:1412:ALA:H	2.19	0.44
1:A:1049:ILE:O	1:A:1050:GLU:C	2.56	0.44
6:H:5:LEU:O	6:H:133:ASN:HB3	2.17	0.44
2:B:1169:MET:HE3	2:B:1205:GLN:HG2	1.98	0.44
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.44
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.98	0.44
2:B:185:THR:H	2:B:188:ASP:HB2	1.81	0.44
1:A:845:LEU:O	1:A:848:ILE:HG13	2.17	0.44
2:B:1038:SER:HB3	2:B:1062:HIS:NE2	2.33	0.44
10:L:61:THR:HG22	10:L:62:LYS:N	2.33	0.44
6:H:49:VAL:CG1	6:H:50:ALA:H	2.27	0.44
4:E:137:GLU:O	4:E:140:LEU:N	2.43	0.44
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	3.00	0.44
7:I:10:CYS:SG	7:I:29:CYS:SG	3.12	0.44
2:B:247:GLY:O	2:B:248:SER:HB3	2.17	0.44
3:C:166:GLU:CG	9:K:10:PHE:CZ	2.96	0.44
9:K:10:PHE:CE1	9:K:11:LEU:HD13	2.49	0.44
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.47	0.44
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.35	0.44
2:B:288:ALA:HA	2:B:331:LEU:HD13	1.99	0.44
2:B:915:THR:HG21	2:B:934:LYS:HG2	2.00	0.44
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.17	0.44
2:B:781:PHE:CE2	2:B:795:ILE:HD11	2.53	0.44
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HE2	2:B:169:ARG:HH12	1.83	0.44
1:A:829:VAL:C	1:A:831:THR:N	2.70	0.44
2:B:371:GLU:N	2:B:371:GLU:OE1	2.49	0.44
11:M:79:UNK:O	11:M:84:UNK:CA	2.65	0.44
1:A:815:PHE:O	1:A:818:MET:N	2.50	0.44
1:A:778:GLY:HA3	2:B:516:ASN:CB	2.46	0.44
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.17	0.44
7:I:106:CYS:O	7:I:107:SER:HB2	2.18	0.44
2:B:690:VAL:HG12	2:B:691:GLU:N	2.32	0.44
1:A:885:THR:HG23	1:A:893:PHE:CE1	2.36	0.44
2:B:549:THR:H	2:B:628:THR:HG22	1.81	0.44
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.53	0.44
1:A:1409:LEU:HA	1:A:1409:LEU:HD23	1.84	0.44
2:B:864:LYS:HD3	2:B:871:THR:CB	2.47	0.44
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.38	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.52	0.44
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.46	0.44
10:L:43:THR:O	10:L:43:THR:HG22	2.18	0.44
2:B:707:PRO:O	2:B:708:GLU:O	2.35	0.44
1:A:825:ILE:C	1:A:827:THR:N	2.70	0.44
1:A:78:PRO:O	1:A:79:GLY:C	2.56	0.44
4:E:138:ALA:C	4:E:140:LEU:H	2.21	0.44
1:A:1347:ALA:O	1:A:1348:LEU:C	2.55	0.44
7:I:92:ARG:CG	7:I:93:LYS:H	2.30	0.44
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.30	0.44
1:A:1415:SER:O	1:A:1416:ALA:C	2.55	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	2.00	0.44
1:A:1046:LEU:O	1:A:1047:SER:C	2.55	0.44
2:B:566:LEU:CD1	2:B:588:GLY:HA2	2.43	0.44
8:J:32:GLU:CD	8:J:32:GLU:H	2.19	0.44
4:E:185:ALA:CB	4:E:190:LEU:HD12	2.47	0.44
2:B:847:ASP:O	3:C:65:HIS:HE1	2.01	0.44
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.32	0.44
4:E:133:GLU:HB3	4:E:135:PHE:HE1	1.83	0.44
5:F:111:LEU:C	5:F:113:GLY:N	2.71	0.44
7:I:74:GLU:OE1	7:I:79:HIS:ND1	2.47	0.44
2:B:361:LEU:O	2:B:363:HIS:O	2.35	0.44
1:A:340:LEU:CD2	2:B:1200:ALA:HB2	2.46	0.44
1:A:69:THR:O	2:B:1174:LYS:HG2	2.17	0.44
6:H:84:ALA:CA	6:H:87:ARG:HB2	2.48	0.44
2:B:377:PHE:C	2:B:379:GLY:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:VAL:O	1:A:1060:PRO:HA	2.18	0.44
2:B:664:THR:HG1	2:B:678:GLU:N	2.14	0.44
1:A:54:ASN:O	1:A:55:ASP:HB2	2.18	0.44
3:C:62:PHE:C	3:C:62:PHE:HD2	2.20	0.44
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.39	0.44
2:B:230:ALA:O	2:B:232:SER:N	2.47	0.44
1:A:525:GLN:HB2	2:B:835:GLN:HG2	2.00	0.44
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.63	0.44
1:A:742:ASN:C	1:A:745:GLN:HB2	2.38	0.44
1:A:401:GLY:H	1:A:435:HIS:HD2	1.66	0.44
2:B:446:LEU:N	2:B:446:LEU:HD23	2.33	0.44
2:B:216:GLU:OE1	2:B:537:LYS:CE	2.66	0.44
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.53	0.44
1:A:881:GLN:NE2	1:A:958:VAL:O	2.46	0.44
1:A:373:THR:HG21	2:B:1105:ALA:O	2.18	0.44
2:B:642:ASP:O	2:B:643:ASP:C	2.56	0.44
1:A:901:LEU:HD13	1:A:919:ILE:CG2	2.48	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.70	0.44
6:H:57:VAL:HG12	6:H:58:THR:N	2.32	0.44
2:B:315:LYS:O	2:B:318:VAL:N	2.46	0.44
1:A:644:LYS:O	1:A:645:LEU:C	2.55	0.44
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.17	0.44
1:A:1121:GLU:O	1:A:1122:PRO:C	2.56	0.44
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.44
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.31	0.44
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.44
4:E:9:ILE:C	4:E:11:ARG:N	2.71	0.44
1:A:412:ARG:CZ	2:B:1108:ARG:NH2	2.81	0.44
2:B:1106:ARG:HG2	2:B:1107:ALA:N	2.31	0.44
9:K:24:ASP:HB3	9:K:30:ALA:CB	2.47	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:OE1	2.17	0.44
2:B:562:GLY:O	2:B:563:MET:C	2.56	0.44
2:B:1171:VAL:HG13	2:B:1191:ILE:HD13	1.99	0.44
1:A:810:PRO:C	2:B:519:TRP:HZ3	2.21	0.44
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.48	0.44
1:A:825:ILE:HD11	2:B:512:ARG:C	2.36	0.44
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.00	0.44
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.44
2:B:1159:ARG:NE	2:B:1193:GLN:NE2	2.33	0.44
2:B:1175:LEU:O	2:B:1176:ASN:CG	2.56	0.44
2:B:1103:ILE:O	2:B:1104:HIS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HG22	1:A:596:THR:N	2.33	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.32	0.44
1:A:709:THR:HG23	7:I:94:ASP:HA	2.00	0.44
9:K:78:THR:O	9:K:79:GLU:C	2.56	0.44
2:B:194:GLU:HA	2:B:194:GLU:OE1	2.18	0.44
2:B:864:LYS:HD3	2:B:871:THR:CA	2.47	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG12	2.00	0.44
1:A:968:GLN:NE2	1:A:1035:TYR:HB2	2.32	0.44
1:A:148:CYS:HB3	1:A:167:CYS:O	2.18	0.44
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.99	0.44
3:C:135:GLN:C	3:C:136:ASP:O	2.56	0.44
2:B:904:ARG:CZ	2:B:948:ILE:HD11	2.48	0.44
1:A:494:SER:HB2	1:A:497:THR:OG1	2.18	0.44
4:E:82:PHE:N	4:E:82:PHE:CD1	2.85	0.44
7:I:50:THR:HG22	7:I:52:ILE:N	2.33	0.43
2:B:274:PRO:O	2:B:276:ILE:N	2.51	0.43
4:E:7:ARG:C	4:E:9:ILE:N	2.71	0.43
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.52	0.43
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.18	0.43
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.00	0.43
1:A:306:ASN:OD1	1:A:313:GLN:NE2	2.51	0.43
10:L:38:LEU:HG	10:L:39:SER:H	1.82	0.43
1:A:458:HIS:ND1	1:A:507:VAL:HG21	2.32	0.43
3:C:9:LYS:HB2	3:C:21:ILE:HB	1.99	0.43
1:A:834:THR:HG21	1:A:1077:THR:HA	2.00	0.43
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.77	0.43
1:A:852:TYR:CE2	5:F:136:ARG:NE	2.86	0.43
2:B:1002:THR:CG2	2:B:1004:GLU:HB2	2.47	0.43
4:E:138:ALA:O	4:E:140:LEU:N	2.50	0.43
3:C:39:ALA:HA	3:C:164:ALA:CB	2.46	0.43
2:B:200:GLY:HA2	2:B:202:TYR:CD2	2.50	0.43
5:F:89:GLU:HB3	5:F:134:ILE:HD13	2.01	0.43
2:B:912:ILE:O	2:B:938:SER:CB	2.59	0.43
9:K:24:ASP:OD1	9:K:26:LYS:N	2.51	0.43
2:B:426:LYS:O	2:B:430:ARG:HG3	2.17	0.43
1:A:1068:ALA:O	1:A:1069:ALA:C	2.55	0.43
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.43
3:C:59:ALA:O	3:C:63:ILE:HG13	2.19	0.43
10:L:45:ALA:O	10:L:46:VAL:CG2	2.64	0.43
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.43
1:A:13:THR:HG23	1:A:1432:GLN:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:C	1:A:614:PHE:CD1	2.92	0.43
2:B:1118:PRO:HD3	2:B:1155:SER:HA	2.00	0.43
6:H:5:LEU:O	6:H:6:PHE:HB2	2.19	0.43
1:A:679:ILE:O	1:A:682:THR:HB	2.18	0.43
9:K:55:LYS:HD3	9:K:78:THR:OG1	2.18	0.43
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.47	0.43
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.47	0.43
3:C:8:VAL:HA	3:C:21:ILE:O	2.18	0.43
2:B:205:ILE:HG12	2:B:461:LEU:HB3	1.99	0.43
2:B:995:ARG:HH11	2:B:995:ARG:HB2	1.81	0.43
3:C:249:ASP:OD1	3:C:253:LYS:HE3	2.19	0.43
3:C:76:ASP:OD2	3:C:128:ASN:N	2.47	0.43
7:I:75:CYS:C	7:I:77:LYS:H	2.20	0.43
2:B:329:THR:O	2:B:332:ASP:HB3	2.18	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.43
2:B:202:TYR:N	2:B:202:TYR:CD2	2.87	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.71	0.43
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.51	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
1:A:633:VAL:HG11	1:A:645:LEU:HD22	2.00	0.43
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.48	0.43
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.39	0.43
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.53	0.43
1:A:1066:VAL:O	1:A:1067:LEU:C	2.56	0.43
2:B:708:GLU:C	2:B:710:LEU:N	2.72	0.43
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.52	0.43
3:C:73:GLN:HE21	3:C:75:MET:N	1.97	0.43
2:B:800:GLN:CB	8:J:52:THR:HG22	2.47	0.43
2:B:214:ALA:HB2	2:B:408:LEU:CD1	2.48	0.43
2:B:1152:MET:SD	2:B:1197:PRO:HD3	2.59	0.43
4:E:168:TYR:CB	4:E:170:LEU:HG	2.49	0.43
2:B:686:ASN:C	2:B:688:GLY:N	2.70	0.43
3:C:251:LEU:HG	9:K:98:LEU:HD11	2.01	0.43
1:A:113:LEU:HG	1:A:218:ASP:OD1	2.19	0.43
7:I:84:VAL:CG1	7:I:84:VAL:O	2.65	0.43
2:B:650:GLU:HG2	2:B:654:ARG:NH1	2.33	0.43
2:B:287:ARG:HG2	2:B:292:ILE:CA	2.27	0.43
7:I:91:ARG:HD3	7:I:91:ARG:HA	1.75	0.43
8:J:53:HIS:CE1	8:J:55:ASP:HA	2.54	0.43
1:A:1384:VAL:O	1:A:1389:PHE:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:HD13	1:A:656:TRP:CD1	2.54	0.43
1:A:535:THR:HG22	1:A:616:VAL:HA	1.98	0.43
4:E:28:TYR:CE2	4:E:64:PRO:HG3	2.53	0.43
6:H:24:CYS:CB	6:H:44:VAL:HG21	2.47	0.43
9:K:92:ASN:O	9:K:93:SER:C	2.56	0.43
4:E:114:ASN:O	4:E:115:ASN:HB3	2.18	0.43
1:A:565:ILE:HD13	1:A:567:LYS:HE2	2.01	0.43
6:H:143:LEU:N	6:H:143:LEU:HD12	2.34	0.43
2:B:955:THR:HA	10:L:54:ARG:O	2.19	0.43
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.53	0.43
2:B:487:THR:O	2:B:488:TYR:C	2.56	0.43
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.71	0.43
7:I:55:THR:HG21	7:I:109:ILE:CD1	2.48	0.43
1:A:86:LEU:HB3	1:A:296:LEU:HD21	2.00	0.43
1:A:741:ASN:HD22	1:A:743:VAL:N	2.16	0.43
2:B:806:THR:C	2:B:808:ALA:N	2.71	0.43
2:B:784:ASN:HD21	2:B:788:ARG:HD2	1.84	0.43
1:A:35:ILE:HD13	1:A:53:LEU:HD23	2.01	0.43
1:A:845:LEU:O	1:A:846:GLU:C	2.57	0.43
2:B:366:GLN:O	2:B:367:LEU:O	2.36	0.43
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.99	0.43
3:C:135:GLN:O	3:C:136:ASP:O	2.37	0.43
2:B:1204:PHE:O	2:B:1207:LEU:HB2	2.19	0.43
7:I:46:HIS:O	7:I:47:GLU:HB2	2.18	0.43
2:B:345:LYS:N	2:B:348:ARG:HE	2.15	0.43
1:A:1155:ASP:O	1:A:1190:PRO:O	2.37	0.43
2:B:1108:ARG:CG	2:B:1108:ARG:O	2.67	0.43
3:C:77:ILE:CG2	3:C:161:LYS:HE3	2.48	0.43
2:B:55:VAL:O	2:B:59:LEU:HB3	2.19	0.43
2:B:834:ASN:HB2	2:B:838:SER:O	2.19	0.43
1:A:42:ASP:OD1	1:A:45:GLN:O	2.36	0.43
1:A:446:ARG:HG2	1:A:446:ARG:NH1	2.28	0.43
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.43
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.43
1:A:131:SER:OG	1:A:132:LYS:N	2.51	0.43
1:A:774:ARG:O	1:A:775:ILE:C	2.57	0.43
1:A:562:THR:HA	1:A:563:PRO:HD3	1.92	0.43
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.13	0.43
7:I:98:VAL:CG1	7:I:99:LEU:N	2.81	0.43
8:J:9:SER:HB2	8:J:45:CYS:HB2	2.01	0.43
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.83	0.43
4:E:69:ILE:O	4:E:73:PRO:HG3	2.19	0.43
4:E:79:TRP:HD1	4:E:96:PHE:HE1	1.67	0.43
1:A:673:GLY:N	1:A:674:PRO:HD2	2.34	0.43
1:A:760:GLN:HB2	2:B:1021:MET:HE1	2.00	0.43
1:A:166:GLY:O	1:A:167:CYS:CB	2.67	0.43
2:B:794:ASN:O	2:B:795:ILE:HD12	2.19	0.43
9:K:95:ILE:O	9:K:98:LEU:HB2	2.19	0.43
2:B:666:TYR:C	2:B:668:ASP:N	2.72	0.43
2:B:101:MET:HE3	2:B:169:ARG:NH2	2.34	0.43
2:B:850:LEU:CD2	2:B:1009:ASP:HB3	2.48	0.43
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.83	0.43
1:A:639:PRO:HG2	1:A:640:GLN:H	1.84	0.43
1:A:1193:LEU:CD2	1:A:1267:MET:HE2	2.48	0.43
1:A:326:ARG:HE	1:A:1406:VAL:HG11	1.82	0.43
3:C:148:ARG:H	3:C:151:GLN:HG3	1.84	0.43
3:C:5:GLY:O	3:C:6:PRO:O	2.37	0.43
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.31	0.43
2:B:877:PRO:O	2:B:878:GLN:HG2	2.19	0.43
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.43
11:M:65:UNK:CA	11:M:78:UNK:O	2.67	0.43
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.31	0.42
1:A:901:LEU:HG	1:A:926:GLN:NE2	2.30	0.42
2:B:955:THR:CG2	10:L:54:ARG:O	2.65	0.42
1:A:48:ALA:O	1:A:49:LYS:CG	2.65	0.42
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.83	0.42
6:H:38:LEU:HD13	6:H:125:LEU:CD1	2.46	0.42
1:A:711:ARG:HA	7:I:97:MET:HE1	2.01	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.67	0.42
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.45	0.42
1:A:99:ILE:O	1:A:102:VAL:HB	2.19	0.42
2:B:546:SER:OG	2:B:631:GLY:N	2.52	0.42
1:A:760:GLN:CB	2:B:1021:MET:HE1	2.49	0.42
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.01	0.42
1:A:984:LYS:O	1:A:988:LEU:HB2	2.19	0.42
2:B:295:GLY:H	2:B:298:LEU:HG	1.84	0.42
2:B:358:LYS:O	2:B:359:GLU:OE1	2.36	0.42
1:A:814:PHE:HB2	2:B:519:TRP:CE3	2.52	0.42
2:B:705:MET:N	2:B:710:LEU:HD12	2.34	0.42
2:B:709:ASP:C	2:B:710:LEU:HD23	2.38	0.42
4:E:113:GLN:HG2	4:E:137:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:137:GLU:O	4:E:138:ALA:C	2.57	0.42
1:A:1348:LEU:CD2	1:A:1372:VAL:HG13	2.39	0.42
1:A:337:ARG:NE	1:A:839:ARG:NH2	2.66	0.42
1:A:151:ASP:OD1	1:A:163:SER:HA	2.19	0.42
1:A:451:HIS:HB2	1:A:454:SER:OG	2.19	0.42
1:A:672:ASP:O	1:A:675:THR:HB	2.19	0.42
1:A:466:SER:HB3	9:K:2:ASN:HD22	1.82	0.42
2:B:1177:HIS:O	2:B:1179:GLN:HG3	2.19	0.42
6:H:84:ALA:CB	6:H:87:ARG:HB2	2.49	0.42
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.53	0.42
2:B:702:LEU:HD22	2:B:737:THR:CG2	2.49	0.42
1:A:853:ASP:OD1	1:A:855:THR:CB	2.64	0.42
1:A:68:GLN:O	1:A:70:CYS:N	2.52	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.18	0.42
1:A:751:SER:O	1:A:752:LYS:CB	2.67	0.42
1:A:30:ILE:O	1:A:31:SER:O	2.37	0.42
2:B:806:THR:O	2:B:808:ALA:N	2.53	0.42
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.18	0.42
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.42
2:B:1177:HIS:C	2:B:1179:GLN:H	2.22	0.42
2:B:1177:HIS:O	2:B:1179:GLN:N	2.52	0.42
2:B:484:ASN:CG	2:B:486:TYR:HE1	2.23	0.42
1:A:134:ARG:O	1:A:137:ALA:N	2.52	0.42
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.00	0.42
2:B:749:LEU:HD22	2:B:753:ALA:CB	2.49	0.42
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.54	0.42
7:I:59:VAL:HG12	7:I:60:GLN:N	2.34	0.42
1:A:813:PHE:CE2	2:B:524:PRO:CG	2.97	0.42
2:B:705:MET:H	2:B:710:LEU:CD1	2.32	0.42
11:M:63:UNK:N	11:M:64:UNK:N	2.66	0.42
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.16	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.42
1:A:457:ALA:O	1:A:507:VAL:HG23	2.19	0.42
6:H:111:LEU:HD23	6:H:127:GLY:O	2.18	0.42
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.49	0.42
4:E:178:ILE:CG2	4:E:214:CYS:HA	2.48	0.42
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.55	0.42
3:C:101:LEU:HD12	3:C:101:LEU:HA	1.89	0.42
5:F:140:ASP:OD1	5:F:141:GLY:N	2.52	0.42
4:E:117:THR:C	4:E:119:SER:N	2.73	0.42
2:B:34:ILE:HG12	2:B:542:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:VAL:HG22	2:B:651:LEU:HD23	2.01	0.42
7:I:103:CYS:HG	7:I:106:CYS:HG	1.67	0.42
2:B:955:THR:HG1	10:L:55:ILE:HA	1.83	0.42
2:B:601:ARG:O	2:B:605:ARG:HG3	2.19	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.54	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:N	2.44	0.42
6:H:83:GLN:C	6:H:85:GLY:N	2.73	0.42
1:A:399:HIS:C	1:A:401:GLY:N	2.71	0.42
2:B:368:GLU:O	2:B:371:GLU:OE1	2.37	0.42
2:B:105:SER:O	2:B:106:ASP:HB2	2.20	0.42
1:A:810:PRO:HG3	2:B:745:PRO:HB2	2.01	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.52	0.42
1:A:541:ILE:N	1:A:541:ILE:HD12	2.34	0.42
2:B:1106:ARG:HH12	2:B:1118:PRO:CA	2.33	0.42
2:B:1106:ARG:HH12	2:B:1118:PRO:HA	1.85	0.42
1:A:89:PRO:HG3	1:A:208:LEU:HD12	2.00	0.42
2:B:864:LYS:CG	2:B:865:LYS:N	2.80	0.42
1:A:982:THR:HB	1:A:985:ASP:CG	2.40	0.42
10:L:27:LEU:HD13	10:L:37:LYS:CB	2.48	0.42
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.83	0.42
9:K:98:LEU:O	9:K:99:GLY:C	2.58	0.42
1:A:474:VAL:HG13	1:A:474:VAL:O	2.19	0.42
2:B:969:ARG:HG2	2:B:970:THR:N	2.33	0.42
6:H:96:VAL:HG13	6:H:143:LEU:HG	2.02	0.42
6:H:12:VAL:HG13	6:H:26:ILE:HG23	2.01	0.42
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.42
1:A:960:ILE:O	1:A:961:ARG:C	2.57	0.42
1:A:591:PHE:HD2	1:A:595:THR:HB	1.83	0.42
6:H:4:THR:O	6:H:5:LEU:HD23	2.19	0.42
1:A:709:THR:O	1:A:712:GLU:N	2.52	0.42
4:E:59:SER:HA	4:E:80:VAL:O	2.19	0.42
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.19	0.42
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.85	0.42
7:I:101:PHE:HD1	7:I:110:PHE:O	2.02	0.42
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.17	0.42
9:K:82:ASP:O	9:K:85:ASP:HB2	2.20	0.42
1:A:1152:ILE:C	7:I:43:VAL:HB	2.39	0.42
1:A:568:PRO:CB	3:C:221:TYR:CZ	3.03	0.42
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	2.20	0.42
1:A:68:GLN:C	1:A:70:CYS:N	2.73	0.42
8:J:53:HIS:CD2	8:J:54:VAL:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:CB	2:B:995:ARG:HH11	2.33	0.42
8:J:21:TYR:CA	8:J:39:LEU:HD11	2.49	0.42
1:A:866:PHE:C	1:A:867:ILE:HG13	2.40	0.42
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.55	0.42
1:A:1126:ALA:O	1:A:1128:GLN:N	2.53	0.42
1:A:725:ALA:HA	1:A:728:LYS:HE2	2.02	0.42
1:A:810:PRO:CB	2:B:705:MET:SD	3.08	0.42
2:B:542:MET:HE2	2:B:747:MET:HE2	2.01	0.42
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.49	0.42
1:A:1187:GLN:HA	1:A:1243:VAL:HG23	2.02	0.42
1:A:1192:LEU:HD11	1:A:1239:ARG:CB	2.37	0.42
2:B:54:PHE:HA	2:B:58:THR:CB	2.47	0.42
1:A:530:GLY:O	1:A:532:ARG:N	2.53	0.42
1:A:533:LYS:C	1:A:535:THR:H	2.23	0.42
1:A:751:SER:OG	2:B:1015:HIS:HE1	2.03	0.42
1:A:366:VAL:HA	1:A:367:PRO:HD2	1.81	0.42
4:E:168:TYR:O	4:E:170:LEU:HD23	2.19	0.42
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.84	0.42
9:K:93:SER:O	9:K:97:LYS:HG3	2.20	0.42
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.49	0.42
4:E:131:THR:HG21	4:E:191:LYS:HE2	2.02	0.42
2:B:887:HIS:HD2	11:M:37:UNK:O	1.47	0.42
3:C:214:ASN:CB	3:C:217:ASP:OD2	2.68	0.42
9:K:103:THR:O	9:K:106:GLU:N	2.53	0.42
4:E:19:VAL:O	4:E:19:VAL:HG12	2.20	0.42
1:A:481:ASP:C	1:A:481:ASP:OD1	2.58	0.42
2:B:346:GLU:O	2:B:347:LYS:C	2.58	0.42
1:A:80:HIS:N	1:A:243:PRO:HB3	2.34	0.42
1:A:76:GLU:O	1:A:78:PRO:CD	2.68	0.42
2:B:276:ILE:HD11	2:B:355:ILE:CD1	2.50	0.42
3:C:27:LEU:HD12	3:C:27:LEU:O	2.20	0.42
3:C:73:GLN:NE2	3:C:75:MET:H	1.97	0.42
1:A:401:GLY:N	1:A:435:HIS:HD2	2.18	0.42
2:B:879:ARG:O	2:B:880:THR:HB	2.20	0.42
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.18	0.42
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42
1:A:782:ARG:NH2	7:I:67:THR:HG22	2.34	0.42
1:A:1317:MET:CA	1:A:1322:ILE:HD11	2.46	0.42
1:A:114:LEU:HD12	1:A:142:CYS:O	2.18	0.42
9:K:71:PHE:CD1	9:K:71:PHE:C	2.93	0.42
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:ASN:OD1	2:B:500:THR:N	2.53	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.95	0.42
3:C:14:SER:HA	9:K:114:LEU:HD22	2.02	0.41
6:H:57:VAL:CG1	6:H:58:THR:N	2.83	0.41
4:E:28:TYR:CE1	4:E:78:LEU:CD1	3.03	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.34	0.41
1:A:843:LYS:HA	1:A:843:LYS:HD3	1.90	0.41
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.18	0.41
7:I:63:GLY:O	7:I:70:ARG:NH2	2.53	0.41
1:A:1349:TYR:O	1:A:1350:LYS:C	2.56	0.41
2:B:737:THR:HG23	7:I:66:PRO:HB3	2.01	0.41
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.84	0.41
1:A:14:VAL:O	1:A:15:LYS:HD3	2.20	0.41
3:C:242:GLN:O	3:C:246:ARG:N	2.52	0.41
1:A:598:LEU:HD22	6:H:25:ARG:CZ	2.50	0.41
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.85	0.41
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.34	0.41
1:A:533:LYS:C	1:A:535:THR:N	2.72	0.41
2:B:269:ILE:HB	2:B:317:CYS:SG	2.60	0.41
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.41
1:A:335:ARG:HA	1:A:335:ARG:HD3	1.87	0.41
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.01	0.41
1:A:629:LEU:CD1	1:A:645:LEU:HD21	2.48	0.41
1:A:108:MET:O	1:A:109:HIS:CB	2.66	0.41
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.34	0.41
1:A:115:LEU:HB2	1:A:122:MET:HE1	2.02	0.41
1:A:474:VAL:HG13	1:A:478:TYR:HE1	1.86	0.41
2:B:843:GLN:HB2	2:B:993:THR:OG1	2.20	0.41
8:J:34:THR:O	8:J:35:ALA:C	2.58	0.41
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.19	0.41
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.34	0.41
1:A:1438:THR:CG2	5:F:92:ARG:HD2	2.50	0.41
8:J:3:VAL:CG2	8:J:18:TRP:CG	3.02	0.41
1:A:960:ILE:HD12	1:A:1021:LEU:CD2	2.50	0.41
1:A:530:GLY:O	1:A:533:LYS:N	2.53	0.41
2:B:913:GLY:HA2	2:B:938:SER:HB2	2.02	0.41
10:L:41:SER:O	10:L:44:ASP:HB2	2.21	0.41
3:C:252:GLN:NE2	9:K:99:GLY:N	2.68	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.55	0.41
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.84	0.41
2:B:850:LEU:HD22	2:B:1009:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:35:PHE:O	9:K:70:ARG:HB2	2.21	0.41
7:I:98:VAL:HG12	7:I:99:LEU:N	2.35	0.41
2:B:120:ARG:HH12	10:L:54:ARG:NH1	2.18	0.41
8:J:52:THR:CG2	8:J:52:THR:O	2.68	0.41
1:A:419:LYS:HG2	11:M:46:UNK:O	2.19	0.41
2:B:315:LYS:O	2:B:317:CYS:N	2.53	0.41
1:A:683:ILE:O	1:A:686:ALA:N	2.53	0.41
4:E:71:LYS:C	4:E:73:PRO:HD3	2.40	0.41
2:B:880:THR:O	2:B:881:ASN:HB2	2.19	0.41
1:A:84:ILE:HG21	1:A:239:LEU:HD23	2.01	0.41
6:H:84:ALA:HA	6:H:87:ARG:CB	2.50	0.41
5:F:138:LEU:HD23	5:F:138:LEU:HA	1.82	0.41
2:B:53:GLN:HG2	2:B:547:VAL:HG13	2.02	0.41
7:I:84:VAL:HG13	7:I:84:VAL:O	2.19	0.41
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.60	0.41
2:B:435:THR:O	2:B:435:THR:HG22	2.20	0.41
2:B:199:MET:N	2:B:199:MET:SD	2.87	0.41
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.44	0.41
1:A:825:ILE:HG21	2:B:512:ARG:HG3	2.01	0.41
1:A:908:LEU:O	1:A:909:ASP:C	2.58	0.41
1:A:913:LEU:CD1	1:A:981:LEU:O	2.69	0.41
3:C:146:LYS:O	3:C:147:LEU:HD23	2.20	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:CB	2.51	0.41
6:H:139:ASN:O	6:H:140:ALA:CB	2.68	0.41
1:A:1322:ILE:HD12	1:A:1327:ILE:HD12	2.03	0.41
1:A:101:LYS:HG2	1:A:139:TRP:CZ2	2.55	0.41
1:A:134:ARG:O	1:A:136:ALA:N	2.53	0.41
2:B:171:PRO:HD2	2:B:457:LEU:HD12	2.03	0.41
10:L:28:LYS:O	10:L:29:TYR:CG	2.74	0.41
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.19	0.41
2:B:702:LEU:CD2	2:B:735:ALA:HB1	2.51	0.41
1:A:1150:SER:HB2	1:A:1195:LEU:CD2	2.49	0.41
1:A:567:LYS:CD	6:H:95:TYR:CD1	3.00	0.41
1:A:574:GLY:O	1:A:577:ILE:HG12	2.21	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.59	0.41
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.41
10:L:34:CYS:HG	10:L:51:CYS:HG	1.57	0.41
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.20	0.41
4:E:100:ILE:O	4:E:101:GLN:C	2.58	0.41
1:A:760:GLN:OE1	2:B:1021:MET:HE2	2.20	0.41
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.50	0.41
7:I:25:LEU:HD12	7:I:26:LEU:N	2.35	0.41
1:A:756:ILE:CG2	1:A:757:ASN:N	2.80	0.41
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.34	0.41
1:A:738:LYS:HZ1	3:C:194:GLU:CA	2.33	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.20	0.41
3:C:29:MET:O	3:C:30:ALA:C	2.58	0.41
1:A:810:PRO:HG3	2:B:745:PRO:CB	2.51	0.41
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.41
1:A:1149:ALA:CB	7:I:47:GLU:N	2.75	0.41
10:L:55:ILE:H	10:L:55:ILE:HG12	1.53	0.41
7:I:7:CYS:HB2	7:I:14:LEU:CD2	2.34	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.57	0.41
1:A:344:ARG:O	2:B:1118:PRO:HD2	2.20	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.41
1:A:928:LEU:O	1:A:929:LEU:C	2.59	0.41
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.60	0.41
1:A:1293:SER:OG	1:A:1294:PRO:CD	2.68	0.41
7:I:16:PRO:HA	7:I:26:LEU:O	2.20	0.41
5:F:138:LEU:HB3	5:F:139:PRO:CD	2.51	0.41
9:K:46:ILE:CG2	9:K:50:LEU:HD12	2.51	0.41
1:A:1098:VAL:O	1:A:1099:PRO:C	2.59	0.41
2:B:1115:THR:CG2	2:B:1199:ALA:HB2	2.50	0.41
1:A:441:PRO:HG2	1:A:441:PRO:O	2.20	0.41
1:A:783:THR:HG21	1:A:815:PHE:HZ	1.19	0.41
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.56	0.41
1:A:825:ILE:CD1	2:B:512:ARG:C	2.89	0.41
2:B:175:ARG:CG	2:B:175:ARG:HH11	2.34	0.41
1:A:403:LYS:O	1:A:404:TYR:O	2.39	0.41
4:E:3:GLN:HG3	4:E:5:ASN:H	1.85	0.41
2:B:911:ILE:HD11	2:B:941:LEU:CB	2.50	0.41
1:A:302:THR:O	1:A:313:GLN:NE2	2.54	0.41
1:A:223:GLY:O	1:A:1415:SER:CA	2.64	0.41
2:B:1152:MET:O	2:B:1156:ASP:O	2.39	0.41
3:C:31:ASN:O	3:C:32:SER:C	2.56	0.41
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.03	0.41
4:E:13:TRP:O	4:E:16:PHE:HB3	2.21	0.41
9:K:106:GLU:O	9:K:110:ASN:ND2	2.54	0.41
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.51	0.41
1:A:765:VAL:HG12	1:A:766:GLY:N	2.35	0.41
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:50:THR:HG22	7:I:52:ILE:HG23	1.99	0.41
1:A:1150:SER:HG	7:I:44:TYR:HE2	1.45	0.41
1:A:542:GLU:OE1	1:A:569:LYS:HE2	2.20	0.41
1:A:79:GLY:C	1:A:243:PRO:HG3	2.41	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.56	0.41
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	3.03	0.41
1:A:598:LEU:HD22	6:H:25:ARG:HH12	1.83	0.41
2:B:418:LYS:O	2:B:420:LEU:N	2.54	0.41
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.21	0.41
1:A:535:THR:O	1:A:536:LEU:C	2.59	0.41
2:B:941:LEU:HD21	2:B:946:ASN:HA	2.02	0.41
2:B:911:ILE:HG21	2:B:966:VAL:HG11	2.01	0.41
2:B:778:MET:HE3	2:B:1094:ARG:HD3	2.00	0.41
1:A:894:GLU:C	1:A:896:ARG:N	2.74	0.41
1:A:458:HIS:CE1	1:A:507:VAL:CG2	3.00	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.66	0.41
1:A:367:PRO:CB	1:A:466:SER:HA	2.47	0.41
2:B:1020:ARG:O	2:B:1021:MET:C	2.58	0.41
2:B:872:GLU:HA	2:B:915:THR:O	2.21	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.56	0.41
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.89	0.41
6:H:138:GLU:HG2	6:H:139:ASN:N	2.35	0.41
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.51	0.41
2:B:205:ILE:CD1	2:B:205:ILE:N	2.84	0.41
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.51	0.41
2:B:240:ILE:C	2:B:253:THR:HG23	2.41	0.41
2:B:380:TYR:O	2:B:384:ARG:HG2	2.21	0.41
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.85	0.41
4:E:116:ILE:CG2	4:E:117:THR:N	2.84	0.41
2:B:578:THR:HG23	2:B:622:LYS:C	2.41	0.41
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	2.01	0.41
1:A:568:PRO:HB3	3:C:221:TYR:OH	2.21	0.41
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.34	0.41
1:A:379:VAL:HG22	1:A:431:LYS:HG2	2.03	0.41
2:B:121:ASN:HD21	2:B:965:LYS:HE3	1.86	0.41
9:K:47:ARG:HH11	9:K:48:ALA:N	2.19	0.41
1:A:443:LEU:HD22	1:A:455:MET:CE	2.48	0.41
2:B:205:ILE:HG21	2:B:462:ALA:HB2	2.03	0.41
2:B:901:PRO:O	2:B:949:VAL:O	2.38	0.41
7:I:6:PHE:HD2	7:I:13:MET:HA	1.86	0.41
1:A:810:PRO:CG	2:B:705:MET:SD	3.06	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:PRO:O	2:B:708:GLU:C	2.59	0.40
1:A:1149:ALA:CA	7:I:47:GLU:H	2.33	0.40
10:L:60:ARG:CG	10:L:61:THR:N	2.62	0.40
1:A:909:ASP:OD1	1:A:910:PRO:HD2	2.21	0.40
2:B:350:GLN:O	2:B:351:TYR:C	2.59	0.40
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.86	0.40
2:B:818:PRO:HG3	8:J:54:VAL:HG21	2.03	0.40
3:C:66:ARG:NH2	8:J:3:VAL:O	2.54	0.40
1:A:871:ASP:CB	4:E:204:THR:CG2	2.99	0.40
1:A:980:ASP:OD2	1:A:1039:LYS:HB3	2.21	0.40
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.36	0.40
2:B:627:PHE:O	2:B:632:ARG:NH1	2.54	0.40
1:A:225:ASN:C	1:A:227:VAL:N	2.71	0.40
2:B:185:THR:N	2:B:188:ASP:HB2	2.36	0.40
9:K:21:ILE:HG12	9:K:33:ILE:HG12	2.03	0.40
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.62	0.40
1:A:18:GLN:O	2:B:1215:ARG:HG3	2.21	0.40
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.36	0.40
1:A:432:VAL:O	1:A:434:ARG:N	2.54	0.40
1:A:784:LEU:HD12	1:A:811:GLN:HB3	2.03	0.40
2:B:120:ARG:HH22	10:L:54:ARG:HD2	1.86	0.40
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.47	0.40
2:B:284:ILE:HG12	2:B:324:ILE:HD12	2.03	0.40
4:E:7:ARG:HG3	4:E:8:ASN:N	2.36	0.40
1:A:14:VAL:HB	1:A:1430:LEU:HD13	2.02	0.40
2:B:244:LEU:HB2	2:B:249:ARG:HA	2.03	0.40
2:B:51:PHE:O	2:B:54:PHE:N	2.54	0.40
6:H:126:GLU:N	6:H:130:ARG:HH12	2.19	0.40
1:A:331:GLY:O	1:A:332:LYS:O	2.39	0.40
4:E:90:VAL:HA	4:E:120:ALA:HB2	2.04	0.40
1:A:921:GLY:O	1:A:922:ASP:C	2.59	0.40
1:A:1107:VAL:CG2	1:A:1383:SER:HA	2.51	0.40
1:A:203:SER:O	1:A:207:ILE:HG12	2.21	0.40
3:C:153:LEU:HD12	3:C:153:LEU:HA	1.91	0.40
1:A:719:VAL:HG22	1:A:774:ARG:HD2	2.03	0.40
2:B:704:ALA:HB2	2:B:738:PHE:CD1	2.56	0.40
1:A:244:PRO:O	1:A:245:PRO:C	2.59	0.40
2:B:167:ILE:O	2:B:168:GLY:O	2.38	0.40
2:B:549:THR:HG22	2:B:550:ASP:N	2.36	0.40
1:A:1436:ILE:CG2	2:B:1142:GLY:HA2	2.51	0.40
2:B:363:HIS:O	2:B:364:ILE:CG1	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.94	0.40
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.57	0.40
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	2.04	0.40
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.85	0.40
1:A:808:LEU:HD12	1:A:808:LEU:N	2.35	0.40
2:B:283:VAL:HG13	2:B:297:ILE:HD12	2.03	0.40
1:A:19:PHE:HA	2:B:1213:THR:O	2.22	0.40
1:A:1107:VAL:HG23	1:A:1383:SER:HA	2.03	0.40
6:H:117:SER:HA	6:H:122:LEU:HD23	2.02	0.40
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.39	0.40
2:B:583:ASN:HD21	2:B:628:THR:CB	2.28	0.40
2:B:1117:GLN:NE2	2:B:1156:ASP:OD2	2.54	0.40
5:F:109:VAL:HG12	5:F:110:ASP:H	1.82	0.40
1:A:88:LYS:HD2	1:A:293:GLU:OE1	2.20	0.40
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.51	0.40
1:A:113:LEU:C	1:A:115:LEU:H	2.23	0.40
1:A:650:GLN:O	1:A:651:LYS:C	2.58	0.40
2:B:484:ASN:ND2	2:B:486:TYR:HD1	2.19	0.40
7:I:34:TYR:C	7:I:35:VAL:HG23	2.41	0.40
4:E:116:ILE:HG22	4:E:117:THR:N	2.36	0.40
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.20	0.40
1:A:1006:ILE:HG22	1:A:1007:ILE:N	2.36	0.40
2:B:495:LEU:HA	2:B:495:LEU:HD23	1.86	0.40
4:E:136:ASN:OD1	4:E:136:ASN:C	2.60	0.40
2:B:737:THR:O	2:B:738:PHE:C	2.60	0.40
1:A:569:LYS:NZ	3:C:221:TYR:O	2.40	0.40
1:A:1116:LEU:CD2	1:A:1316:VAL:HG21	2.51	0.40
7:I:99:LEU:HB2	7:I:112:SER:OG	2.21	0.40
7:I:99:LEU:O	7:I:111:THR:HG23	2.21	0.40
3:C:66:ARG:HB3	8:J:5:VAL:HG21	2.04	0.40
2:B:801:LYS:HE2	8:J:51:LEU:O	2.22	0.40
1:A:531:ILE:CG2	1:A:532:ARG:N	2.84	0.40
2:B:992:ILE:CD1	2:B:994:TYR:CE2	3.04	0.40
6:H:82:PRO:HB2	6:H:83:GLN:H	1.78	0.40
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.50	0.40
1:A:477:PRO:CG	1:A:521:MET:HG2	2.52	0.40
1:A:1158:PRO:HB3	1:A:1241:ARG:HH12	1.84	0.40
9:K:92:ASN:C	9:K:94:ILE:N	2.75	0.40
1:A:1394:THR:CG2	1:A:1398:MET:CE	3.00	0.40
1:A:848:ILE:HG23	1:A:864:ILE:HD12	2.03	0.40
1:A:1378:GLN:O	1:A:1380:GLY:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.96	0.40
4:E:72:PHE:CD1	4:E:72:PHE:N	2.89	0.40

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1362/1733 (79%)	1020 (75%)	252 (18%)	90 (7%)	1	25
2	B	1077/1224 (88%)	836 (78%)	172 (16%)	69 (6%)	2	26
3	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	2	27
4	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	35
5	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	4	39
6	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	9
7	I	114/122 (93%)	90 (79%)	15 (13%)	9 (8%)	1	19
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	2	26
9	K	112/120 (93%)	96 (86%)	16 (14%)	0	100	100
10	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3459/4173 (83%)	2647 (76%)	587 (17%)	225 (6%)	1	26

All (225) Ramachandran outliers are listed below:

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

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1205/1520 (79%)	1128 (94%)	77 (6%)	22	61
2	B	952/1061 (90%)	886 (93%)	66 (7%)	19	59
3	C	234/274 (85%)	222 (95%)	12 (5%)	29	67
4	E	196/197 (100%)	189 (96%)	7 (4%)	42	75
5	F	74/137 (54%)	68 (92%)	6 (8%)	15	52
6	H	117/128 (91%)	112 (96%)	5 (4%)	35	71
7	I	113/116 (97%)	104 (92%)	9 (8%)	15	53
8	J	60/65 (92%)	56 (93%)	4 (7%)	20	59
9	K	99/102 (97%)	90 (91%)	9 (9%)	12	46
10	L	40/57 (70%)	35 (88%)	5 (12%)	6	31
All	All	3090/3657 (84%)	2890 (94%)	200 (6%)	21	60

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1380/1733 (79%)	0.05	37 (2%) 58 48	47, 179, 269, 300	0
2	B	1097/1224 (89%)	0.13	46 (4%) 40 31	26, 192, 280, 300	0
3	C	266/318 (83%)	-0.05	4 (1%) 76 67	45, 168, 245, 293	0
4	E	214/215 (99%)	0.14	13 (6%) 25 18	76, 206, 284, 300	0
5	F	84/155 (54%)	0.03	1 (1%) 81 73	61, 160, 231, 277	0
6	H	133/146 (91%)	0.43	6 (4%) 37 29	119, 207, 300, 300	0
7	I	118/122 (96%)	0.90	21 (17%) 2 3	133, 246, 300, 300	0
8	J	65/70 (92%)	-0.03	0 100 100	76, 169, 231, 270	0
9	K	114/120 (95%)	-0.12	1 (0%) 85 80	72, 155, 241, 274	0
10	L	46/70 (65%)	0.78	7 (15%) 3 4	129, 222, 288, 300	0
11	M	0/86	-	-	-	-
All	All	3517/4259 (82%)	0.12	136 (3%) 43 34	26, 186, 278, 300	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	26	THR	9.1
2	B	919	SER	8.3
10	L	25	ALA	8.0
2	B	881	ASN	6.7
7	I	41	PRO	6.5
1	A	1176	LEU	5.4
1	A	1175	SER	5.3
1	A	1125	ALA	5.2
2	B	882	THR	5.1
1	A	170	THR	5.1
2	B	366	GLN	5.1
7	I	74	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLY	4.7
6	H	83	GLN	4.5
1	A	60	SER	4.4
2	B	729	ILE	4.4
2	B	866	TYR	4.3
7	I	118	ARG	3.9
2	B	133	LYS	3.9
1	A	153	PRO	3.9
1	A	313	GLN	3.9
4	E	51	GLY	3.8
6	H	146	ARG	3.8
1	A	44	THR	3.8
10	L	50	ASP	3.8
7	I	8	ARG	3.7
7	I	116	ASN	3.7
7	I	40	SER	3.6
4	E	52	ARG	3.6
2	B	715	ALA	3.6
2	B	868	MET	3.5
2	B	164	LYS	3.5
2	B	733	HIS	3.5
4	E	93	MET	3.4
2	B	359	GLU	3.4
7	I	119	THR	3.4
2	B	432	MET	3.4
2	B	880	THR	3.4
2	B	722	ASP	3.3
2	B	877	PRO	3.3
2	B	734	HIS	3.3
2	B	730	ARG	3.3
2	B	437	GLU	3.2
2	B	869	SER	3.2
1	A	424	ILE	3.2
1	A	1126	ALA	3.2
1	A	1232	ASN	3.2
7	I	102	VAL	3.2
2	B	345	LYS	3.2
7	I	42	LEU	3.1
2	B	723	VAL	3.1
4	E	97	VAL	3.1
4	E	53	PRO	3.1
2	B	435	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	132	VAL	3.0
4	E	2	ASP	3.0
2	B	918	ILE	3.0
2	B	1173	ALA	2.9
1	A	88	LYS	2.9
7	I	73	ARG	2.9
3	C	267	GLN	2.9
7	I	2	THR	2.9
1	A	1172	LEU	2.9
2	B	732	SER	2.8
2	B	428	ILE	2.8
2	B	134	LYS	2.8
1	A	144	THR	2.8
1	A	419	LYS	2.8
1	A	152	VAL	2.8
1	A	428	TYR	2.8
10	L	27	LEU	2.7
7	I	43	VAL	2.7
2	B	90	ILE	2.7
7	I	76	PRO	2.7
6	H	35	GLN	2.7
7	I	84	VAL	2.7
10	L	37	LYS	2.6
2	B	865	LYS	2.6
7	I	110	PHE	2.6
1	A	141	LEU	2.6
1	A	821	ARG	2.6
2	B	358	LYS	2.6
1	A	1231	ASP	2.6
1	A	49	LYS	2.6
7	I	57	GLY	2.6
4	E	50	MET	2.6
1	A	171	GLN	2.5
2	B	714	GLU	2.5
2	B	466	TRP	2.5
2	B	678	GLU	2.5
2	B	477	ALA	2.5
2	B	724	ASP	2.5
1	A	421	ALA	2.5
2	B	725	PRO	2.5
1	A	420	ARG	2.4
4	E	116	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
6	H	85	GLY	2.4
2	B	569	TYR	2.4
2	B	467	GLY	2.4
4	E	121	MET	2.4
4	E	88	VAL	2.4
7	I	81	ARG	2.4
4	E	118	PRO	2.4
1	A	53	LEU	2.3
7	I	120	GLN	2.3
3	C	268	ASP	2.3
1	A	50	ILE	2.3
10	L	45	ALA	2.3
2	B	870	ILE	2.3
2	B	512	ARG	2.3
5	F	104	ASN	2.3
1	A	115	LEU	2.2
1	A	1169	ILE	2.2
10	L	38	LEU	2.2
7	I	34	TYR	2.2
6	H	110	ASP	2.2
1	A	223	GLY	2.2
2	B	735	ALA	2.2
2	B	893	LEU	2.2
1	A	149	GLU	2.2
1	A	1153	TYR	2.2
7	I	9	ASP	2.1
7	I	83	ASN	2.1
1	A	280	GLU	2.1
1	A	199	LEU	2.1
9	K	74	ARG	2.1
1	A	1236	LEU	2.1
6	H	84	ALA	2.1
1	A	114	LEU	2.1
3	C	215	GLU	2.1
2	B	92	PHE	2.1
1	A	314	ALA	2.1
4	E	29	PHE	2.0
3	C	106	GLU	2.0
2	B	247	GLY	2.0
4	E	100	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
12	ZN	I	203	1/1	0.45	0.62	0.17	166,166,166,166	0
12	ZN	A	1735	1/1	0.89	0.12	-1.03	166,166,166,166	0
12	ZN	C	319	1/1	0.98	0.15	-1.05	166,166,166,166	0
12	ZN	A	1734	1/1	0.92	0.11	-1.72	166,166,166,166	0
12	ZN	J	101	1/1	0.99	0.14	-1.76	166,166,166,166	0
12	ZN	L	105	1/1	0.95	0.10	-2.00	175,175,175,175	0
12	ZN	I	204	1/1	0.84	0.09	-2.19	166,166,166,166	0
12	ZN	B	1307	1/1	0.93	0.13	-	166,166,166,166	0
12	ZN	M	209	1/1	0.36	0.27	-	156,156,156,156	0
13	MG	A	1736	1/1	0.88	0.39	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.