



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SFO
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COMPLEX
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-02-20
Resolution : 3.61 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

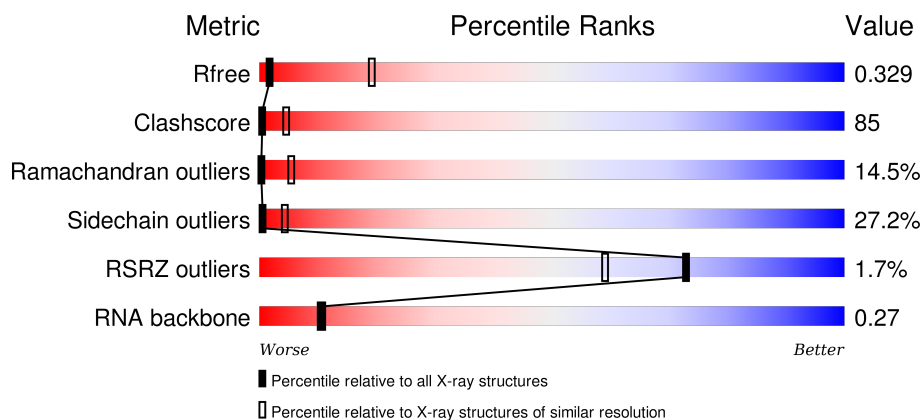
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)
RNA backbone	2183	1058 (4.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	R	10	<div> <div>20%</div> <div>40%</div> <div>40%</div> <div>20%</div> </div>
2	T	14	<div> <div>29%</div> <div>50%</div> <div>43%</div> <div>7%</div> </div>
3	A	1733	<div> <div>%</div> <div>12%</div> <div>39%</div> <div>23%</div> <div>6%</div> <div>20%</div> </div>
4	B	1224	<div> <div>%</div> <div>15%</div> <div>48%</div> <div>21%</div> <div>6%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	318	
6	E	215	
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28647 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 RNA chain called RNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1106	Total	C	N	O	S	0	0	0
			8793	5568	1538	1632	55			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

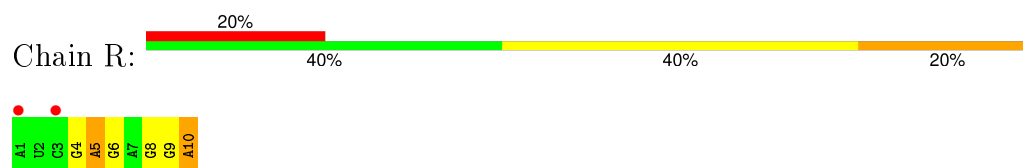
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

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

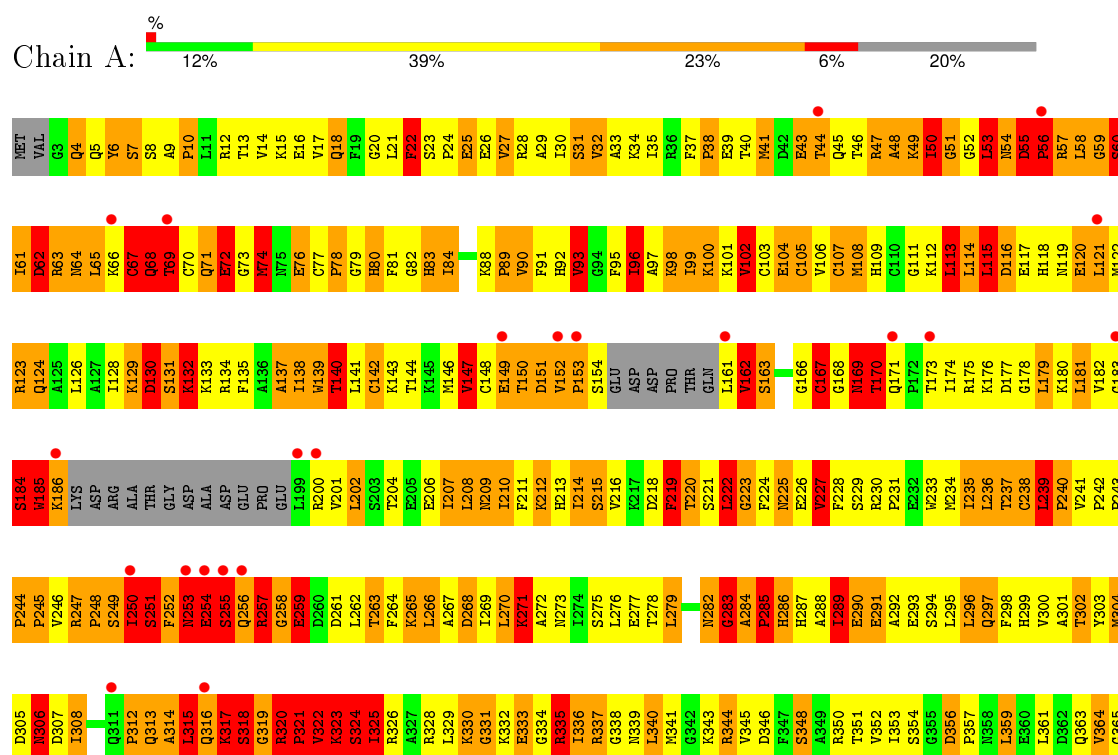
• Molecule 1: RNA STRAND



• Molecule 2: DNA STRAND



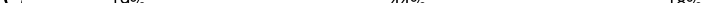
• Molecule 3: DNA-directed RNA polymerase II largest subunit

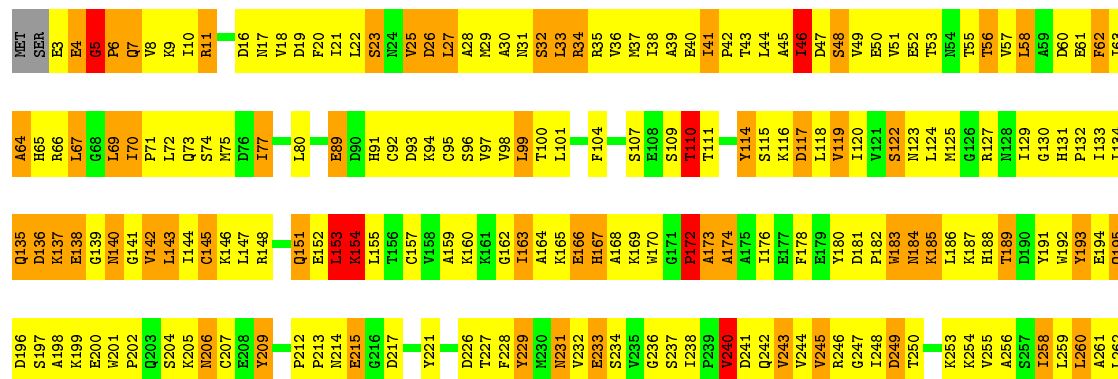


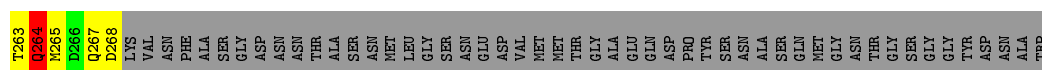
E1307	L1254	A1125	V1064	M1004	D939	E979	M818		K687	B618	D587	S494	W430	F367
T1308	E1255	A1126	G1065	E1005	R940	R980	G819	S751	K688	H619	G588	E495	K431	F368
D1309	E1256	L1127	V1066	L1086	R941	Q881	G820	K752	K689	H620	V589	E496	V432	K368
G1310	D1257	Q1128	L1067	I1007	F942	S882	R821	F753	V690	T621	V590	T497	E433	S369
V1311	P1190	Q1129	A1068	E1108	L943	L383	G823	S754	L691	V622	P561	R498	R434	L370
M1312	W1191	Q1130	A1069	M1009	R944	D884	G824	F755	D692		T562	A499	H435	L374
L1313	L1192	L1132	Q1070	A1010	E945	T885	L824	L756	V693		P563	E500	L436	T375
S1314	L1193	K1132		Q1011	E946	T886	L825		T694		A564	E501	M437	T376
E1315	L1194	L1133	G1073	R1012	F947	G887	D826		R695	L629	V566	L504	D438	
E1316	I1195	I1134	E1074	D1013		G888	T827	A759	E696		K567	C505	P441	F377
M1317	E1196	P1075	P1076	A1014	A952	S889	A828		E697		P568	A506	V442	V379
T1318	D1257	P1076	T1077	V1015	N953	D890	R829	G764	Q698	V633	K569	A507	L443	V380
V1319	L1197	S1136	A1077	L1016	K954	A891	K830	V765	A699	T634	P570		F444	T381
P1320	D1198	I1138	Q1078	L1037	P855	A892	T831		R700					P382
G1321	A1200	M1079	Q1078	F1018	L956	F993	A832	Q768	L702	P639	L571	T511	N445	
L1322	H1140	T1080	T1080	C1019	P957	E994	E833	Q769	L702		W572	V512	R446	V383
D1323	M1202	T1141	L1081	L1020	V958	K895	T834	Q770		Q640	S573	S513	Q447	N384
P1324	N1203	T1142	ASN	C1021	N959	R896	G835	E771	K705	V641	G574	P514	P448	T385
T1325	D1264	L1143	THR	L1022	T960	X897	X836		H706	C642	K575	O515	S449	D386
R1326	M1265	V1146	PHE	R1023	R861	R898	I837	R774	G707	A643	Q576	S516	L450	R387
T1327	D1206	H1S	HIS	S1024	R962	R999	Q838	I775	T709		L577	H517	H451	T388
M1328	L1207	T1147	PHE	R1025	L963	D900	R839	A776	T709	L645	S578	P519	K452	T389
T1329	T1208	I1148	ALA	L1026	L964	L901	R840	F777	L710		S579		M453	Q390
E1330	M1209	A1149	GLY	A1027	Q965	L902	L841	G778	R712		V580	E520	S454	L391
M1331	G1210	S1150	VAL	T1028	N966	L903	V842	F779	E711	N648	A581	N521	M455	
F1332	Q1211	E1151	ALA	R1029	A967	T904	K843	V780	S713	Q650	I582	G522	M456	N394
T1333	T1212	I1152	SER	R1030	Q968	D905	A844	D781	F714		P583			G395
L1334	G1213	Y1153	K1092	V1031	Q969	H906	L845	R782	L721	V652		V524	A457	F396
M1335	R1214	Y1154	K1093	L1032	T970	T907	E846	T783	L716	V653	I586	G525	H458	N397
M1336	R1215	D1155	V1094	Q1033	F971	L908	D847	L784	N717	N654	H587	D526	V462	E398
E1337	P1156	P1156	L1095	E1034	R872	D909	I848	T785	V718	P655	L588	T527	L463	R399
V1338	D1157	S1096	S1096	Y1035	L973	P910	M849	H786	V719	H656	Q589	L528	P464	P400
L1339	Q1218	G1097	G1097	R1036	S911	S911		F787	R720		R590	G529	Y465	G401
G1340	T1219	R1159	V1098	L1037	D974	L912	Y852	K789	F721	L658	F591	E530	S466	A402
E1342	F1220	R1160	P1099	T1038	P978	L913	D853		L722		D592	L531	K403	
L1343	K1221	T1161	R1100	K1039	S979	E914	N854		N723	N860	E593	R532	R469	V404
A1343	N1222	V1162	L1101	Q1040	D880	S915	T855	Y792	E724	G661	G594	K533	L470	V405
M1283	D1223	I1163	K1102	A1041	L981	G916	T856	S793	A725	P662	T595	L534	M471	T406
R1344	L1224	P1164	E1103	F1042	T982	S917	R857	F794	R726		T596	L536	L472	R407
A1346	F1225	E1165	L1104	D1043	L983	E918	N858	E795	D727	G665	L587	L536	S473	D408
L1347	V1226	D1166	L1105	V1044	K984	L919	S859	S796	R728				V474	S409
E1287	V1227	E1167	N1106	V1045	D985	L920	L860		K738	G667	S599	D538	T475	
D1288	V1228	E1168	V1107	L1047	L986	G921	G861	V600	A729		P600	T539	S476	R412
R1289	S1229	I1169	A1108	S1047	V987	D922	N862	E901	L732	T669	K601	F540	P477	T413
K1290	E1230	I1170	K1109	M1048	L988	L923	V863	N802	A733		D602	L541	Y478	D414
V1291	Q1171	M1110	M1110	I1049	G989	K924	I864	S803	E734	A671	N603	E542	M479	L415
P1292	L1172	M1111	E1050	E1050	V990	L925	Q865	Y804	V735	D672	M604	D543	R416	L416
N1293	D1233	K1112	A1051	K991	K991	Q926	F866	L805	N736	G673	M605	D544	D481	Y417
V1355	E1234	F1174	T1113	Q1052	D992	V927	I867	R606	L737	P674	L606	O545	F482	S418
L1356	K1235	S1175	P1114	F1053	L993	L928	V868	G907	K738	T675	I607	V546	D483	K419
A1357	L1236	L1176	S1115	L1054	Q994	L929	G869	L808	D739	H676	I608	L547	G484	R420
S1358	I1237	L1116	L1116	R1055	E995	D930	E870	T809	L740		D609	N548	D485	R421
D1359	ASP	T1117	T1117	S1056	N996	E931	D871	P810	N741	T679	G610	N549	E486	A422
	GLU	GLU	GLU	V1057	L997	E932	G872	Q811	N742	T680	Q611	L550	M487	D423
Y1362	C1240	GLU	L1119	V1058	L998	K933	M873	P812	V743	D681	I613	N551	N488	R424
E1363	ALA	ALA	Y1120	H1059	V999	K934	D874	F813	K744	T682	T612	N552	L489	Q425
M1364	GLU	E1121	E1121	P1060	L1000	Q935	A875	P814	Q745	T683	P614	V553	H490	L426
T1365	GLN	P1122	P1122	G1061	R1001	L936	A876	P815	M746	A684	G615	P554	V491	Q427
L1366	ARG	SER	G1123	E1062	K1002	V937	H877	H816	V747	B685	V616	P555	P492	Y428
H1367	PHE	H1124	H1124	M1063	K1003	K938	I878	A817	M748	A686	V617	N556	Q493	G429



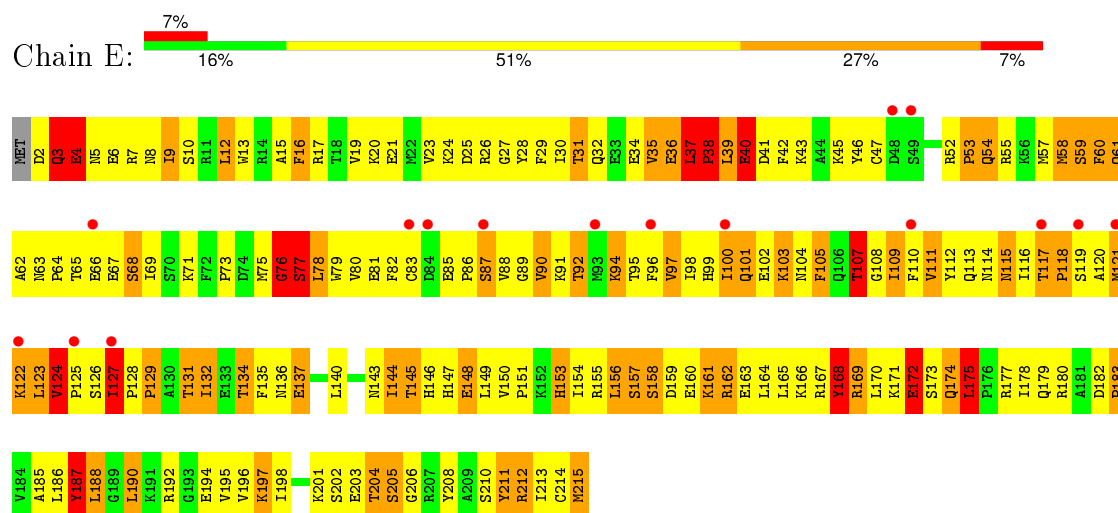


Chain C:  19% 44% 18% • 16%

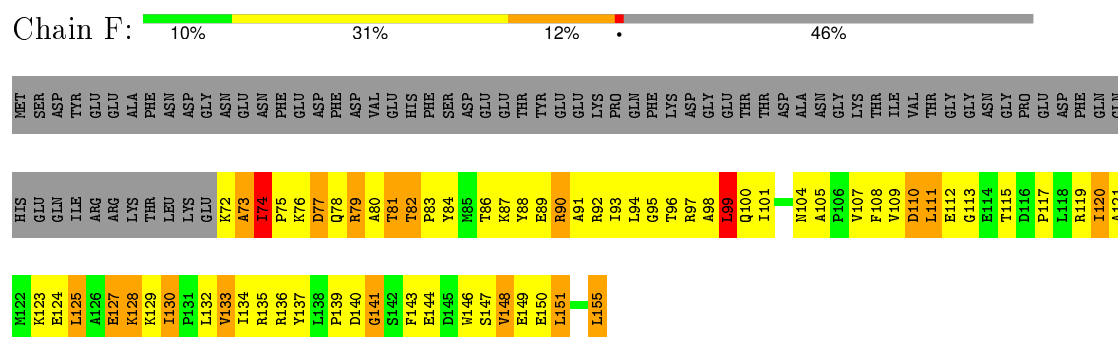




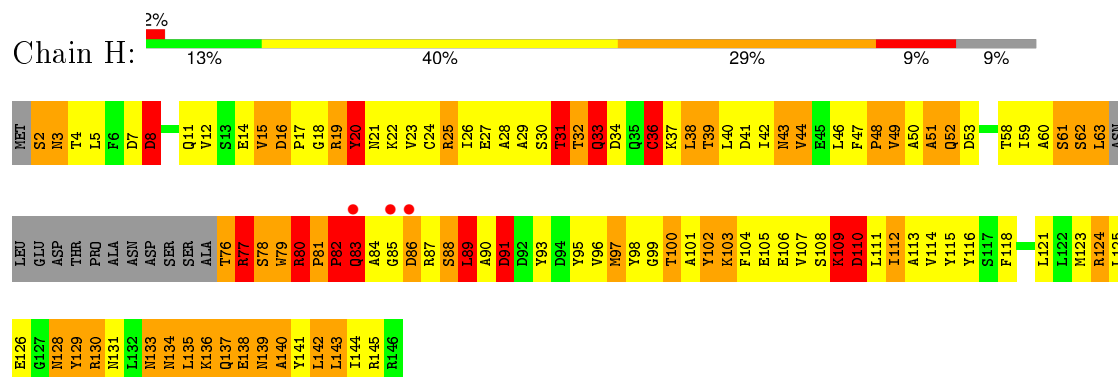
- Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



- Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



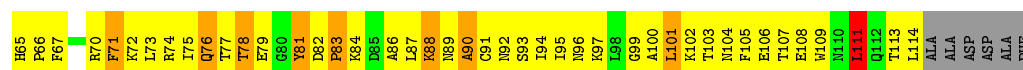
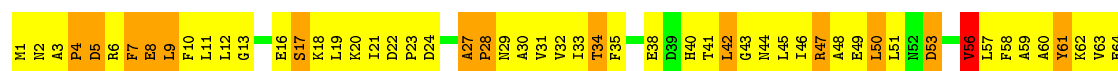
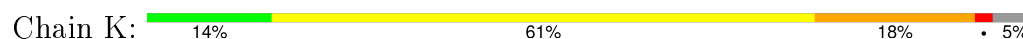
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide



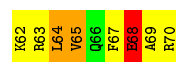
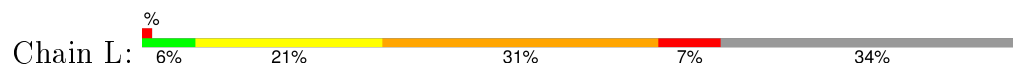
- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.08Å 221.26Å 193.69Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	39.86 – 3.61 39.86 – 3.60	Depositor EDS
% Data completeness (in resolution range)	92.7 (39.86-3.61) 92.7 (39.86-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.315 , 0.343 0.309 , 0.329	Depositor DCC
R_{free} test set	7393 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 80020 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	28647	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	R	0.67	0/244	0.83	0/380
2	T	0.75	0/311	1.39	3/477 (0.6%)
3	A	0.88	15/11163 (0.1%)	1.45	167/15091 (1.1%)
4	B	0.84	7/8964 (0.1%)	1.38	114/12086 (0.9%)
5	C	0.78	0/2133	1.24	13/2891 (0.4%)
6	E	0.90	2/1788 (0.1%)	1.40	14/2406 (0.6%)
7	F	0.83	0/691	1.28	7/933 (0.8%)
8	H	0.85	1/1086 (0.1%)	1.59	20/1470 (1.4%)
9	I	1.03	2/989 (0.2%)	1.64	23/1331 (1.7%)
10	J	0.78	0/541	1.44	7/727 (1.0%)
11	K	0.74	0/937	1.20	5/1265 (0.4%)
12	L	0.99	1/366 (0.3%)	1.78	12/485 (2.5%)
All	All	0.86	28/29213 (0.1%)	1.41	385/39542 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	5
3	A	1	6
4	B	0	7
5	C	0	2
6	E	0	1
9	I	0	1
All	All	1	22

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	319	GLY	C-O	10.97	1.41	1.23
3	A	255	SER	CA-CB	8.59	1.65	1.52
3	A	320	ARG	CA-CB	8.38	1.72	1.53
3	A	320	ARG	CG-CD	7.83	1.71	1.51
4	B	595	ARG	CG-CD	7.49	1.70	1.51
3	A	185	TRP	CB-CG	7.02	1.62	1.50
6	E	4	GLU	CB-CG	7.00	1.65	1.52
4	B	595	ARG	CB-CG	6.96	1.71	1.52
3	A	90	VAL	CB-CG1	-6.79	1.38	1.52
3	A	277	GLU	CB-CG	6.79	1.65	1.52
3	A	320	ARG	C-N	6.75	1.47	1.34
6	E	172	GLU	CB-CG	6.31	1.64	1.52
3	A	323	LYS	N-CA	6.26	1.58	1.46
3	A	1255	GLU	CB-CG	6.26	1.64	1.52
8	H	79	TRP	CB-CG	-5.94	1.39	1.50
12	L	68	GLU	CB-CG	5.80	1.63	1.52
3	A	255	SER	CB-OG	5.78	1.49	1.42
9	I	4	PHE	CB-CG	-5.57	1.41	1.51
4	B	1224	PHE	CB-CG	5.49	1.60	1.51
4	B	315	LYS	CB-CG	5.42	1.67	1.52
4	B	275	TYR	CB-CG	5.37	1.59	1.51
9	I	29	CYS	CB-SG	5.32	1.91	1.82
4	B	431	TYR	CD1-CE1	5.20	1.47	1.39
3	A	67	CYS	CB-SG	5.19	1.91	1.82
3	A	1315	GLU	CB-CG	5.15	1.61	1.52
3	A	1280	GLU	CB-CG	5.05	1.61	1.52
4	B	223	VAL	CB-CG2	-5.02	1.42	1.52
3	A	325	ILE	N-CA	5.02	1.56	1.46

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	321	PRO	N-CA-C	-18.56	63.84	112.10
3	A	322	VAL	N-CA-C	14.54	150.26	111.00
10	J	10	CYS	CA-CB-SG	12.01	135.61	114.00
3	A	315	LEU	CA-CB-CG	11.82	142.50	115.30
4	B	478	GLY	N-CA-C	-11.76	83.71	113.10
3	A	821	ARG	N-CA-C	-11.71	79.39	111.00
4	B	431	TYR	N-CA-C	-11.40	80.23	111.00
3	A	259	GLU	N-CA-C	11.33	141.58	111.00
9	I	78	CYS	CA-CB-SG	11.17	134.10	114.00
4	B	637	LEU	N-CA-C	10.98	140.64	111.00
4	B	647	GLY	N-CA-C	10.76	140.01	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	322	VAL	CB-CA-C	-10.69	91.10	111.40
3	A	258	GLY	N-CA-C	10.58	139.54	113.10
9	I	120	GLN	N-CA-C	10.58	139.56	111.00
4	B	635	ARG	N-CA-C	10.53	139.44	111.00
3	A	320	ARG	CA-CB-CG	-10.52	90.26	113.40
4	B	479	VAL	N-CA-C	-9.91	84.24	111.00
4	B	69	LEU	N-CA-C	9.64	137.03	111.00
4	B	868	MET	N-CA-C	-9.34	85.79	111.00
9	I	78	CYS	N-CA-CB	-9.19	94.05	110.60
3	A	257	ARG	N-CA-C	8.96	135.18	111.00
3	A	283	GLY	N-CA-C	8.96	135.49	113.10
3	A	55	ASP	N-CA-C	8.95	135.15	111.00
3	A	316	GLN	CB-CA-C	8.87	128.14	110.40
9	I	79	HIS	N-CA-C	8.87	134.96	111.00
3	A	170	THR	N-CA-C	8.79	134.73	111.00
3	A	249	SER	N-CA-C	8.66	134.38	111.00
3	A	121	LEU	N-CA-C	-8.55	87.91	111.00
9	I	75	CYS	N-CA-C	-8.44	88.20	111.00
4	B	468	GLU	N-CA-C	8.44	133.79	111.00
6	E	205	SER	N-CA-C	-8.42	88.26	111.00
8	H	137	GLN	N-CA-C	8.34	133.52	111.00
3	A	53	LEU	CA-CB-CG	8.32	134.45	115.30
3	A	1172	LEU	N-CA-C	8.25	133.28	111.00
3	A	1000	LEU	CA-CB-CG	-8.23	96.38	115.30
3	A	78	PRO	N-CA-C	-8.18	90.83	112.10
4	B	484	ASN	N-CA-C	-8.17	88.93	111.00
4	B	893	LEU	CA-CB-CG	8.15	134.05	115.30
4	B	230	ALA	C-N-CD	-8.14	102.68	120.60
4	B	430	ARG	N-CA-C	8.13	132.96	111.00
8	H	16	ASP	N-CA-C	8.12	132.92	111.00
9	I	8	ARG	N-CA-C	-8.06	89.24	111.00
3	A	317	LYS	C-N-CA	7.99	141.68	121.70
3	A	251	SER	N-CA-C	7.99	132.57	111.00
4	B	370	PHE	N-CA-C	-7.97	89.48	111.00
3	A	43	GLU	N-CA-C	-7.93	89.59	111.00
4	B	475	SER	N-CA-C	-7.93	89.59	111.00
4	B	212	LEU	CA-CB-CG	-7.91	97.12	115.30
4	B	168	GLY	N-CA-C	7.89	132.82	113.10
8	H	80	ARG	N-CA-C	-7.88	89.73	111.00
4	B	981	ALA	N-CA-C	7.88	132.26	111.00
5	C	89	GLU	N-CA-C	-7.87	89.75	111.00
4	B	712	PRO	N-CA-C	-7.84	91.70	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	LEU	CA-CB-CG	-7.84	97.27	115.30
3	A	1176	LEU	CA-CB-CG	7.83	133.31	115.30
3	A	254	GLU	C-N-CA	7.83	141.26	121.70
3	A	1111	MET	N-CA-C	7.80	132.07	111.00
8	H	133	ASN	N-CA-C	7.79	132.05	111.00
3	A	223	GLY	N-CA-C	7.71	132.38	113.10
3	A	324	SER	N-CA-C	7.71	131.81	111.00
3	A	183	GLY	N-CA-C	7.67	132.26	113.10
3	A	102	VAL	CB-CA-C	-7.66	96.84	111.40
8	H	85	GLY	N-CA-C	-7.63	94.02	113.10
3	A	163	SER	N-CA-C	7.62	131.59	111.00
3	A	318	SER	N-CA-C	-7.62	90.43	111.00
10	J	64	ASN	N-CA-C	7.60	131.52	111.00
3	A	317	LYS	N-CA-C	7.57	131.43	111.00
4	B	941	LEU	CA-CB-CG	7.57	132.70	115.30
3	A	895	LYS	CD-CE-NZ	7.49	128.93	111.70
4	B	492	LEU	CA-CB-CG	-7.45	98.16	115.30
4	B	54	PHE	N-CA-C	-7.43	90.95	111.00
3	A	536	LEU	CA-CB-CG	7.42	132.37	115.30
3	A	98	LYS	N-CA-C	-7.40	91.02	111.00
4	B	1223	ASP	N-CA-C	7.38	130.92	111.00
3	A	173	THR	N-CA-C	-7.34	91.17	111.00
3	A	253	ASN	N-CA-C	7.30	130.71	111.00
8	H	100	THR	N-CA-C	-7.29	91.32	111.00
3	A	890	ASP	N-CA-C	-7.29	91.33	111.00
3	A	1392	SER	N-CA-C	7.28	130.66	111.00
4	B	1154	ALA	N-CA-C	-7.25	91.41	111.00
4	B	296	GLU	N-CA-C	-7.25	91.44	111.00
4	B	1221	SER	N-CA-C	7.24	130.53	111.00
6	E	157	SER	N-CA-C	7.23	130.51	111.00
4	B	275	TYR	CA-CB-CG	7.22	127.11	113.40
4	B	247	GLY	N-CA-C	7.22	131.14	113.10
4	B	706	GLN	N-CA-C	-7.22	91.52	111.00
4	B	43	LEU	CA-CB-CG	-7.21	98.73	115.30
3	A	532	ARG	N-CA-C	7.20	130.43	111.00
3	A	239	LEU	CA-CB-CG	7.16	131.78	115.30
4	B	276	ILE	CB-CA-C	-7.15	97.29	111.60
3	A	1067	LEU	CA-CB-CG	-7.15	98.86	115.30
3	A	50	ILE	CB-CA-C	-7.13	97.34	111.60
3	A	1081	LEU	CA-CB-CG	7.12	131.67	115.30
4	B	181	LEU	CA-CB-CG	-7.12	98.93	115.30
3	A	316	GLN	C-N-CA	7.11	139.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	39	LEU	CA-CB-CG	-7.11	98.95	115.30
4	B	595	ARG	NE-CZ-NH1	7.11	123.85	120.30
3	A	330	LYS	N-CA-C	7.10	130.18	111.00
4	B	838	SER	N-CA-C	-7.10	91.84	111.00
8	H	121	LEU	N-CA-C	-7.09	91.87	111.00
4	B	167	ILE	CB-CA-C	-7.07	97.47	111.60
9	I	10	CYS	CA-CB-SG	7.04	126.68	114.00
12	L	57	LEU	CA-CB-CG	-7.03	99.13	115.30
8	H	134	ASN	N-CA-C	-7.00	92.08	111.00
9	I	10	CYS	N-CA-C	6.99	129.87	111.00
8	H	83	GLN	N-CA-C	-6.98	92.14	111.00
3	A	81	PHE	N-CA-C	6.98	129.84	111.00
3	A	316	GLN	CA-CB-CG	-6.97	98.06	113.40
12	L	60	ARG	N-CA-C	-6.97	92.19	111.00
3	A	179	LEU	CA-CB-CG	6.93	131.23	115.30
3	A	531	ILE	N-CA-C	-6.92	92.33	111.00
4	B	473	MET	CA-C-N	-6.90	102.01	117.20
4	B	474	SER	N-CA-C	-6.90	92.36	111.00
5	C	167	HIS	N-CA-C	-6.89	92.41	111.00
4	B	99	LYS	N-CA-C	-6.87	92.46	111.00
4	B	21	GLU	N-CA-C	6.86	129.53	111.00
12	L	41	SER	N-CA-C	6.84	129.47	111.00
9	I	77	LYS	C-N-CA	6.81	138.72	121.70
3	A	1269	GLU	N-CA-C	6.79	129.33	111.00
3	A	1311	VAL	N-CA-C	6.77	129.28	111.00
5	C	7	GLN	N-CA-C	6.76	129.26	111.00
3	A	236	LEU	CA-CB-CG	-6.73	99.82	115.30
3	A	550	LEU	CA-CB-CG	6.72	130.76	115.30
3	A	1229	SER	N-CA-C	-6.68	92.96	111.00
3	A	1207	LEU	N-CA-C	6.66	128.97	111.00
3	A	284	ALA	N-CA-C	6.65	128.96	111.00
3	A	236	LEU	N-CA-C	6.65	128.95	111.00
4	B	868	MET	CG-SD-CE	6.65	110.83	100.20
4	B	1128	LEU	CA-CB-CG	-6.64	100.02	115.30
7	F	151	LEU	CA-CB-CG	-6.64	100.03	115.30
4	B	265	SER	N-CA-C	6.62	128.86	111.00
3	A	451	HIS	CB-CA-C	-6.61	97.19	110.40
3	A	93	VAL	N-CA-C	6.60	128.82	111.00
4	B	95	ILE	N-CA-C	-6.57	93.26	111.00
4	B	764	SER	C-N-CD	6.56	142.18	128.40
4	B	250	PHE	CB-CG-CD1	-6.55	116.21	120.80
4	B	702	LEU	CA-CB-CG	-6.54	100.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5	ASN	N-CA-C	-6.53	93.38	111.00
3	A	254	GLU	CB-CA-C	6.51	123.43	110.40
4	B	431	TYR	CA-CB-CG	6.51	125.78	113.40
10	J	64	ASN	C-N-CD	-6.51	106.27	120.60
3	A	1285	MET	CA-CB-CG	6.50	124.34	113.30
9	I	55	THR	N-CA-C	-6.49	93.49	111.00
9	I	26	LEU	N-CA-C	6.47	128.48	111.00
3	A	908	LEU	CA-CB-CG	6.46	130.17	115.30
4	B	335	GLY	N-CA-C	-6.46	96.95	113.10
3	A	896	ARG	N-CA-C	6.46	128.43	111.00
3	A	978	PRO	N-CA-C	6.43	128.81	112.10
4	B	981	ALA	CA-C-N	-6.43	103.06	117.20
3	A	286	HIS	N-CA-C	6.42	128.32	111.00
3	A	254	GLU	CA-C-N	-6.41	103.10	117.20
4	B	461	LEU	CA-CB-CG	-6.39	100.59	115.30
3	A	533	LYS	CA-CB-CG	6.39	127.46	113.40
3	A	120	GLU	N-CA-C	6.39	128.25	111.00
3	A	974	ASP	N-CA-C	6.34	128.13	111.00
3	A	1256	GLU	N-CA-C	6.33	128.09	111.00
3	A	315	LEU	CB-CG-CD2	-6.33	100.25	111.00
3	A	973	ILE	N-CA-C	6.32	128.05	111.00
3	A	222	LEU	CA-CB-CG	6.30	129.80	115.30
4	B	37	PHE	N-CA-C	-6.30	93.98	111.00
4	B	429	PHE	N-CA-C	-6.29	94.01	111.00
4	B	723	VAL	CB-CA-C	-6.29	99.45	111.40
4	B	637	LEU	CA-C-N	-6.29	103.37	117.20
3	A	318	SER	N-CA-CB	6.28	119.93	110.50
4	B	884	ARG	N-CA-C	-6.27	94.07	111.00
4	B	636	PRO	CA-N-CD	-6.27	102.72	111.50
3	A	710	LEU	CA-CB-CG	6.27	129.71	115.30
3	A	320	ARG	C-N-CD	-6.26	106.82	120.60
11	K	16	GLU	N-CA-C	-6.26	94.09	111.00
3	A	1405	THR	N-CA-C	6.26	127.90	111.00
4	B	723	VAL	N-CA-C	6.25	127.87	111.00
4	B	323	VAL	N-CA-C	-6.24	94.16	111.00
6	E	12	LEU	CA-CB-CG	-6.23	100.97	115.30
8	H	109	LYS	CA-C-N	-6.23	103.50	117.20
4	B	330	ALA	N-CA-C	-6.21	94.23	111.00
3	A	588	LEU	CA-CB-CG	-6.20	101.05	115.30
4	B	432	MET	N-CA-C	6.20	127.74	111.00
4	B	252	SER	N-CA-C	6.20	127.73	111.00
8	H	31	THR	N-CA-C	-6.18	94.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	53	PRO	C-N-CA	-6.17	106.26	121.70
11	K	20	LYS	N-CA-C	-6.16	94.37	111.00
4	B	473	MET	CB-CA-C	6.16	122.71	110.40
3	A	1445	ILE	N-CA-C	6.15	127.61	111.00
3	A	289	ILE	N-CA-C	-6.15	94.40	111.00
9	I	118	ARG	CB-CA-C	-6.13	98.14	110.40
3	A	398	GLU	N-CA-C	-6.12	94.47	111.00
4	B	1168	LEU	N-CA-C	6.12	127.52	111.00
4	B	473	MET	CB-CG-SD	6.11	130.73	112.40
7	F	105	ALA	N-CA-C	-6.09	94.54	111.00
3	A	7	SER	N-CA-C	-6.08	94.57	111.00
4	B	250	PHE	N-CA-C	-6.08	94.58	111.00
3	A	547	LEU	CA-CB-CG	-6.08	101.32	115.30
9	I	74	GLU	N-CA-C	-6.08	94.59	111.00
6	E	54	GLN	CA-CB-CG	-6.08	100.03	113.40
8	H	110	ASP	N-CA-CB	-6.07	99.67	110.60
6	E	107	THR	N-CA-C	6.06	127.36	111.00
4	B	1096	ARG	N-CA-C	-6.06	94.65	111.00
4	B	222	ILE	CA-C-N	-6.05	103.89	117.20
8	H	62	SER	N-CA-C	6.04	127.32	111.00
3	A	67	CYS	N-CA-C	-6.04	94.69	111.00
9	I	18	GLU	N-CA-C	6.03	127.27	111.00
12	L	44	ASP	N-CA-C	-6.02	94.75	111.00
4	B	68	THR	N-CA-C	6.00	127.19	111.00
3	A	152	VAL	N-CA-C	5.99	127.18	111.00
5	C	109	SER	N-CA-C	5.98	127.14	111.00
3	A	1121	GLU	N-CA-C	-5.98	94.86	111.00
3	A	906	HIS	CB-CA-C	-5.97	98.46	110.40
2	T	3	DG	N9-C1'-C2'	-5.97	101.26	112.60
12	L	49	LYS	C-N-CA	5.96	136.59	121.70
9	I	118	ARG	N-CA-C	5.94	127.04	111.00
3	A	1053	PHE	N-CA-C	-5.94	94.97	111.00
3	A	257	ARG	CG-CD-NE	5.93	124.26	111.80
4	B	511	PRO	N-CA-C	5.93	127.51	112.10
3	A	740	LEU	CA-CB-CG	-5.93	101.67	115.30
3	A	702	LEU	CA-CB-CG	5.92	128.92	115.30
4	B	1184	GLY	N-CA-C	-5.92	98.30	113.10
4	B	250	PHE	CB-CG-CD2	5.91	124.94	120.80
2	T	6	DC	N1-C1'-C2'	-5.88	101.42	112.60
4	B	638	PHE	N-CA-CB	5.88	121.19	110.60
4	B	222	ILE	C-N-CA	5.88	136.40	121.70
4	B	1066	SER	N-CA-C	5.88	126.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	161	LEU	CA-CB-CG	5.88	128.81	115.30
3	A	1381	LEU	N-CA-C	-5.87	95.14	111.00
3	A	590	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	A	708	MET	CA-CB-CG	5.87	123.28	113.30
3	A	895	LYS	CA-CB-CG	5.86	126.30	113.40
3	A	1094	VAL	N-CA-C	5.86	126.81	111.00
5	C	139	GLY	N-CA-C	5.85	127.73	113.10
5	C	173	ALA	N-CA-C	5.85	126.80	111.00
3	A	177	ASP	N-CA-C	-5.84	95.22	111.00
4	B	648	HIS	N-CA-C	5.82	126.72	111.00
3	A	227	VAL	N-CA-C	5.82	126.71	111.00
4	B	638	PHE	CB-CA-C	-5.81	98.78	110.40
3	A	569	LYS	N-CA-C	-5.80	95.33	111.00
3	A	4	GLN	N-CA-C	-5.80	95.35	111.00
3	A	320	ARG	CB-CA-C	5.79	121.98	110.40
4	B	276	ILE	N-CA-C	5.79	126.63	111.00
3	A	249	SER	C-N-CA	5.78	136.16	121.70
3	A	315	LEU	CB-CA-C	-5.78	99.21	110.20
3	A	1155	ASP	N-CA-C	-5.78	95.40	111.00
3	A	340	LEU	CA-CB-CG	-5.76	102.05	115.30
5	C	183	TRP	N-CA-C	-5.76	95.45	111.00
3	A	568	PRO	N-CA-C	5.72	126.97	112.10
10	J	3	VAL	C-N-CA	-5.72	97.99	122.00
3	A	285	PRO	N-CA-C	5.71	126.95	112.10
4	B	1166	CYS	CA-CB-SG	5.69	124.25	114.00
3	A	1005	GLU	N-CA-C	5.69	126.36	111.00
3	A	1391	ARG	CG-CD-NE	5.68	123.73	111.80
6	E	175	LEU	CA-CB-CG	5.66	128.31	115.30
2	T	7	DC	N1-C1'-C2'	-5.65	101.87	112.60
3	A	152	VAL	C-N-CD	-5.64	108.19	120.60
3	A	993	LEU	N-CA-C	-5.64	95.77	111.00
4	B	431	TYR	CB-CA-C	5.63	121.67	110.40
7	F	77	ASP	CB-CA-C	-5.62	99.16	110.40
11	K	81	TYR	CA-CB-CG	5.60	124.04	113.40
12	L	52	GLY	N-CA-C	5.60	127.10	113.10
4	B	865	LYS	CD-CE-NZ	5.59	124.57	111.70
7	F	130	ILE	C-N-CD	-5.58	108.31	120.60
3	A	22	PHE	N-CA-C	5.58	126.06	111.00
7	F	127	GLU	N-CA-C	-5.58	95.94	111.00
8	H	133	ASN	CB-CA-C	-5.58	99.25	110.40
3	A	1017	LEU	CA-CB-CG	-5.56	102.51	115.30
4	B	1157	ALA	N-CA-C	-5.56	95.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	197	LYS	N-CA-C	-5.55	96.01	111.00
9	I	58	VAL	N-CA-C	-5.53	96.06	111.00
4	B	132	VAL	N-CA-C	5.53	125.93	111.00
3	A	60	SER	N-CA-C	5.52	125.92	111.00
4	B	305	VAL	N-CA-C	5.50	125.84	111.00
3	A	67	CYS	CA-CB-SG	5.49	123.89	114.00
9	I	5	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	A	972	HIS	C-N-CA	5.48	135.41	121.70
4	B	326	ASP	N-CA-C	5.48	125.80	111.00
3	A	391	LEU	CA-CB-CG	5.48	127.90	115.30
8	H	20	TYR	CB-CA-C	-5.48	99.45	110.40
12	L	58	LYS	N-CA-C	5.48	125.79	111.00
4	B	744	HIS	C-N-CD	-5.46	108.58	120.60
3	A	980	ASP	CB-CA-C	5.45	121.30	110.40
6	E	76	GLY	N-CA-C	5.45	126.72	113.10
5	C	153	LEU	N-CA-C	-5.45	96.30	111.00
4	B	473	MET	CA-CB-CG	-5.44	104.05	113.30
8	H	128	ASN	N-CA-C	5.44	125.69	111.00
3	A	321	PRO	N-CA-CB	-5.44	96.62	102.60
3	A	130	ASP	N-CA-C	5.43	125.67	111.00
4	B	637	LEU	O-C-N	5.42	131.37	122.70
4	B	427	ASP	N-CA-C	-5.42	96.38	111.00
3	A	1283	VAL	N-CA-C	5.41	125.61	111.00
7	F	99	LEU	CA-CB-CG	5.41	127.75	115.30
3	A	50	ILE	N-CA-C	5.41	125.61	111.00
3	A	113	LEU	N-CA-C	-5.41	96.41	111.00
3	A	1122	PRO	N-CA-C	5.40	126.14	112.10
4	B	764	SER	N-CA-C	5.40	125.58	111.00
9	I	36	GLU	CA-CB-CG	5.40	125.28	113.40
4	B	223	VAL	N-CA-CB	-5.39	99.63	111.50
4	B	711	GLU	C-N-CD	-5.39	108.73	120.60
5	C	154	LYS	CD-CE-NZ	5.39	124.11	111.70
4	B	646	LEU	CA-CB-CG	5.39	127.70	115.30
11	K	111	LEU	CA-CB-CG	5.39	127.70	115.30
4	B	253	THR	N-CA-C	5.38	125.53	111.00
3	A	181	LEU	CA-CB-CG	-5.37	102.95	115.30
9	I	78	CYS	N-CA-C	5.37	125.48	111.00
4	B	591	ARG	N-CA-C	-5.35	96.56	111.00
3	A	58	LEU	CA-CB-CG	5.34	127.59	115.30
3	A	256	GLN	C-N-CA	5.34	135.06	121.70
4	B	636	PRO	CA-C-N	-5.34	105.45	117.20
3	A	316	GLN	CA-C-N	-5.34	105.46	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1270	ASN	N-CA-C	-5.34	96.59	111.00
3	A	56	PRO	N-CA-C	5.33	125.97	112.10
9	I	49	ILE	N-CA-C	-5.33	96.61	111.00
3	A	888	GLY	N-CA-C	5.32	126.40	113.10
4	B	634	TYR	C-N-CA	-5.32	108.41	121.70
9	I	11	ASN	N-CA-CB	5.32	120.17	110.60
7	F	74	ILE	C-N-CD	-5.31	108.91	120.60
10	J	5	VAL	N-CA-C	-5.31	96.66	111.00
12	L	30	ILE	N-CA-C	-5.31	96.66	111.00
3	A	317	LYS	CA-C-N	-5.31	105.53	117.20
3	A	380	VAL	CB-CA-C	-5.31	101.32	111.40
5	C	217	ASP	CB-CG-OD1	-5.31	113.53	118.30
3	A	599	SER	C-N-CD	5.30	139.53	128.40
3	A	901	LEU	CA-CB-CG	-5.29	103.12	115.30
4	B	1180	PHE	N-CA-C	5.29	125.28	111.00
12	L	39	SER	N-CA-C	-5.29	96.72	111.00
4	B	1193	GLN	N-CA-C	-5.28	96.73	111.00
8	H	110	ASP	N-CA-C	-5.28	96.74	111.00
12	L	27	LEU	CA-CB-CG	5.28	127.44	115.30
10	J	2	ILE	N-CA-C	5.27	125.23	111.00
3	A	1289	ARG	N-CA-C	5.27	125.23	111.00
4	B	1192	TYR	N-CA-C	5.27	125.22	111.00
4	B	595	ARG	CB-CG-CD	5.26	125.29	111.60
3	A	74	MET	N-CA-C	5.25	125.17	111.00
3	A	253	ASN	C-N-CA	5.24	134.79	121.70
3	A	252	PHE	CA-C-N	-5.23	105.69	117.20
4	B	883	LEU	N-CA-C	5.23	125.11	111.00
3	A	918	GLU	N-CA-C	-5.21	96.93	111.00
3	A	1227	ILE	CB-CA-C	-5.21	101.19	111.60
4	B	854	LEU	CA-CB-CG	-5.20	103.34	115.30
4	B	167	ILE	N-CA-C	-5.19	96.98	111.00
10	J	10	CYS	N-CA-CB	-5.19	101.27	110.60
3	A	481	ASP	N-CA-CB	5.18	119.93	110.60
3	A	1112	LYS	N-CA-C	5.18	125.00	111.00
6	E	53	PRO	N-CA-C	5.18	125.58	112.10
3	A	867	ILE	CB-CA-C	-5.18	101.23	111.60
3	A	1278	ASN	N-CA-C	5.18	124.99	111.00
4	B	901	PRO	N-CA-C	5.17	125.55	112.10
4	B	239	GLU	CA-CB-CG	5.16	124.76	113.40
8	H	141	TYR	N-CA-C	-5.16	97.06	111.00
4	B	707	PRO	N-CA-C	-5.16	98.69	112.10
5	C	5	GLY	N-CA-C	5.16	125.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	17	ARG	CG-CD-NE	-5.16	100.97	111.80
5	C	9	LYS	N-CA-C	-5.15	97.09	111.00
3	A	384	ASN	N-CA-C	5.14	124.88	111.00
12	L	41	SER	N-CA-CB	-5.14	102.79	110.50
3	A	250	ILE	N-CA-C	5.14	124.88	111.00
3	A	1313	LEU	N-CA-C	-5.14	97.12	111.00
4	B	461	LEU	CB-CG-CD1	-5.14	102.27	111.00
6	E	132	ILE	CG1-CB-CG2	5.13	122.69	111.40
3	A	255	SER	CB-CA-C	5.13	119.84	110.10
3	A	147	VAL	CB-CA-C	-5.12	101.67	111.40
4	B	61	ASP	CB-CA-C	-5.12	100.16	110.40
9	I	3	THR	CA-CB-CG2	-5.12	105.23	112.40
3	A	417	TYR	N-CA-C	-5.12	97.19	111.00
3	A	1109	LYS	N-CA-C	-5.12	97.19	111.00
4	B	510	LYS	N-CA-C	5.12	124.81	111.00
3	A	1294	PRO	N-CA-C	-5.11	98.81	112.10
3	A	1127	ASP	N-CA-C	-5.11	97.20	111.00
4	B	1214	PRO	N-CA-C	-5.11	98.83	112.10
8	H	62	SER	N-CA-CB	-5.10	102.85	110.50
11	K	56	VAL	CB-CA-C	-5.09	101.72	111.40
3	A	1002	GLY	N-CA-C	5.09	125.83	113.10
3	A	1403	GLU	N-CA-C	5.09	124.74	111.00
3	A	254	GLU	CA-CB-CG	-5.08	102.23	113.40
4	B	122	LEU	CA-CB-CG	5.08	126.98	115.30
4	B	238	ALA	N-CA-C	-5.08	97.29	111.00
3	A	602	ASP	N-CA-C	-5.07	97.30	111.00
8	H	36	CYS	N-CA-C	5.07	124.69	111.00
4	B	888	GLY	N-CA-C	5.07	125.76	113.10
6	E	192	ARG	N-CA-C	-5.07	97.32	111.00
3	A	1285	MET	CB-CG-SD	5.06	127.59	112.40
4	B	578	THR	N-CA-C	-5.05	97.35	111.00
5	C	217	ASP	CB-CG-OD2	5.04	122.84	118.30
3	A	115	LEU	CA-CB-CG	5.04	126.89	115.30
3	A	878	ILE	N-CA-C	5.02	124.56	111.00
3	A	154	SER	N-CA-C	5.02	124.55	111.00
3	A	447	GLN	C-N-CD	5.01	138.93	128.40
3	A	137	ALA	N-CA-C	-5.00	97.49	111.00
12	L	48	CYS	CA-CB-SG	5.00	123.01	114.00

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	A	322	VAL	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1035	TYR	Sidechain
3	A	320	ARG	Mainchain
3	A	322	VAL	Mainchain
3	A	376	TYR	Sidechain
3	A	6	TYR	Sidechain
3	A	814	PHE	Sidechain
4	B	250	PHE	Sidechain
4	B	275	TYR	Sidechain
4	B	431	TYR	Sidechain
4	B	636	PRO	Mainchain
4	B	638	PHE	Sidechain
4	B	797	TYR	Sidechain
4	B	798	TYR	Sidechain
5	C	114	TYR	Sidechain
5	C	209	TYR	Sidechain
6	E	187	TYR	Sidechain
9	I	4	PHE	Sidechain
2	T	10	DT	Sidechain
2	T	11	DC	Sidechain
2	T	13	DA	Sidechain
2	T	6	DC	Sidechain
2	T	8	DT	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	217	0	110	18	0
2	T	279	0	160	43	0
3	A	10969	0	11070	2106	0
4	B	8793	0	8823	1592	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2095	0	2051	337	0
6	E	1752	0	1776	303	0
7	F	679	0	701	127	0
8	H	1068	0	1040	193	0
9	I	971	0	929	162	0
10	J	532	0	542	125	0
11	K	919	0	929	175	0
12	L	364	0	387	65	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28647	0	28518	4856	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 85.

All (4856) 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)
3:A:853:ASP:OD1	3:A:855:THR:HB	1.32	1.25
3:A:90:VAL:HG12	3:A:297:GLN:NE2	1.49	1.24
4:B:635:ARG:HB2	4:B:636:PRO:CD	1.65	1.21
3:A:321:PRO:O	3:A:322:VAL:HG22	1.41	1.18
3:A:351:THR:HG23	4:B:1103:ILE:HD12	1.23	1.18
3:A:61:ILE:O	3:A:63:ARG:N	1.78	1.17
3:A:312:PRO:O	3:A:313:GLN:HG3	1.44	1.16
4:B:477:ALA:HB3	4:B:479:VAL:HG22	1.21	1.16
3:A:855:THR:HG21	3:A:857:ARG:HE	1.11	1.16
3:A:67:CYS:O	3:A:70:CYS:HB3	1.39	1.16
4:B:1175:LEU:O	4:B:1176:ASN:HB2	1.40	1.16
2:T:2:DC:H2'	2:T:3:DG:C8	1.82	1.15
4:B:174:LEU:HD22	4:B:204:ILE:HD11	1.20	1.15
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	1.87	1.14
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.13	1.14
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.19	1.14
4:B:120:ARG:HD2	4:B:955:THR:HG21	1.22	1.14
4:B:635:ARG:CB	4:B:636:PRO:HD3	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:471:LYS:HG3	4:B:472:ALA:H	0.97	1.14
3:A:899:VAL:HG12	3:A:929:LEU:HD12	1.27	1.14
3:A:913:LEU:CD1	3:A:914:GLU:H	1.59	1.13
6:E:52:ARG:HB3	6:E:53:PRO:HD2	1.23	1.13
5:C:3:GLU:HG3	5:C:4:GLU:H	1.01	1.13
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.26	1.13
4:B:955:THR:HG22	4:B:956:THR:H	1.07	1.13
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.63	1.13
7:F:155:LEU:H	7:F:155:LEU:HD23	1.04	1.12
3:A:278:THR:O	3:A:278:THR:HG22	1.50	1.12
3:A:913:LEU:HD12	3:A:914:GLU:N	1.64	1.11
5:C:22:LEU:CD2	5:C:25:VAL:HG21	1.80	1.11
3:A:892:ALA:HA	3:A:895:LYS:HB2	1.20	1.11
4:B:167:ILE:HG23	4:B:424:LEU:HD13	1.14	1.10
3:A:1161:THR:HG22	3:A:1163:ILE:H	0.96	1.10
3:A:320:ARG:HD2	3:A:320:ARG:H	0.99	1.10
4:B:882:THR:HG21	4:B:935:ARG:HA	1.30	1.10
4:B:474:SER:HA	4:B:476:ARG:HG3	1.29	1.10
10:J:43:ARG:HG3	10:J:46:CYS:HB2	1.32	1.09
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.10	1.09
4:B:1171:VAL:HG12	4:B:1172:ILE:H	1.14	1.09
4:B:549:THR:HG22	4:B:550:ASP:H	0.99	1.09
4:B:658:ILE:HA	4:B:661:LEU:HD12	1.35	1.09
4:B:471:LYS:HG3	4:B:472:ALA:N	1.63	1.09
3:A:630:ILE:HD12	3:A:630:ILE:H	1.15	1.09
4:B:711:GLU:H	4:B:712:PRO:HD3	1.05	1.08
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.13	1.08
3:A:59:GLY:HA2	3:A:67:CYS:SG	1.91	1.08
4:B:65:GLU:HG2	4:B:66:ASP:N	1.51	1.08
3:A:49:LYS:O	3:A:50:ILE:HG12	1.54	1.08
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	1.87	1.08
3:A:169:ASN:H	3:A:169:ASN:ND2	1.37	1.08
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.53	1.08
3:A:169:ASN:HD22	3:A:169:ASN:N	1.47	1.08
3:A:89:PRO:O	3:A:204:THR:HG21	1.52	1.08
4:B:169:ARG:HB2	4:B:454:THR:HG23	1.35	1.08
3:A:261:ASP:HB3	3:A:323:LYS:CD	1.83	1.07
10:J:10:CYS:SG	10:J:43:ARG:HD2	1.93	1.07
4:B:1099:VAL:HG12	4:B:1103:ILE:HD11	1.33	1.07
3:A:649:ILE:O	3:A:653:VAL:HG23	1.53	1.07
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.14	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:380:VAL:HG21	3:A:430:TRP:H	1.20	1.07
3:A:1169:ILE:HD12	3:A:1169:ILE:H	1.16	1.07
3:A:322:VAL:CG1	3:A:323:LYS:HD3	1.83	1.07
4:B:1103:ILE:HD13	4:B:1103:ILE:N	1.70	1.07
3:A:7:SER:HB3	4:B:1193:GLN:NE2	1.67	1.07
4:B:287:ARG:HG2	4:B:292:ILE:HD13	1.37	1.07
6:E:46:TYR:HE2	6:E:58:MET:HA	1.14	1.06
3:A:868:TYR:HE1	3:A:1064:VAL:HG11	1.00	1.06
4:B:65:GLU:CG	4:B:66:ASP:H	1.67	1.06
8:H:32:THR:HG22	8:H:33:GLN:HG2	1.32	1.06
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.09	1.06
11:K:53:ASP:O	11:K:56:VAL:HG23	1.55	1.06
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.19	1.06
3:A:265:LYS:HE2	3:A:323:LYS:HE2	1.35	1.06
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	1.69	1.06
3:A:380:VAL:CG2	3:A:430:TRP:H	1.67	1.05
3:A:114:LEU:O	3:A:115:LEU:HD23	1.53	1.05
3:A:406:ILE:CD1	3:A:431:LYS:HB2	1.84	1.05
4:B:464:GLY:HA3	4:B:478:GLY:HA2	1.38	1.05
3:A:71:GLN:O	3:A:73:GLY:N	1.89	1.05
9:I:10:CYS:HB3	9:I:31:THR:HG21	1.13	1.05
4:B:917:PRO:HA	4:B:933:SER:O	1.54	1.05
4:B:635:ARG:HD2	4:B:636:PRO:HD3	1.32	1.05
3:A:1025:ARG:HG2	3:A:1025:ARG:HH11	1.20	1.05
3:A:913:LEU:HD12	3:A:914:GLU:H	0.93	1.05
3:A:981:LEU:HD21	3:A:1039:LYS:HA	1.32	1.05
4:B:235:SER:O	4:B:236:HIS:ND1	1.87	1.05
5:C:60:ASP:HB3	12:L:67:PHE:CE1	1.91	1.05
3:A:315:LEU:HD12	3:A:319:GLY:HA2	1.39	1.04
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.37	1.04
4:B:254:LEU:HD22	4:B:361:LEU:HD11	1.39	1.04
3:A:320:ARG:N	3:A:320:ARG:HD2	1.70	1.04
3:A:565:ILE:HG23	3:A:567:LYS:HE3	1.33	1.04
3:A:1214:GLU:O	3:A:1218:GLN:HG2	1.57	1.03
3:A:406:ILE:HD13	3:A:431:LYS:HB2	1.04	1.03
3:A:146:MET:O	3:A:170:THR:HG22	1.54	1.03
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.40	1.03
6:E:28:TYR:HE1	6:E:78:LEU:HD13	1.18	1.03
3:A:278:THR:O	3:A:279:LEU:HD23	1.58	1.03
7:F:73:ALA:O	7:F:74:ILE:HG12	1.56	1.03
3:A:1422:ARG:HH21	4:B:1220:ARG:HD3	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:265:LYS:NZ	3:A:322:VAL:HG21	1.72	1.03
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.36	1.03
3:A:901:LEU:HD23	3:A:907:THR:CG2	1.89	1.03
3:A:452:LYS:HB2	4:B:1141:HIS:CE1	1.93	1.03
4:B:280:ILE:HG21	4:B:285:ILE:HG12	1.39	1.03
3:A:783:THR:HG22	3:A:784:LEU:HG	1.37	1.03
5:C:60:ASP:HB3	12:L:67:PHE:HE1	1.18	1.03
3:A:320:ARG:CB	3:A:321:PRO:HB3	1.87	1.02
3:A:1004:ASN:HD22	6:E:167:ARG:CD	1.72	1.02
3:A:320:ARG:HB2	3:A:321:PRO:HB3	1.03	1.02
4:B:329:THR:HA	4:B:332:ASP:HB2	1.36	1.02
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.40	1.02
5:C:3:GLU:HG3	5:C:4:GLU:N	1.74	1.02
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.40	1.02
3:A:567:LYS:HB3	8:H:96:VAL:N	1.75	1.02
12:L:51:CYS:SG	12:L:51:CYS:O	2.18	1.01
9:I:17:ARG:HG2	9:I:18:GLU:H	1.21	1.01
4:B:634:TYR:HE1	4:B:692:TYR:CD1	1.78	1.01
3:A:531:ILE:HG12	3:A:622:VAL:HG11	1.36	1.01
9:I:17:ARG:HG2	9:I:18:GLU:N	1.72	1.01
4:B:635:ARG:HB2	4:B:636:PRO:HD3	1.03	1.01
4:B:284:ILE:HD12	4:B:324:ILE:HD12	1.42	1.01
11:K:49:GLU:HG3	11:K:94:ILE:HD11	1.41	1.01
3:A:215:SER:HB3	3:A:218:ASP:OD2	1.59	1.01
2:T:6:DC:H2"	2:T:7:DC:H5'	1.41	1.01
3:A:1312:ASN:O	3:A:1316:VAL:HG23	1.61	1.01
3:A:91:PHE:HD2	3:A:297:GLN:OE1	1.43	1.01
4:B:473:MET:C	4:B:475:SER:H	1.46	1.01
3:A:1445:ILE:HD12	3:A:1445:ILE:H	1.23	1.01
3:A:65:LEU:HD23	3:A:65:LEU:H	1.25	1.01
4:B:701:ILE:HB	4:B:740:HIS:HE1	1.22	1.00
6:E:65:THR:OG1	6:E:67:GLU:HB3	1.61	1.00
5:C:133:ILE:O	5:C:134:ILE:HD13	1.59	1.00
4:B:108:VAL:HG12	4:B:109:THR:H	1.27	1.00
3:A:351:THR:HG22	3:A:352:VAL:H	1.26	1.00
2:T:1:DA:H2"	2:T:2:DC:O5'	1.57	1.00
3:A:1067:LEU:HD21	3:A:1367:HIS:HE1	1.23	1.00
6:E:64:PRO:CG	6:E:76:GLY:HA2	1.92	1.00
3:A:1079:MET:O	3:A:1080:THR:OG1	1.78	1.00
4:B:167:ILE:CG2	4:B:424:LEU:HD13	1.90	1.00
5:C:46:ILE:HD13	5:C:159:ALA:HB2	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1165:ILE:HG22	4:B:1166:CYS:N	1.75	1.00
3:A:1134:ILE:O	3:A:1138:ILE:HG12	1.61	1.00
3:A:320:ARG:HH21	4:B:471:LYS:HB3	1.25	1.00
3:A:567:LYS:HB3	8:H:96:VAL:H	1.22	0.99
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.03	0.99
3:A:530:GLY:C	3:A:532:ARG:N	2.03	0.99
7:F:81:THR:HG22	7:F:136:ARG:NH1	1.76	0.99
4:B:1084:GLN:NE2	5:C:191:TYR:HA	1.77	0.99
9:I:10:CYS:CB	9:I:31:THR:HG21	1.92	0.99
6:E:46:TYR:CE2	6:E:58:MET:HA	1.96	0.99
3:A:367:PRO:HG2	3:A:370:ILE:HD12	1.44	0.99
4:B:1002:THR:HG21	4:B:1006:ILE:HB	1.41	0.99
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.89	0.98
4:B:256:VAL:HG11	4:B:382:ILE:CD1	1.93	0.98
4:B:955:THR:HG22	4:B:956:THR:N	1.72	0.98
6:E:113:GLN:HA	6:E:137:GLU:HG3	1.45	0.98
3:A:99:ILE:HA	3:A:102:VAL:CG2	1.93	0.98
4:B:1103:ILE:HD13	4:B:1103:ILE:H	1.27	0.98
3:A:901:LEU:HA	3:A:907:THR:HG23	1.44	0.98
4:B:168:GLY:HA2	4:B:454:THR:OG1	1.64	0.98
5:C:229:TYR:HD1	5:C:229:TYR:N	1.62	0.98
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.46	0.98
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.42	0.98
11:K:51:LEU:CD1	11:K:59:ALA:HB3	1.93	0.98
3:A:406:ILE:HD13	3:A:431:LYS:CB	1.93	0.97
3:A:302:THR:HG23	3:A:313:GLN:HE22	1.26	0.97
3:A:1004:ASN:HD22	6:E:167:ARG:HD2	0.84	0.97
4:B:563:MET:O	4:B:563:MET:HG3	1.61	0.97
4:B:711:GLU:N	4:B:712:PRO:HD3	1.76	0.97
3:A:1116:LEU:H	3:A:1308:THR:HB	1.24	0.97
5:C:258:ILE:HD11	11:K:42:LEU:HD21	1.45	0.97
8:H:81:PRO:HB2	8:H:82:PRO:CD	1.94	0.97
4:B:274:PRO:O	4:B:276:ILE:N	1.97	0.97
3:A:609:ASP:O	3:A:611:GLN:N	1.98	0.97
5:C:260:LEU:O	5:C:264:GLN:HG3	1.64	0.97
3:A:134:ARG:HD3	3:A:221:SER:O	1.63	0.97
4:B:698:GLU:O	4:B:701:ILE:HD12	1.63	0.97
3:A:528:LEU:HA	3:A:531:ILE:HG22	1.42	0.97
4:B:846:ILE:HG23	4:B:974:PRO:HG2	1.43	0.97
3:A:889:SER:HB2	3:A:892:ALA:H	1.28	0.96
4:B:549:THR:HG22	4:B:550:ASP:N	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:194:GLU:O	5:C:195:GLN:HG3	1.64	0.96
4:B:977:GLY:CA	4:B:1099:VAL:HG21	1.95	0.96
3:A:406:ILE:HD12	3:A:406:ILE:H	1.28	0.96
3:A:55:ASP:HA	3:A:58:LEU:HB2	1.46	0.96
4:B:780:VAL:HG21	10:J:56:LEU:CD1	1.95	0.96
2:T:5:DT:H2''	2:T:6:DC:H5'	1.44	0.96
4:B:521:LEU:CD2	4:B:635:ARG:HG2	1.95	0.96
3:A:709:THR:HG22	3:A:711:ARG:H	1.27	0.96
3:A:1228:TRP:HB3	3:A:1238:ILE:HD13	1.47	0.96
2:T:2:DC:H2'	2:T:3:DG:H8	1.25	0.96
4:B:899:ILE:HD11	4:B:911:ILE:HG12	1.47	0.96
3:A:528:LEU:O	3:A:528:LEU:HD12	1.65	0.96
3:A:794:PRO:HG2	3:A:795:GLU:HG2	1.47	0.96
6:E:126:SER:O	6:E:128:PRO:HD3	1.66	0.96
3:A:321:PRO:O	3:A:322:VAL:HG13	1.66	0.96
3:A:452:LYS:HB2	4:B:1141:HIS:HE1	1.28	0.96
8:H:106:GLU:C	8:H:108:SER:H	1.57	0.96
3:A:321:PRO:O	3:A:322:VAL:CG2	2.13	0.95
3:A:7:SER:CB	4:B:1193:GLN:NE2	2.29	0.95
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.45	0.95
3:A:148:CYS:O	3:A:149:GLU:O	1.84	0.95
3:A:320:ARG:HB2	3:A:321:PRO:CB	1.96	0.95
3:A:1392:SER:O	3:A:1393:ASN:ND2	1.97	0.95
4:B:635:ARG:CD	4:B:636:PRO:HD3	1.96	0.95
3:A:55:ASP:O	3:A:57:ARG:N	1.99	0.95
3:A:213:HIS:O	3:A:214:ILE:O	1.84	0.95
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.04	0.95
4:B:477:ALA:HB3	4:B:479:VAL:CG2	1.97	0.94
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.49	0.94
11:K:58:PHE:HE2	11:K:74:ARG:HE	0.98	0.94
3:A:1161:THR:HG22	3:A:1163:ILE:N	1.81	0.94
4:B:473:MET:C	4:B:475:SER:N	2.19	0.94
3:A:58:LEU:HD22	3:A:243:PRO:HB3	1.49	0.94
3:A:886:ILE:HG12	3:A:943:LEU:HD12	1.49	0.94
3:A:899:VAL:HG12	3:A:929:LEU:CD1	1.97	0.94
8:H:82:PRO:O	8:H:83:GLN:HB2	1.67	0.94
7:F:81:THR:CG2	7:F:136:ARG:HD3	1.96	0.94
3:A:208:LEU:O	3:A:209:ASN:O	1.85	0.94
4:B:167:ILE:HG23	4:B:424:LEU:CD1	1.97	0.94
3:A:90:VAL:HG13	3:A:297:GLN:HB2	1.48	0.94
3:A:90:VAL:HG12	3:A:297:GLN:HE21	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:320:ARG:CD	3:A:320:ARG:H	1.81	0.94
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.32	0.94
4:B:345:LYS:O	4:B:347:LYS:N	2.01	0.94
3:A:351:THR:CG2	4:B:1103:ILE:HD12	1.96	0.94
3:A:58:LEU:CD2	3:A:243:PRO:HB3	1.98	0.94
3:A:1116:LEU:HD22	3:A:1311:VAL:HG22	1.49	0.93
3:A:265:LYS:HE3	3:A:323:LYS:HG3	1.48	0.93
3:A:99:ILE:HA	3:A:102:VAL:HG23	1.46	0.93
3:A:1171:GLN:HB2	3:A:1172:LEU:HD23	1.51	0.93
2:T:1:DA:H2'	2:T:1:DA:N3	1.81	0.93
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.48	0.93
4:B:796:LEU:HB3	4:B:799:PRO:HD3	1.46	0.93
5:C:57:VAL:CG1	10:J:60:PHE:HB2	1.98	0.93
5:C:36:VAL:HG23	11:K:41:THR:HG21	1.50	0.93
4:B:550:ASP:OD1	4:B:551:PRO:HD2	1.67	0.93
4:B:477:ALA:CB	4:B:479:VAL:HG22	1.99	0.93
3:A:1362:TYR:CD1	3:A:1363:VAL:N	2.36	0.93
11:K:32:VAL:HG23	11:K:74:ARG:HG3	1.49	0.93
3:A:312:PRO:O	3:A:313:GLN:CG	2.17	0.93
9:I:10:CYS:SG	9:I:31:THR:HG22	2.08	0.93
3:A:58:LEU:O	3:A:59:GLY:O	1.86	0.93
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.84	0.93
3:A:530:GLY:C	3:A:532:ARG:H	1.58	0.93
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.48	0.93
4:B:1081:LEU:O	5:C:189:THR:HG23	1.69	0.93
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.14	0.93
3:A:855:THR:HG21	3:A:857:ARG:NE	1.83	0.92
3:A:908:LEU:HD11	3:A:983:ILE:HD11	1.49	0.92
4:B:737:THR:HG21	9:I:66:PRO:O	1.70	0.92
5:C:134:ILE:CD1	5:C:141:GLY:HA3	1.99	0.92
6:E:52:ARG:CB	6:E:53:PRO:HD2	1.95	0.92
4:B:708:GLU:HG3	4:B:709:ASP:H	1.34	0.92
5:C:115:SER:HB3	5:C:141:GLY:O	1.69	0.92
4:B:102:VAL:HG21	4:B:112:LEU:HD22	1.48	0.92
9:I:29:CYS:SG	9:I:31:THR:HB	2.10	0.92
6:E:28:TYR:CE1	6:E:78:LEU:HD13	2.04	0.92
4:B:737:THR:HG23	9:I:66:PRO:CB	1.99	0.92
3:A:1053:PHE:O	3:A:1055:ARG:N	2.02	0.92
3:A:391:LEU:HD13	3:A:400:PRO:O	1.70	0.92
3:A:590:ARG:HB3	3:A:605:MET:H	1.31	0.92
3:A:1362:TYR:HD1	3:A:1363:VAL:H	1.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:45:ALA:HA	5:C:72:LEU:HD12	1.51	0.92
4:B:234:ILE:H	4:B:234:ILE:HD13	1.33	0.92
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	1.99	0.92
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.51	0.92
8:H:108:SER:O	8:H:109:LYS:HB2	1.65	0.92
4:B:701:ILE:CB	4:B:740:HIS:HE1	1.82	0.91
4:B:955:THR:CG2	4:B:956:THR:H	1.81	0.91
3:A:718:VAL:O	3:A:722:LEU:HD12	1.70	0.91
4:B:112:LEU:HD12	4:B:113:TYR:H	1.33	0.91
3:A:107:CYS:HB3	3:A:114:LEU:HD22	1.48	0.91
3:A:1277:GLU:HG3	3:A:1278:ASN:ND2	1.83	0.91
4:B:727:LYS:HD3	4:B:1049:ASP:OD1	1.69	0.91
4:B:102:VAL:CG2	4:B:112:LEU:HD22	2.00	0.91
4:B:912:ILE:HD11	4:B:966:VAL:CG2	2.00	0.91
4:B:549:THR:CG2	4:B:550:ASP:H	1.84	0.91
3:A:830:LYS:HE3	3:A:1098:VAL:HG21	1.53	0.91
3:A:133:LYS:O	3:A:137:ALA:HB2	1.71	0.91
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.50	0.91
4:B:25:ILE:HD12	4:B:651:LEU:HD12	1.50	0.91
11:K:49:GLU:HG3	11:K:94:ILE:CD1	2.00	0.91
8:H:113:ALA:HA	8:H:125:LEU:O	1.71	0.91
8:H:97:MET:HB2	8:H:118:PHE:CD2	2.06	0.90
3:A:1434:ALA:HB1	3:A:1436:ILE:HD12	1.50	0.90
3:A:185:TRP:O	3:A:186:LYS:HB2	1.69	0.90
11:K:57:LEU:HD12	11:K:76:GLN:CG	2.01	0.90
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.49	0.90
3:A:894:GLU:C	3:A:896:ARG:H	1.73	0.90
3:A:261:ASP:CB	3:A:323:LYS:HD2	2.01	0.90
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.52	0.90
11:K:57:LEU:HD12	11:K:76:GLN:HG3	1.53	0.90
4:B:984:HIS:HD2	4:B:1024:ALA:HB3	1.36	0.90
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.54	0.90
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.02	0.90
3:A:406:ILE:HD12	3:A:406:ILE:N	1.86	0.90
4:B:701:ILE:HB	4:B:740:HIS:CE1	2.07	0.90
3:A:20:GLY:O	3:A:21:LEU:HD23	1.72	0.90
7:F:101:ILE:HD11	7:F:121:ALA:HB2	1.54	0.90
3:A:944:ARG:HG2	3:A:1298:TYR:OH	1.72	0.89
12:L:55:ILE:O	12:L:56:LEU:HB2	1.72	0.89
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.54	0.89
3:A:33:ALA:HB2	3:A:82:GLY:HA2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:805:LEU:C	3:A:805:LEU:HD12	1.91	0.89
3:A:888:GLY:O	3:A:889:SER:O	1.90	0.89
6:E:112:TYR:CE1	6:E:136:ASN:HB2	2.07	0.89
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.52	0.89
4:B:479:VAL:O	4:B:480:SER:HB3	1.69	0.89
3:A:528:LEU:C	3:A:530:GLY:H	1.70	0.89
4:B:332:ASP:O	4:B:334:ILE:N	2.05	0.89
6:E:111:VAL:O	6:E:111:VAL:HG12	1.72	0.89
3:A:90:VAL:HG11	3:A:297:GLN:CA	2.01	0.89
3:A:353:ILE:HD13	3:A:487:MET:CE	2.02	0.89
4:B:114:PRO:HD3	4:B:124:TYR:CE1	2.07	0.89
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.72	0.89
7:F:98:ALA:HA	7:F:101:ILE:HD12	1.54	0.89
6:E:131:THR:HG22	6:E:132:ILE:H	1.35	0.89
4:B:788:ARG:CB	4:B:788:ARG:HH11	1.86	0.89
4:B:322:PHE:CZ	9:I:30:ARG:HD2	2.07	0.89
4:B:471:LYS:O	4:B:473:MET:N	2.06	0.89
10:J:9:SER:OG	10:J:45:CYS:HB2	1.73	0.88
6:E:54:GLN:O	6:E:57:MET:HB3	1.71	0.88
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.54	0.88
3:A:531:ILE:HD13	3:A:622:VAL:HG21	1.54	0.88
3:A:523:ILE:HD13	3:A:622:VAL:HG22	1.55	0.88
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.03	0.88
3:A:535:THR:HG21	3:A:617:VAL:H	1.36	0.88
4:B:129:PHE:CE2	4:B:166:PHE:HB2	2.09	0.88
11:K:65:HIS:HD2	11:K:67:PHE:H	1.20	0.88
6:E:23:VAL:HG13	6:E:28:TYR:HD1	1.38	0.88
2:T:6:DC:H2''	2:T:7:DC:C5'	2.03	0.88
4:B:278:GLN:HG2	4:B:279:ASP:H	1.37	0.88
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.07	0.88
3:A:868:TYR:HE1	3:A:1064:VAL:CG1	1.86	0.88
3:A:1291:VAL:HG13	3:A:1292:PRO:HD2	1.52	0.88
4:B:798:TYR:HD2	10:J:4:PRO:HG3	1.39	0.88
3:A:1355:VAL:HG12	3:A:1356:ILE:N	1.89	0.88
3:A:809:THR:HG23	3:A:812:GLU:OE1	1.72	0.88
9:I:25:LEU:HD12	9:I:26:LEU:H	1.36	0.88
4:B:1002:THR:CG2	4:B:1006:ILE:HB	2.04	0.88
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.32	0.88
3:A:169:ASN:HD22	3:A:169:ASN:H	0.89	0.88
9:I:10:CYS:SG	9:I:31:THR:CG2	2.62	0.88
5:C:44:LEU:CB	5:C:77:ILE:HD11	1.99	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:322:VAL:CB	3:A:323:LYS:HD3	2.04	0.88
5:C:71:PRO:HB2	5:C:133:ILE:HD12	1.53	0.88
3:A:261:ASP:HB3	3:A:323:LYS:HD2	1.50	0.88
4:B:329:THR:CA	4:B:332:ASP:HB2	2.03	0.88
5:C:46:ILE:HG21	5:C:157:CYS:HB3	1.56	0.88
4:B:316:PRO:HA	4:B:319:GLU:HG3	1.54	0.88
9:I:17:ARG:CG	9:I:18:GLU:H	1.86	0.87
5:C:258:ILE:CD1	11:K:42:LEU:HD21	2.04	0.87
3:A:590:ARG:HB3	3:A:605:MET:N	1.89	0.87
3:A:1373:ASP:O	3:A:1377:THR:HG23	1.73	0.87
6:E:37:LEU:O	6:E:38:PRO:O	1.92	0.87
4:B:469:GLN:O	4:B:471:LYS:N	2.05	0.87
3:A:1404:GLU:O	3:A:1408:ILE:HG12	1.72	0.87
4:B:788:ARG:HB3	4:B:788:ARG:NH1	1.89	0.87
3:A:265:LYS:NZ	3:A:322:VAL:CG2	2.36	0.87
3:A:455:MET:O	3:A:456:MET:HG2	1.74	0.87
3:A:793:SER:HB2	3:A:794:PRO:HD2	1.57	0.87
3:A:894:GLU:O	3:A:896:ARG:N	2.07	0.87
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.04	0.87
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.09	0.87
4:B:130:VAL:HG12	4:B:132:VAL:HG23	1.56	0.87
3:A:504:LEU:HD11	7:F:91:ALA:CB	2.05	0.87
5:C:70:ILE:CD1	5:C:144:ILE:HD11	2.05	0.87
4:B:1177:HIS:O	4:B:1179:GLN:N	2.06	0.87
4:B:1107:ALA:O	4:B:1108:ARG:HB3	1.75	0.87
5:C:46:ILE:HD11	5:C:72:LEU:HD11	1.57	0.86
5:C:114:TYR:CD2	5:C:140:ASN:HB2	2.10	0.86
4:B:230:ALA:HB3	4:B:231:PRO:HD3	1.56	0.86
4:B:1072:MET:HE3	4:B:1085:ILE:HG21	1.57	0.86
3:A:72:GLU:HA	3:A:72:GLU:OE1	1.73	0.86
4:B:299:GLU:OE1	4:B:572:HIS:HB3	1.75	0.86
5:C:133:ILE:HD11	5:C:237:SER:HA	1.57	0.86
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.57	0.86
4:B:955:THR:OG1	12:L:55:ILE:HA	1.74	0.86
4:B:957:ASN:HB3	4:B:961:LEU:HD12	1.57	0.86
3:A:565:ILE:HG23	3:A:567:LYS:CE	2.06	0.86
5:C:70:ILE:HD12	5:C:144:ILE:HD11	1.56	0.86
3:A:401:GLY:H	3:A:435:HIS:HD2	1.23	0.86
3:A:262:LEU:O	3:A:266:LEU:HB2	1.75	0.86
4:B:1156:ASP:HB3	4:B:1198:TYR:H	1.39	0.86
6:E:168:TYR:C	6:E:169:ARG:HG2	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:955:THR:HG23	12:L:54:ARG:O	1.74	0.86
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.00	0.86
3:A:1015:VAL:CG1	3:A:1019:CYS:SG	2.64	0.86
3:A:583:PRO:O	3:A:610:GLY:HA3	1.75	0.86
6:E:187:TYR:HD2	6:E:188:LEU:HD23	1.40	0.86
3:A:1127:ASP:HB2	3:A:1130:GLN:HB3	1.58	0.86
4:B:120:ARG:CD	4:B:955:THR:HG21	2.05	0.86
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.40	0.85
4:B:996:ARG:NH2	5:C:38:ILE:HD12	1.91	0.85
4:B:363:HIS:O	4:B:364:ILE:HB	1.75	0.85
4:B:322:PHE:CD1	4:B:322:PHE:O	2.29	0.85
8:H:139:ASN:O	8:H:140:ALA:HB2	1.75	0.85
10:J:7:CYS:HA	10:J:49:MET:HE3	1.57	0.85
4:B:860:MET:HG2	4:B:861:ASP:N	1.91	0.85
4:B:91:SER:OG	4:B:133:LYS:HB2	1.75	0.85
3:A:90:VAL:CG1	3:A:297:GLN:HB2	2.06	0.85
4:B:474:SER:CA	4:B:476:ARG:HG3	2.04	0.85
3:A:630:ILE:N	3:A:630:ILE:HD12	1.90	0.85
3:A:1256:GLU:O	3:A:1258:HIS:N	2.09	0.85
3:A:1445:ILE:HD12	3:A:1445:ILE:N	1.90	0.85
5:C:229:TYR:CD1	5:C:229:TYR:N	2.36	0.85
5:C:10:ILE:HD13	5:C:20:PHE:HB3	1.58	0.85
10:J:10:CYS:SG	10:J:43:ARG:CD	2.64	0.85
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.06	0.85
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.55	0.85
3:A:898:ARG:HB2	3:A:933:TYR:HE1	1.42	0.85
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.12	0.85
4:B:466:TRP:N	4:B:475:SER:OG	2.08	0.85
7:F:147:SER:OG	7:F:150:GLU:HG3	1.76	0.85
9:I:25:LEU:HD12	9:I:26:LEU:N	1.89	0.85
3:A:858:ASN:C	3:A:858:ASN:HD22	1.79	0.85
3:A:179:LEU:CD1	3:A:297:GLN:HG2	2.07	0.85
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.12	0.85
5:C:44:LEU:HD12	5:C:160:LYS:O	1.76	0.85
4:B:634:TYR:CE1	4:B:692:TYR:CD1	2.64	0.85
4:B:129:PHE:CE2	4:B:166:PHE:CB	2.60	0.85
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.11	0.85
3:A:320:ARG:NH2	4:B:469:GLN:O	2.08	0.85
4:B:1099:VAL:CG1	4:B:1103:ILE:HD11	2.06	0.85
5:C:3:GLU:CG	5:C:4:GLU:H	1.88	0.85
4:B:902:GLY:O	12:L:65:VAL:HG11	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:PHE:CD2	3:A:297:GLN:OE1	2.29	0.84
4:B:230:ALA:N	4:B:231:PRO:HD2	1.91	0.84
11:K:12:LEU:HD12	11:K:12:LEU:H	1.38	0.84
4:B:475:SER:O	4:B:477:ALA:N	2.10	0.84
4:B:65:GLU:CG	4:B:66:ASP:N	2.33	0.84
3:A:1319:VAL:HB	3:A:1322:ILE:HD12	1.59	0.84
3:A:12:ARG:HD3	4:B:1192:TYR:HE2	1.40	0.84
4:B:29:ASP:HB3	4:B:658:ILE:HD13	1.57	0.84
4:B:736:THR:O	4:B:736:THR:HG22	1.77	0.84
3:A:929:LEU:HD21	3:A:983:ILE:CG2	2.07	0.84
4:B:236:HIS:HD2	4:B:389:ALA:HB2	1.42	0.84
4:B:801:LYS:HG2	10:J:52:THR:HG23	1.58	0.84
3:A:779:PHE:CE1	3:A:785:PRO:HD3	2.13	0.84
3:A:1362:TYR:HD1	3:A:1363:VAL:N	1.72	0.84
4:B:256:VAL:HG11	4:B:382:ILE:HD11	1.57	0.84
3:A:925:LEU:C	3:A:927:VAL:H	1.78	0.84
4:B:431:TYR:CE1	4:B:447:ALA:HB2	2.13	0.84
11:K:92:ASN:HA	11:K:95:ILE:HD12	1.56	0.84
3:A:635:ARG:NH2	3:A:877:HIS:ND1	2.26	0.84
4:B:62:ILE:HD12	4:B:418:LYS:HE2	1.59	0.84
3:A:1422:ARG:HH21	4:B:1220:ARG:CD	1.90	0.84
3:A:380:VAL:HG21	3:A:430:TRP:N	1.93	0.84
3:A:322:VAL:HB	3:A:323:LYS:HD3	1.58	0.84
9:I:7:CYS:N	9:I:14:LEU:HD21	1.93	0.84
8:H:106:GLU:C	8:H:108:SER:N	2.29	0.84
3:A:922:ASP:OD1	3:A:923:LEU:N	2.09	0.84
3:A:981:LEU:CD2	3:A:1039:LYS:HA	2.08	0.84
3:A:821:ARG:O	3:A:825:ILE:HG12	1.78	0.84
3:A:955:PRO:O	3:A:956:LEU:HG	1.78	0.83
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.04	0.83
9:I:15:TYR:HB3	9:I:16:PRO:CD	2.08	0.83
3:A:151:ASP:OD1	3:A:163:SER:HA	1.78	0.83
3:A:103:CYS:C	3:A:105:CYS:H	1.77	0.83
4:B:708:GLU:O	4:B:710:LEU:N	2.10	0.83
4:B:577:ALA:HB1	4:B:589:VAL:HG13	1.59	0.83
3:A:1200:ALA:O	3:A:1203:ASN:N	2.09	0.83
3:A:322:VAL:HG12	3:A:323:LYS:HD3	1.59	0.83
3:A:1291:VAL:CG1	3:A:1292:PRO:HD2	2.07	0.83
6:E:116:ILE:O	6:E:118:PRO:HD3	1.77	0.83
4:B:707:PRO:HB3	4:B:741:CYS:SG	2.18	0.83
4:B:744:HIS:HD2	4:B:746:SER:OG	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:474:SER:O	4:B:476:ARG:HB2	1.79	0.83
3:A:59:GLY:CA	3:A:67:CYS:SG	2.67	0.83
3:A:925:LEU:C	3:A:927:VAL:N	2.26	0.83
4:B:635:ARG:CB	4:B:636:PRO:CD	2.40	0.83
4:B:744:HIS:CD2	4:B:746:SER:OG	2.31	0.83
3:A:265:LYS:HE3	3:A:323:LYS:CG	2.08	0.83
4:B:474:SER:HA	4:B:476:ARG:CG	2.07	0.83
4:B:1104:HIS:HB2	4:B:1122:ARG:HB2	1.60	0.83
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.08	0.83
3:A:343:LYS:NZ	4:B:1197:PRO:HB3	1.93	0.83
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.25	0.83
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.61	0.83
4:B:1076:HIS:ND1	11:K:40:HIS:HD2	1.76	0.83
3:A:888:GLY:O	3:A:940:ARG:NH2	2.10	0.83
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.09	0.83
4:B:108:VAL:HG12	4:B:109:THR:N	1.94	0.83
6:E:64:PRO:HG3	6:E:76:GLY:HA2	1.59	0.83
3:A:451:HIS:O	4:B:1137:CYS:SG	2.36	0.83
3:A:1322:ILE:O	3:A:1324:PRO:HD3	1.78	0.83
7:F:111:LEU:O	7:F:113:GLY:N	2.10	0.83
7:F:155:LEU:N	7:F:155:LEU:HD23	1.84	0.83
4:B:555:ILE:HD11	4:B:582:VAL:HG11	1.61	0.83
4:B:1162:ILE:HD13	4:B:1168:LEU:C	1.97	0.83
8:H:84:ALA:C	8:H:86:ASP:H	1.79	0.83
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.59	0.83
9:I:50:THR:CG2	9:I:52:ILE:HG22	2.09	0.83
3:A:321:PRO:HD2	3:A:322:VAL:HA	1.58	0.82
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	1.93	0.82
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.08	0.82
3:A:207:ILE:HA	3:A:210:ILE:HG13	1.61	0.82
3:A:765:VAL:HG22	3:A:802:ASN:O	1.79	0.82
4:B:682:SER:O	4:B:686:ASN:ND2	2.12	0.82
3:A:302:THR:CG2	3:A:313:GLN:HE22	1.93	0.82
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.09	0.82
4:B:1099:VAL:HG12	4:B:1103:ILE:CD1	2.09	0.82
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.60	0.82
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.15	0.82
5:C:22:LEU:HD21	5:C:25:VAL:HG21	1.59	0.82
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.14	0.82
3:A:996:ASN:O	3:A:998:LEU:HB2	1.79	0.82
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1161:THR:HG22	3:A:1162:VAL:N	1.92	0.82
3:A:779:PHE:CZ	3:A:785:PRO:HD3	2.15	0.82
4:B:168:GLY:CA	4:B:454:THR:OG1	2.28	0.82
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.09	0.82
6:E:161:LYS:O	6:E:163:GLU:N	2.12	0.82
7:F:155:LEU:H	7:F:155:LEU:CD2	1.84	0.82
8:H:32:THR:HG22	8:H:33:GLN:CG	2.09	0.82
4:B:65:GLU:HG2	4:B:66:ASP:H	0.73	0.82
8:H:12:VAL:HG13	8:H:28:ALA:HB2	1.62	0.82
11:K:46:ILE:HG23	11:K:50:LEU:HD12	1.60	0.82
6:E:65:THR:C	6:E:67:GLU:H	1.81	0.81
12:L:43:THR:O	12:L:43:THR:CG2	2.27	0.81
3:A:590:ARG:HG3	3:A:590:ARG:HH11	1.45	0.81
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.62	0.81
7:F:132:LEU:O	7:F:148:VAL:HG23	1.80	0.81
3:A:1161:THR:CG2	3:A:1163:ILE:H	1.86	0.81
4:B:472:ALA:O	4:B:474:SER:N	2.13	0.81
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.62	0.81
3:A:68:GLN:C	3:A:70:CYS:H	1.79	0.81
3:A:907:THR:HG22	3:A:908:LEU:H	1.45	0.81
4:B:563:MET:HA	4:B:589:VAL:O	1.81	0.81
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.03	0.81
11:K:90:ALA:O	11:K:94:ILE:HD13	1.80	0.81
3:A:219:PHE:O	3:A:222:LEU:HD12	1.78	0.81
3:A:834:THR:HG21	3:A:1077:THR:CA	2.10	0.81
6:E:113:GLN:HB3	6:E:137:GLU:OE1	1.80	0.81
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.62	0.81
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.60	0.81
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.42	0.81
3:A:265:LYS:CE	3:A:323:LYS:HE2	2.10	0.81
2:T:2:DC:C2'	2:T:3:DG:H8	1.92	0.81
4:B:882:THR:CG2	4:B:935:ARG:HA	2.08	0.81
5:C:58:LEU:HD21	10:J:57:ILE:HD13	1.60	0.81
12:L:43:THR:O	12:L:43:THR:HG22	1.79	0.81
10:J:51:LEU:O	10:J:51:LEU:HD12	1.81	0.81
3:A:898:ARG:HD2	3:A:899:VAL:N	1.96	0.81
8:H:142:LEU:HD12	8:H:143:LEU:N	1.96	0.81
8:H:93:TYR:CD1	8:H:143:LEU:HB2	2.15	0.81
3:A:1042:PHE:CE2	3:A:1046:LEU:HD12	2.15	0.81
4:B:737:THR:CG2	9:I:66:PRO:CB	2.58	0.81
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1101:LEU:HG	3:A:1105:LEU:CD1	2.11	0.81
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.80	0.81
3:A:1173:HIS:HD2	3:A:1227:ILE:HG23	1.45	0.81
6:E:43:LYS:O	6:E:47:CYS:HB2	1.81	0.81
3:A:278:THR:CG2	3:A:278:THR:O	2.24	0.81
3:A:119:ASN:O	3:A:122:MET:HB3	1.81	0.81
5:C:66:ARG:NH2	10:J:3:VAL:O	2.14	0.81
9:I:47:GLU:OE1	9:I:50:THR:HG23	1.81	0.81
6:E:171:LYS:HB2	6:E:174:GLN:HG3	1.63	0.81
4:B:830:TYR:CE1	4:B:1000:PRO:HB3	2.16	0.81
3:A:58:LEU:CD2	3:A:80:HIS:O	2.29	0.81
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.81	0.81
5:C:134:ILE:HD12	5:C:141:GLY:CA	2.11	0.81
4:B:175:ARG:HH11	4:B:175:ARG:HG2	1.44	0.81
3:A:1242:VAL:HG12	3:A:1243:VAL:N	1.96	0.81
3:A:13:THR:HB	3:A:15:LYS:NZ	1.96	0.81
3:A:705:LYS:HG3	3:A:713:SER:HB3	1.62	0.81
3:A:1342:GLU:HG2	6:E:212:ARG:HH12	1.45	0.81
11:K:49:GLU:CG	11:K:94:ILE:HD11	2.11	0.81
3:A:546:VAL:HG12	3:A:550:LEU:CD2	2.11	0.81
3:A:1052:GLN:O	3:A:1053:PHE:O	1.97	0.81
3:A:901:LEU:HA	3:A:907:THR:CG2	2.11	0.80
7:F:75:PRO:O	7:F:79:ARG:HD2	1.81	0.80
4:B:984:HIS:CD2	4:B:1024:ALA:HB3	2.15	0.80
7:F:109:VAL:HG12	7:F:110:ASP:H	1.42	0.80
4:B:1077:THR:CG2	4:B:1079:LYS:H	1.94	0.80
11:K:50:LEU:HD21	11:K:75:ILE:HD13	1.63	0.80
9:I:10:CYS:HB3	9:I:31:THR:CG2	2.05	0.80
3:A:65:LEU:HD23	3:A:65:LEU:N	1.96	0.80
8:H:89:LEU:C	8:H:91:ASP:H	1.81	0.80
3:A:908:LEU:O	3:A:909:ASP:O	1.98	0.80
3:A:14:VAL:H	3:A:1432:GLN:NE2	1.80	0.80
3:A:1101:LEU:O	3:A:1105:LEU:HD12	1.80	0.80
8:H:139:ASN:O	8:H:140:ALA:CB	2.28	0.80
2:T:4:DA:H5'	3:A:832:ALA:HA	1.64	0.80
3:A:445:ASN:ND2	3:A:446:ARG:N	2.30	0.80
3:A:130:ASP:O	3:A:131:SER:C	2.18	0.80
4:B:806:THR:N	4:B:809:MET:HE3	1.96	0.80
3:A:783:THR:O	3:A:784:LEU:HD23	1.82	0.80
4:B:737:THR:HG23	9:I:66:PRO:HB3	1.63	0.80
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:173:ALA:O	5:C:174:ALA:HB3	1.81	0.80
5:C:52:GLU:OE2	5:C:154:LYS:HG2	1.81	0.80
3:A:649:ILE:O	3:A:653:VAL:CG2	2.30	0.80
3:A:1409:LEU:HD13	4:B:1207:LEU:HD21	1.63	0.80
8:H:3:ASN:CG	8:H:4:THR:H	1.81	0.80
12:L:68:GLU:OE1	12:L:68:GLU:O	2.00	0.80
3:A:146:MET:O	3:A:170:THR:CG2	2.29	0.80
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.11	0.80
3:A:239:LEU:HD12	3:A:240:PRO:O	1.82	0.80
3:A:261:ASP:CG	3:A:323:LYS:HD2	2.02	0.80
10:J:36:LEU:HD12	10:J:47:ARG:HG2	1.64	0.80
5:C:98:VAL:C	5:C:99:LEU:HD23	2.01	0.80
4:B:521:LEU:HD23	4:B:635:ARG:HG2	1.64	0.80
3:A:886:ILE:HD11	3:A:943:LEU:HB2	1.64	0.80
4:B:794:ASN:HD22	4:B:794:ASN:N	1.80	0.80
3:A:697:ALA:HB2	3:A:702:LEU:HG	1.62	0.79
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.62	0.79
11:K:65:HIS:CD2	11:K:67:PHE:H	1.99	0.79
3:A:305:ASP:OD1	3:A:306:ASN:N	2.15	0.79
4:B:1175:LEU:O	4:B:1176:ASN:CB	2.27	0.79
4:B:788:ARG:CB	4:B:788:ARG:NH1	2.45	0.79
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.11	0.79
3:A:1284:MET:HA	3:A:1306:LEU:HD23	1.64	0.79
3:A:322:VAL:HB	3:A:323:LYS:HG2	1.63	0.79
3:A:313:GLN:O	3:A:314:ALA:HB2	1.80	0.79
3:A:919:ILE:O	3:A:920:LEU:C	2.20	0.79
4:B:806:THR:HG22	4:B:808:ALA:H	1.48	0.79
3:A:785:PRO:HB2	4:B:701:ILE:HD11	1.64	0.79
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.12	0.79
4:B:1182:CYS:O	4:B:1183:LYS:O	2.01	0.79
8:H:41:ASP:O	8:H:42:ILE:HD13	1.82	0.79
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.16	0.79
3:A:504:LEU:HD11	7:F:91:ALA:HB2	1.64	0.79
3:A:522:GLY:C	3:A:523:ILE:HD12	2.01	0.79
3:A:569:LYS:HG2	3:A:571:LEU:HD11	1.64	0.79
4:B:800:GLN:HG2	10:J:52:THR:HG21	1.63	0.79
3:A:575:LYS:HD3	3:A:612:ILE:HD11	1.65	0.79
6:E:170:LEU:HD13	6:E:175:LEU:CD2	2.12	0.79
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.65	0.79
3:A:7:SER:HB3	4:B:1193:GLN:HE22	1.44	0.79
4:B:68:THR:O	4:B:69:LEU:HD23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:ARG:CG	9:I:18:GLU:N	2.45	0.79
3:A:849:MET:HE1	3:A:1061:GLY:HA2	1.63	0.79
3:A:58:LEU:HD22	3:A:243:PRO:CB	2.11	0.79
6:E:164:LEU:HD13	6:E:211:TYR:CE2	2.18	0.79
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.63	0.79
3:A:531:ILE:CG1	3:A:622:VAL:HG11	2.11	0.79
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.46	0.79
5:C:182:PRO:HB2	5:C:207:CYS:SG	2.22	0.79
4:B:124:TYR:OH	4:B:179:CYS:HA	1.83	0.79
3:A:598:LEU:HD13	8:H:25:ARG:NH1	1.97	0.79
3:A:343:LYS:HZ1	4:B:1197:PRO:HB3	1.48	0.79
3:A:68:GLN:NE2	3:A:80:HIS:NE2	2.31	0.79
3:A:58:LEU:HD21	3:A:80:HIS:O	1.83	0.79
3:A:567:LYS:CB	8:H:96:VAL:H	1.96	0.79
3:A:120:GLU:HG2	3:A:120:GLU:O	1.81	0.79
3:A:1273:LEU:O	3:A:1274:ARG:HB3	1.82	0.78
4:B:1076:HIS:ND1	11:K:40:HIS:CD2	2.51	0.78
9:I:33:SER:O	9:I:34:TYR:O	2.01	0.78
5:C:93:ASP:O	5:C:127:ARG:NH2	2.16	0.78
4:B:815:ARG:HH11	4:B:815:ARG:HG3	1.48	0.78
11:K:7:PHE:HA	11:K:10:PHE:CZ	2.18	0.78
4:B:174:LEU:CD2	4:B:204:ILE:HD11	2.10	0.78
4:B:1171:VAL:HG12	4:B:1172:ILE:N	1.95	0.78
3:A:114:LEU:HD13	3:A:171:GLN:NE2	1.97	0.78
5:C:244:VAL:O	5:C:248:ILE:HG13	1.83	0.78
3:A:868:TYR:CE1	3:A:1064:VAL:HG21	2.18	0.78
3:A:676:MET:SD	3:A:679:ILE:HD12	2.22	0.78
6:E:30:ILE:HG23	6:E:34:GLU:OE1	1.83	0.78
5:C:92:CYS:SG	5:C:94:LYS:CB	2.72	0.78
3:A:1228:TRP:HB3	3:A:1238:ILE:CD1	2.13	0.78
4:B:167:ILE:HD12	4:B:424:LEU:HD11	1.65	0.78
6:E:96:PHE:O	6:E:98:ILE:N	2.17	0.78
3:A:12:ARG:HD3	4:B:1192:TYR:CE2	2.18	0.78
4:B:834:ASN:O	4:B:1013:ASN:HB2	1.82	0.78
2:T:2:DC:C2'	2:T:3:DG:C8	2.65	0.78
4:B:474:SER:C	4:B:476:ARG:N	2.26	0.78
11:K:40:HIS:CE1	11:K:63:VAL:HG11	2.18	0.78
3:A:326:ARG:CG	3:A:1406:VAL:HG21	2.14	0.78
3:A:107:CYS:CB	3:A:114:LEU:HD22	2.13	0.78
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.19	0.78
4:B:129:PHE:CD2	4:B:166:PHE:HB2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:ILE:HD12	8:H:95:TYR:CZ	2.19	0.78
9:I:42:LEU:HD12	9:I:43:VAL:N	1.98	0.78
7:F:111:LEU:C	7:F:113:GLY:H	1.86	0.78
8:H:5:LEU:HD22	8:H:133:ASN:O	1.84	0.78
9:I:19:ASP:O	9:I:23:ASN:HA	1.84	0.78
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.66	0.78
5:C:134:ILE:HD11	5:C:141:GLY:HA3	1.62	0.78
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.18	0.78
3:A:1222:ASN:O	3:A:1223:ASP:HB3	1.81	0.78
3:A:1279:ILE:O	3:A:1279:ILE:HG22	1.81	0.78
4:B:1171:VAL:CG1	4:B:1172:ILE:H	1.96	0.78
4:B:365:THR:HG23	4:B:367:LEU:H	1.49	0.78
5:C:196:ASP:O	5:C:200:GLU:HB2	1.84	0.78
11:K:93:SER:O	11:K:97:LYS:HG3	1.83	0.78
9:I:7:CYS:CA	9:I:14:LEU:HD21	2.13	0.78
4:B:711:GLU:N	4:B:712:PRO:CD	2.47	0.77
4:B:954:VAL:O	12:L:55:ILE:O	2.01	0.77
4:B:273:LEU:HB2	4:B:276:ILE:HD12	1.64	0.77
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.64	0.77
4:B:751:VAL:HG12	4:B:752:ALA:N	1.99	0.77
3:A:1189:SER:OG	3:A:1190:PRO:HD2	1.84	0.77
6:E:162:ARG:HH21	6:E:166:LYS:HZ3	1.30	0.77
10:J:43:ARG:CG	10:J:46:CYS:HB2	2.12	0.77
3:A:913:LEU:HD12	3:A:915:SER:H	1.48	0.77
4:B:169:ARG:HB2	4:B:454:THR:CG2	2.14	0.77
3:A:852:TYR:CE1	7:F:136:ARG:HG2	2.19	0.77
4:B:770:GLN:HG2	4:B:983:ARG:O	1.84	0.77
4:B:1116:ARG:HG3	4:B:1198:TYR:CD2	2.19	0.77
3:A:1150:SER:OG	3:A:1264:GLU:OE1	2.02	0.77
3:A:1329:THR:HG22	3:A:1331:SER:H	1.50	0.77
9:I:42:LEU:HD12	9:I:43:VAL:H	1.47	0.77
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.67	0.77
3:A:320:ARG:CD	3:A:320:ARG:N	2.41	0.77
9:I:6:PHE:HB3	9:I:12:ASN:O	1.84	0.77
5:C:227:THR:HG22	5:C:229:TYR:CE1	2.18	0.77
3:A:1155:ASP:OD2	3:A:1162:VAL:HG23	1.84	0.77
3:A:265:LYS:HZ2	3:A:322:VAL:CG2	1.97	0.77
12:L:48:CYS:HB3	12:L:51:CYS:O	1.85	0.77
3:A:1120:LEU:HD23	3:A:1125:ALA:O	1.85	0.77
4:B:645:SER:O	4:B:647:GLY:N	2.16	0.77
4:B:112:LEU:HD12	4:B:113:TYR:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:64:PRO:HG2	6:E:76:GLY:HA2	1.67	0.77
4:B:759:PRO:HD2	4:B:1046:PRO:HG3	1.67	0.77
4:B:911:ILE:HG22	4:B:912:ILE:HG13	1.65	0.77
5:C:56:THR:HG21	5:C:145:CYS:SG	2.24	0.77
4:B:635:ARG:CG	4:B:636:PRO:HD3	2.13	0.77
5:C:4:GLU:HG3	5:C:5:GLY:H	1.50	0.77
5:C:46:ILE:CD1	5:C:72:LEU:HD11	2.15	0.77
9:I:19:ASP:HB2	9:I:24:ARG:HG3	1.67	0.77
7:F:81:THR:HG22	7:F:136:ARG:HH11	1.50	0.77
4:B:1084:GLN:OE1	4:B:1084:GLN:N	2.18	0.77
4:B:635:ARG:HD2	4:B:636:PRO:CD	2.14	0.77
4:B:640:VAL:O	4:B:650:GLU:O	2.03	0.77
4:B:956:THR:OG1	4:B:961:LEU:O	2.02	0.77
3:A:247:ARG:HH11	3:A:263:THR:HG23	1.49	0.77
3:A:630:ILE:CD1	3:A:630:ILE:H	1.92	0.76
3:A:852:TYR:CE2	3:A:1060:PRO:HB2	2.20	0.76
5:C:227:THR:HG22	5:C:229:TYR:HE1	1.51	0.76
5:C:229:TYR:HD1	5:C:229:TYR:H	1.33	0.76
3:A:855:THR:CG2	3:A:857:ARG:HE	1.94	0.76
3:A:492:PRO:C	3:A:493:GLN:HE21	1.87	0.76
4:B:1184:GLY:O	4:B:1186:ASP:N	2.18	0.76
3:A:898:ARG:HA	3:A:933:TYR:CD1	2.21	0.76
3:A:26:GLU:O	3:A:29:ALA:N	2.17	0.76
6:E:127:ILE:HG12	6:E:127:ILE:O	1.84	0.76
3:A:588:LEU:HD12	3:A:589:GLN:H	1.51	0.76
3:A:1171:GLN:HB2	3:A:1172:LEU:CD2	2.16	0.76
3:A:1193:LEU:HD12	3:A:1194:ARG:N	2.00	0.76
3:A:265:LYS:HZ3	3:A:322:VAL:HG21	1.45	0.76
3:A:672:ASP:CB	3:A:736:ASN:OD1	2.33	0.76
7:F:135:ARG:HG2	7:F:137:TYR:HE1	1.50	0.76
3:A:96:ILE:HG22	3:A:97:ALA:N	2.00	0.76
8:H:89:LEU:O	8:H:91:ASP:N	2.18	0.76
3:A:1168:GLU:O	3:A:1170:ILE:N	2.19	0.76
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.83	0.76
4:B:46:GLN:HG3	4:B:47:GLN:H	1.50	0.76
3:A:868:TYR:CE2	3:A:1366:ARG:HD3	2.21	0.76
4:B:427:ASP:HA	4:B:430:ARG:HH11	1.50	0.76
5:C:99:LEU:HD23	5:C:99:LEU:N	2.01	0.76
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.48	0.76
5:C:242:GLN:O	5:C:246:ARG:HG3	1.85	0.76
3:A:30:ILE:HG13	4:B:1183:LYS:HZ1	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:ILE:CG2	11:K:50:LEU:HD12	2.16	0.76
3:A:573:SER:O	3:A:576:GLN:HB2	1.85	0.76
11:K:12:LEU:HD12	11:K:12:LEU:N	2.00	0.76
3:A:528:LEU:C	3:A:530:GLY:N	2.38	0.76
3:A:84:ILE:HG22	3:A:241:VAL:CG2	2.16	0.76
7:F:107:VAL:HG11	7:F:111:LEU:HD11	1.66	0.76
8:H:134:ASN:O	8:H:135:LEU:O	2.04	0.76
4:B:859:TYR:OH	4:B:941:LEU:HD22	1.86	0.76
3:A:106:VAL:CG1	3:A:107:CYS:N	2.49	0.76
3:A:107:CYS:SG	3:A:108:MET:N	2.58	0.76
4:B:521:LEU:HD21	4:B:635:ARG:HG2	1.67	0.75
3:A:902:LEU:HD11	3:A:926:GLN:HG3	1.67	0.75
9:I:29:CYS:SG	9:I:31:THR:CB	2.74	0.75
3:A:1154:TYR:HE1	9:I:18:GLU:HG2	1.50	0.75
10:J:10:CYS:HB2	10:J:45:CYS:SG	2.25	0.75
3:A:896:ARG:HD2	3:A:897:TYR:HE1	1.51	0.75
3:A:901:LEU:O	3:A:903:ASN:N	2.20	0.75
4:B:1072:MET:CE	4:B:1085:ILE:HG21	2.17	0.75
6:E:198:ILE:HD11	6:E:212:ARG:HG3	1.68	0.75
3:A:1242:VAL:CG1	3:A:1243:VAL:H	1.92	0.75
3:A:546:VAL:HG12	3:A:550:LEU:HD21	1.68	0.75
3:A:608:ILE:O	3:A:609:ASP:O	2.04	0.75
3:A:1120:LEU:HB3	3:A:1124:HIS:O	1.86	0.75
3:A:1206:ASP:O	3:A:1274:ARG:NH1	2.19	0.75
4:B:640:VAL:HG23	4:B:740:HIS:N	2.00	0.75
3:A:868:TYR:CD1	3:A:1064:VAL:HG21	2.22	0.75
3:A:352:VAL:HG12	3:A:353:ILE:N	2.00	0.75
4:B:99:LYS:HB3	4:B:180:TYR:CE2	2.21	0.75
6:E:13:TRP:CE3	6:E:39:LEU:HD13	2.22	0.75
5:C:5:GLY:O	5:C:7:GLN:HG2	1.87	0.75
12:L:48:CYS:CB	12:L:51:CYS:O	2.34	0.75
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.66	0.75
4:B:385:LEU:O	4:B:385:LEU:HG	1.86	0.75
3:A:1444:MET:HB2	7:F:133:VAL:HG12	1.67	0.75
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.01	0.75
4:B:1024:ALA:HA	4:B:1027:ILE:HD12	1.67	0.75
4:B:556:THR:HG22	4:B:557:PHE:N	2.02	0.75
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.50	0.75
4:B:806:THR:HG22	4:B:808:ALA:N	2.00	0.75
7:F:125:LEU:HB2	7:F:130:ILE:HD12	1.69	0.75
3:A:321:PRO:O	3:A:322:VAL:CG1	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:THR:OG1	3:A:1211:GLN:OE1	2.03	0.75
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.87	0.75
3:A:886:ILE:HG12	3:A:943:LEU:CD1	2.16	0.75
6:E:111:VAL:CG1	6:E:111:VAL:O	2.35	0.75
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.52	0.75
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.51	0.75
4:B:482:VAL:O	4:B:482:VAL:HG23	1.87	0.74
3:A:648:ASN:O	3:A:652:VAL:HG23	1.86	0.74
3:A:445:ASN:HD22	3:A:446:ARG:N	1.85	0.74
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.87	0.74
3:A:1101:LEU:HG	3:A:1105:LEU:HD11	1.69	0.74
9:I:111:THR:HG22	9:I:113:ASP:H	1.52	0.74
8:H:7:ASP:O	8:H:8:ASP:HB2	1.87	0.74
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	1.84	0.74
4:B:421:PHE:O	4:B:425:THR:HB	1.86	0.74
11:K:33:ILE:HD12	11:K:73:LEU:HD23	1.67	0.74
3:A:399:HIS:O	3:A:435:HIS:CD2	2.40	0.74
3:A:90:VAL:CG1	3:A:297:GLN:NE2	2.41	0.74
4:B:899:ILE:HD11	4:B:911:ILE:CG1	2.18	0.74
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.17	0.74
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.63	0.74
11:K:40:HIS:CE1	11:K:63:VAL:CG1	2.70	0.74
4:B:955:THR:CG2	4:B:956:THR:N	2.44	0.74
4:B:96:TYR:N	4:B:129:PHE:O	2.21	0.74
11:K:87:LEU:O	11:K:90:ALA:HB3	1.86	0.74
3:A:152:VAL:O	3:A:162:VAL:HG23	1.87	0.74
9:I:50:THR:HG22	9:I:52:ILE:H	1.52	0.74
4:B:546:SER:OG	4:B:631:GLY:N	2.19	0.74
3:A:680:THR:HG22	3:A:681:GLU:N	2.00	0.74
5:C:241:ASP:O	5:C:245:VAL:HG23	1.87	0.74
3:A:1025:ARG:CG	3:A:1025:ARG:HH11	2.00	0.74
4:B:986:GLN:HE21	4:B:1016:ALA:HB1	1.51	0.74
4:B:464:GLY:CA	4:B:478:GLY:HA2	2.15	0.74
4:B:428:ILE:C	4:B:430:ARG:N	2.35	0.74
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.70	0.74
3:A:37:PHE:H	3:A:52:GLY:HA2	1.53	0.74
3:A:4:GLN:HE22	4:B:1159:ARG:H	1.33	0.74
4:B:174:LEU:HD12	4:B:179:CYS:SG	2.28	0.74
4:B:128:LEU:HB3	4:B:167:ILE:O	1.87	0.74
9:I:31:THR:HG22	9:I:32:CYS:N	2.03	0.74
3:A:1025:ARG:HA	3:A:1030:ARG:NH1	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:58:LEU:N	5:C:58:LEU:HD23	2.03	0.74
4:B:1165:ILE:CG2	4:B:1166:CYS:N	2.48	0.74
3:A:401:GLY:N	3:A:435:HIS:HD2	1.84	0.74
4:B:247:GLY:O	4:B:248:SER:HB2	1.86	0.74
11:K:27:ALA:HB1	11:K:28:PRO:CD	2.17	0.74
3:A:794:PRO:HG2	3:A:795:GLU:H	1.52	0.74
3:A:90:VAL:CG1	3:A:297:GLN:CB	2.66	0.74
3:A:868:TYR:CE1	3:A:1064:VAL:CG1	2.68	0.74
1:R:8:G:O2'	1:R:9:G:H5'	1.87	0.74
3:A:635:ARG:HH21	3:A:877:HIS:HA	1.53	0.74
4:B:247:GLY:O	4:B:248:SER:CB	2.36	0.74
3:A:902:LEU:O	3:A:903:ASN:HB2	1.88	0.74
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.70	0.74
3:A:569:LYS:HG2	3:A:571:LEU:CD1	2.17	0.74
3:A:1004:ASN:C	3:A:1004:ASN:OD1	2.27	0.74
5:C:145:CYS:HA	10:J:2:ILE:HD11	1.67	0.74
1:R:9:G:C4'	4:B:1097:HIS:NE2	2.51	0.74
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.23	0.74
4:B:291:ILE:CG2	4:B:297:ILE:HD13	2.18	0.73
5:C:58:LEU:HD11	10:J:2:ILE:HD12	1.70	0.73
1:R:10:A:H8	1:R:10:A:OP2	1.70	0.73
3:A:1355:VAL:CG1	3:A:1356:ILE:N	2.51	0.73
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.01	0.73
5:C:37:MET:SD	5:C:232:VAL:HG21	2.27	0.73
4:B:862:GLN:O	4:B:914:LYS:NZ	2.20	0.73
12:L:46:VAL:O	12:L:47:ARG:HB2	1.87	0.73
3:A:151:ASP:OD1	3:A:163:SER:CA	2.36	0.73
3:A:43:GLU:O	3:A:46:THR:HB	1.87	0.73
3:A:320:ARG:HH21	4:B:471:LYS:CB	2.01	0.73
3:A:523:ILE:HD13	3:A:622:VAL:CG2	2.18	0.73
1:R:9:G:H4'	4:B:1097:HIS:NE2	2.04	0.73
8:H:108:SER:O	8:H:109:LYS:CB	2.36	0.73
4:B:310:MET:O	4:B:313:MET:HB2	1.88	0.73
3:A:1355:VAL:HG12	3:A:1356:ILE:H	1.51	0.73
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.18	0.73
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.02	0.73
3:A:179:LEU:HD13	3:A:297:GLN:HG2	1.71	0.73
4:B:843:GLN:HA	4:B:846:ILE:HD12	1.68	0.73
11:K:40:HIS:HE1	11:K:63:VAL:CG1	2.01	0.73
12:L:29:TYR:HB3	12:L:56:LEU:HD22	1.70	0.73
9:I:99:LEU:HB2	9:I:112:SER:CB	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:194:GLU:O	6:E:213:ILE:HD12	1.88	0.73
3:A:92:HIS:HB2	3:A:236:LEU:CD1	2.19	0.73
3:A:599:SER:O	3:A:601:LYS:N	2.22	0.73
10:J:45:CYS:O	10:J:48:ARG:HG3	1.88	0.73
8:H:42:ILE:O	8:H:44:VAL:HG23	1.89	0.73
3:A:541:ILE:HG22	3:A:546:VAL:HG22	1.70	0.73
11:K:58:PHE:HE2	11:K:74:ARG:NE	1.82	0.73
5:C:69:LEU:O	10:J:6:ARG:HD2	1.87	0.73
5:C:120:ILE:HD11	5:C:130:GLY:O	1.88	0.73
4:B:541:LEU:HD12	4:B:747:MET:HE1	1.70	0.73
9:I:96:SER:HB2	9:I:98:VAL:HG23	1.69	0.73
6:E:162:ARG:NH2	6:E:166:LYS:NZ	2.36	0.73
3:A:1067:LEU:HD21	3:A:1367:HIS:CE1	2.15	0.73
4:B:369:GLY:O	4:B:370:PHE:HD1	1.71	0.73
6:E:179:GLN:HB2	6:E:182:ASP:HB2	1.68	0.73
4:B:698:GLU:O	4:B:701:ILE:CD1	2.37	0.73
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.24	0.73
4:B:287:ARG:CG	4:B:292:ILE:HD13	2.16	0.73
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.24	0.73
3:A:475:THR:HG22	3:A:476:SER:H	1.53	0.73
4:B:1152:MET:O	4:B:1157:ALA:HB2	1.88	0.73
3:A:421:ALA:HA	3:A:424:ILE:HD11	1.70	0.73
8:H:11:GLN:N	8:H:29:ALA:O	2.21	0.73
3:A:929:LEU:HD21	3:A:983:ILE:HG23	1.70	0.73
4:B:882:THR:HG22	4:B:883:LEU:N	2.02	0.73
3:A:170:THR:HG22	3:A:171:GLN:H	1.53	0.73
3:A:1422:ARG:NH2	4:B:1220:ARG:HD3	1.99	0.73
4:B:1165:ILE:HG22	4:B:1166:CYS:H	1.50	0.73
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.69	0.73
3:A:1428:VAL:HG13	4:B:1151:LEU:CD2	2.19	0.73
3:A:1161:THR:HG22	3:A:1162:VAL:H	1.54	0.72
3:A:35:ILE:HG22	3:A:270:LEU:HD13	1.71	0.72
4:B:227:LYS:N	4:B:395:GLN:OE1	2.21	0.72
3:A:1154:TYR:CE2	3:A:1156:PRO:HB3	2.23	0.72
4:B:55:VAL:HG12	4:B:56:ASP:N	2.02	0.72
3:A:1169:ILE:HD12	3:A:1169:ILE:N	2.00	0.72
4:B:708:GLU:C	4:B:710:LEU:H	1.91	0.72
3:A:553:VAL:HG13	3:A:648:ASN:HB3	1.70	0.72
3:A:1067:LEU:CD2	3:A:1367:HIS:HE1	2.00	0.72
4:B:1203:LEU:CD1	4:B:1207:LEU:HG	2.19	0.72
4:B:783:THR:HG22	10:J:63:TYR:HE1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.37	0.72
3:A:675:THR:O	3:A:679:ILE:HG13	1.90	0.72
8:H:93:TYR:CD1	8:H:143:LEU:CB	2.72	0.72
9:I:33:SER:O	9:I:35:VAL:HG23	1.89	0.72
4:B:751:VAL:HG12	4:B:752:ALA:H	1.54	0.72
3:A:873:MET:HG2	3:A:957:PRO:CG	2.19	0.72
4:B:708:GLU:HG3	4:B:709:ASP:N	2.04	0.72
4:B:817:LEU:N	4:B:818:PRO:HD3	2.02	0.72
3:A:1156:PRO:O	3:A:1158:PRO:HD3	1.90	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.90	0.72
9:I:103:CYS:O	9:I:104:LEU:HD23	1.89	0.72
4:B:868:MET:O	4:B:869:SER:OG	2.04	0.72
3:A:1209:MET:SD	3:A:1236:LEU:HD22	2.29	0.72
6:E:178:ILE:HG12	6:E:179:GLN:N	2.03	0.72
4:B:129:PHE:CE2	4:B:166:PHE:HB3	2.24	0.72
6:E:124:VAL:H	6:E:125:PRO:HD2	1.54	0.72
3:A:1154:TYR:CE1	9:I:18:GLU:HG2	2.25	0.72
3:A:444:PHE:CE2	3:A:470:LEU:HD23	2.24	0.72
9:I:19:ASP:CB	9:I:24:ARG:HG3	2.20	0.72
4:B:123:THR:HG22	4:B:125:SER:HB3	1.70	0.72
3:A:1018:PHE:O	3:A:1021:LEU:HB3	1.88	0.72
3:A:1434:ALA:O	3:A:1436:ILE:N	2.21	0.72
3:A:660:ASN:C	3:A:660:ASN:HD22	1.92	0.72
4:B:830:TYR:HE1	4:B:1000:PRO:HB3	1.53	0.72
4:B:166:PHE:CD2	4:B:166:PHE:C	2.61	0.72
5:C:57:VAL:HB	5:C:58:LEU:HD23	1.70	0.72
4:B:98:THR:O	4:B:126:SER:CB	2.38	0.72
3:A:378:GLU:OE1	3:A:434:ARG:NH1	2.22	0.72
4:B:638:PHE:CD1	4:B:743:ILE:HD13	2.24	0.72
4:B:474:SER:O	4:B:475:SER:C	2.28	0.72
10:J:52:THR:O	10:J:54:VAL:HG23	1.90	0.72
9:I:41:PRO:O	9:I:43:VAL:HG23	1.89	0.72
3:A:185:TRP:HH2	3:A:200:ARG:HD3	1.55	0.72
6:E:37:LEU:HG	6:E:37:LEU:O	1.88	0.72
4:B:56:ASP:C	4:B:57:TYR:HD1	1.93	0.72
10:J:7:CYS:CA	10:J:49:MET:HE3	2.19	0.72
4:B:112:LEU:O	4:B:180:TYR:HE1	1.73	0.72
3:A:565:ILE:HG12	3:A:567:LYS:HZ1	1.54	0.72
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.72	0.72
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.38	0.72
3:A:351:THR:HG23	4:B:1103:ILE:CD1	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1196:ILE:HB	4:B:1197:PRO:HD2	1.72	0.71
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.10	0.71
4:B:426:LYS:O	4:B:430:ARG:HD2	1.91	0.71
4:B:356:LEU:HD23	4:B:356:LEU:N	2.04	0.71
4:B:796:LEU:HB3	4:B:799:PRO:CD	2.19	0.71
3:A:1424:VAL:HG22	3:A:1436:ILE:HD11	1.71	0.71
8:H:51:ALA:O	8:H:52:GLN:C	2.28	0.71
4:B:63:ILE:CD1	4:B:95:ILE:HD12	2.21	0.71
4:B:291:ILE:HG22	4:B:297:ILE:HD13	1.73	0.71
9:I:15:TYR:O	9:I:27:PHE:HD2	1.73	0.71
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.72	0.71
3:A:103:CYS:C	3:A:105:CYS:N	2.44	0.71
4:B:527:THR:OG1	4:B:528:PRO:HD2	1.90	0.71
3:A:1194:ARG:NH2	3:A:1237:ILE:CD1	2.54	0.71
4:B:1006:ILE:HD11	10:J:45:CYS:SG	2.30	0.71
3:A:1436:ILE:O	3:A:1439:GLY:N	2.24	0.71
3:A:417:TYR:O	3:A:418:SER:HB3	1.90	0.71
4:B:723:VAL:O	4:B:724:ASP:C	2.29	0.71
3:A:403:LYS:HB2	3:A:404:TYR:CD1	2.26	0.71
3:A:1227:ILE:HG22	3:A:1228:TRP:H	1.53	0.71
3:A:1116:LEU:N	3:A:1308:THR:HB	2.03	0.71
3:A:785:PRO:HG2	4:B:703:ILE:HD12	1.72	0.71
11:K:102:LYS:O	11:K:106:GLU:HG3	1.90	0.71
3:A:530:GLY:O	3:A:531:ILE:C	2.29	0.71
3:A:244:PRO:O	3:A:247:ARG:N	2.23	0.71
4:B:952:VAL:HG22	4:B:966:VAL:HG13	1.73	0.71
4:B:287:ARG:NH1	4:B:324:ILE:O	2.24	0.71
3:A:475:THR:HG22	3:A:476:SER:N	2.05	0.71
3:A:984:LYS:O	3:A:988:LEU:HB2	1.89	0.71
4:B:37:PHE:O	4:B:39:ARG:N	2.23	0.71
3:A:265:LYS:HE2	3:A:323:LYS:CE	2.18	0.71
3:A:68:GLN:O	3:A:70:CYS:N	2.24	0.71
3:A:869:GLY:O	3:A:870:GLU:HB2	1.88	0.71
4:B:34:ILE:HD11	4:B:743:ILE:HG22	1.72	0.71
4:B:63:ILE:HD13	4:B:95:ILE:HD12	1.71	0.71
4:B:1155:SER:OG	4:B:1156:ASP:N	2.21	0.71
11:K:53:ASP:O	11:K:56:VAL:CG2	2.35	0.71
4:B:788:ARG:HB2	4:B:788:ARG:HH11	1.56	0.71
3:A:1007:ILE:O	3:A:1010:ALA:N	2.22	0.71
3:A:970:THR:HG22	3:A:970:THR:O	1.89	0.71
6:E:39:LEU:O	6:E:40:GLU:C	2.28	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:39:LEU:O	6:E:41:ASP:N	2.24	0.70
3:A:255:SER:HB3	4:B:918:ILE:HG23	1.73	0.70
3:A:530:GLY:O	3:A:532:ARG:N	2.22	0.70
2:T:4:DA:H2'	2:T:5:DT:H72	1.73	0.70
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.06	0.70
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.72	0.70
11:K:91:CYS:O	11:K:94:ILE:HB	1.91	0.70
7:F:83:PRO:HG2	7:F:84:TYR:HD1	1.55	0.70
3:A:1161:THR:CG2	3:A:1162:VAL:H	2.04	0.70
4:B:27:ALA:O	4:B:28:GLU:C	2.26	0.70
4:B:179:CYS:SG	4:B:181:LEU:HD12	2.30	0.70
8:H:44:VAL:HG12	8:H:44:VAL:O	1.92	0.70
3:A:106:VAL:HG12	3:A:107:CYS:N	2.05	0.70
3:A:92:HIS:O	3:A:95:PHE:HB2	1.91	0.70
4:B:857:ARG:NH2	4:B:942:ARG:NH1	2.38	0.70
3:A:242:PRO:O	3:A:247:ARG:NH2	2.20	0.70
4:B:1060:ARG:O	4:B:1063:GLY:N	2.24	0.70
3:A:322:VAL:HB	3:A:323:LYS:CD	2.20	0.70
3:A:302:THR:OG1	3:A:313:GLN:NE2	2.24	0.70
3:A:381:THR:HG22	3:A:383:TYR:HB2	1.72	0.70
3:A:107:CYS:N	3:A:114:LEU:HD21	2.06	0.70
3:A:14:VAL:N	3:A:1432:GLN:HE22	1.85	0.70
5:C:237:SER:O	5:C:238:ILE:HG13	1.89	0.70
5:C:131:HIS:O	5:C:132:PRO:C	2.28	0.70
3:A:1041:ALA:O	3:A:1044:TRP:HB3	1.91	0.70
7:F:98:ALA:CA	7:F:101:ILE:HD12	2.21	0.70
3:A:39:GLU:O	3:A:53:LEU:HB2	1.91	0.70
3:A:40:THR:O	3:A:41:MET:HG3	1.90	0.70
4:B:115:GLN:O	4:B:119:LEU:HD12	1.91	0.70
3:A:894:GLU:C	3:A:896:ARG:N	2.43	0.70
3:A:875:ALA:HA	3:A:878:ILE:HD12	1.71	0.70
8:H:109:LYS:HB3	8:H:110:ASP:CG	2.10	0.70
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	1.72	0.70
3:A:971:PHE:HB2	3:A:973:ILE:HD13	1.72	0.70
3:A:901:LEU:HD23	3:A:907:THR:HG21	1.71	0.70
4:B:274:PRO:O	4:B:276:ILE:HG13	1.92	0.70
3:A:834:THR:HG21	3:A:1077:THR:CB	2.21	0.70
3:A:805:LEU:C	3:A:805:LEU:CD1	2.60	0.70
4:B:1060:ARG:O	4:B:1062:HIS:N	2.25	0.70
3:A:1285:MET:HG2	3:A:1307:GLU:OE2	1.91	0.70
3:A:1213:GLY:HA2	3:A:1216:ILE:HD12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:LEU:HD12	3:A:297:GLN:HG2	1.73	0.70
3:A:120:GLU:HG3	3:A:123:ARG:HD3	1.74	0.70
4:B:1084:GLN:HG2	5:C:201:TRP:CH2	2.27	0.70
3:A:1143:LEU:O	3:A:1146:VAL:HG23	1.91	0.70
5:C:11:ARG:HE	5:C:21:ILE:HD11	1.56	0.70
3:A:1006:ILE:HD11	6:E:163:GLU:OE2	1.92	0.70
7:F:72:LYS:O	7:F:73:ALA:HB2	1.90	0.70
2:T:6:DC:C2'	2:T:7:DC:H5'	2.18	0.70
6:E:113:GLN:O	6:E:114:ASN:ND2	2.25	0.70
3:A:247:ARG:O	3:A:247:ARG:CG	2.39	0.70
3:A:1017:LEU:HB2	6:E:205:SER:HA	1.74	0.70
3:A:1152:ILE:HG22	3:A:1152:ILE:O	1.90	0.70
3:A:261:ASP:HB3	3:A:323:LYS:CG	2.22	0.70
3:A:322:VAL:HB	3:A:323:LYS:CG	2.21	0.70
4:B:992:ILE:CD1	11:K:67:PHE:HE2	2.04	0.70
3:A:325:ILE:O	3:A:329:LEU:HG	1.92	0.70
4:B:423:LYS:NZ	4:B:423:LYS:HB2	2.07	0.70
3:A:607:ILE:HG12	3:A:612:ILE:HA	1.72	0.70
3:A:599:SER:HB3	3:A:603:ASN:H	1.57	0.70
6:E:29:PHE:O	6:E:30:ILE:HG13	1.91	0.70
4:B:642:ASP:O	4:B:644:GLU:N	2.25	0.69
4:B:634:TYR:CE1	4:B:692:TYR:HD1	2.09	0.69
4:B:739:THR:OG1	4:B:740:HIS:CE1	2.44	0.69
12:L:29:TYR:O	12:L:30:ILE:HG13	1.91	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.06	0.69
3:A:590:ARG:NH2	3:A:620:LYS:O	2.25	0.69
6:E:198:ILE:CD1	6:E:212:ARG:HG3	2.22	0.69
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.73	0.69
3:A:1200:ALA:O	3:A:1202:MET:N	2.25	0.69
4:B:501:PRO:O	4:B:502:ILE:HB	1.92	0.69
3:A:818:MET:O	3:A:819:GLY:O	2.10	0.69
4:B:840:ILE:HG12	4:B:992:ILE:HG22	1.74	0.69
4:B:893:LEU:HD21	4:B:913:GLY:N	2.07	0.69
6:E:131:THR:CG2	6:E:132:ILE:H	1.90	0.69
4:B:30:SER:O	4:B:34:ILE:HD13	1.91	0.69
3:A:321:PRO:O	3:A:322:VAL:CB	2.40	0.69
4:B:1103:ILE:CD1	4:B:1103:ILE:N	2.42	0.69
3:A:302:THR:CG2	3:A:313:GLN:NE2	2.54	0.69
3:A:1028:THR:O	3:A:1029:ARG:C	2.31	0.69
4:B:882:THR:HG21	4:B:935:ARG:CA	2.17	0.69
4:B:373:ARG:HA	4:B:566:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:115:ASN:C	6:E:116:ILE:HG12	2.13	0.69
4:B:313:MET:HG3	4:B:390:LEU:HD21	1.74	0.69
5:C:110:THR:HG22	5:C:110:THR:O	1.91	0.69
3:A:450:LEU:HD12	3:A:450:LEU:H	1.58	0.69
4:B:899:ILE:HD11	4:B:911:ILE:HG23	1.74	0.69
3:A:901:LEU:HB2	3:A:926:GLN:HG2	1.75	0.69
6:E:35:VAL:O	6:E:37:LEU:N	2.25	0.69
3:A:1126:ALA:O	3:A:1128:GLN:N	2.25	0.69
4:B:1104:HIS:CG	4:B:1122:ARG:HB2	2.28	0.69
6:E:60:PHE:CE2	6:E:80:VAL:HG21	2.27	0.69
3:A:380:VAL:CG2	3:A:430:TRP:N	2.50	0.69
5:C:148:ARG:NH1	10:J:64:ASN:HA	2.06	0.69
10:J:52:THR:O	10:J:53:HIS:C	2.31	0.69
3:A:964:ILE:HD12	3:A:1037:LEU:HD21	1.75	0.69
10:J:45:CYS:SG	10:J:46:CYS:N	2.65	0.69
4:B:175:ARG:HH11	4:B:175:ARG:CG	2.05	0.69
4:B:446:LEU:O	4:B:447:ALA:HB3	1.92	0.69
4:B:168:GLY:HA2	4:B:454:THR:HG1	1.55	0.69
4:B:284:ILE:O	4:B:287:ARG:N	2.26	0.69
3:A:1148:ILE:HD11	3:A:1198:ASP:HB2	1.75	0.69
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.57	0.69
3:A:1113:THR:HG22	3:A:1113:THR:O	1.92	0.69
3:A:1161:THR:CG2	3:A:1162:VAL:N	2.56	0.69
3:A:1169:ILE:H	3:A:1169:ILE:CD1	1.90	0.69
3:A:1195:LEU:HD11	3:A:1267:MET:HE3	1.73	0.69
4:B:429:PHE:O	4:B:433:GLN:OE1	2.11	0.69
4:B:420:LEU:HD21	4:B:468:GLU:OE2	1.92	0.69
3:A:622:VAL:HG22	3:A:622:VAL:O	1.93	0.69
4:B:365:THR:HG23	4:B:366:GLN:N	2.06	0.69
4:B:800:GLN:CG	10:J:52:THR:HG21	2.23	0.69
4:B:1095:LEU:C	4:B:1096:ARG:O	2.27	0.69
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.28	0.69
3:A:582:ILE:HG22	3:A:610:GLY:HA2	1.74	0.69
3:A:129:LYS:O	3:A:130:ASP:HB2	1.91	0.69
7:F:120:ILE:HG22	7:F:121:ALA:N	2.07	0.69
4:B:98:THR:O	4:B:126:SER:HB2	1.92	0.69
9:I:2:THR:O	9:I:3:THR:C	2.30	0.69
3:A:1116:LEU:HD21	3:A:1312:ASN:H	1.58	0.69
3:A:261:ASP:CB	3:A:323:LYS:CD	2.63	0.69
3:A:751:SER:HB2	4:B:1015:HIS:HE1	1.57	0.69
4:B:993:THR:O	4:B:994:TYR:HD2	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:LEU:C	8:H:143:LEU:HG	2.13	0.69
3:A:946:VAL:HG22	6:E:201:LYS:HB3	1.75	0.69
4:B:1084:GLN:NE2	5:C:191:TYR:CA	2.55	0.69
3:A:98:LYS:O	3:A:100:LYS:N	2.25	0.69
3:A:1377:THR:C	3:A:1379:GLY:H	1.95	0.69
3:A:321:PRO:CG	3:A:322:VAL:N	2.54	0.69
3:A:115:LEU:HD11	3:A:142:CYS:HB3	1.74	0.69
4:B:236:HIS:CD2	4:B:389:ALA:HB2	2.26	0.69
10:J:59:LYS:O	10:J:62:ARG:HB2	1.93	0.69
5:C:46:ILE:HA	5:C:159:ALA:HA	1.75	0.69
8:H:113:ALA:CA	8:H:125:LEU:O	2.41	0.69
3:A:321:PRO:HD2	3:A:322:VAL:CA	2.17	0.68
5:C:173:ALA:O	5:C:174:ALA:CB	2.40	0.68
4:B:451:LYS:O	4:B:452:THR:C	2.31	0.68
3:A:886:ILE:CD1	3:A:943:LEU:HB2	2.22	0.68
9:I:34:TYR:CD2	9:I:35:VAL:N	2.62	0.68
3:A:456:MET:HG3	3:A:478:TYR:OH	1.94	0.68
7:F:120:ILE:O	7:F:123:LYS:N	2.25	0.68
3:A:151:ASP:OD1	3:A:162:VAL:O	2.10	0.68
6:E:7:ARG:C	6:E:9:ILE:H	1.95	0.68
9:I:55:THR:HG23	9:I:58:VAL:CG2	2.23	0.68
3:A:874:ASP:OD1	3:A:876:ALA:N	2.27	0.68
4:B:121:ASN:N	4:B:121:ASN:HD22	1.90	0.68
4:B:114:PRO:CG	4:B:181:LEU:HD11	2.24	0.68
3:A:532:ARG:HG2	3:A:533:LYS:N	2.07	0.68
3:A:26:GLU:HA	3:A:29:ALA:HB3	1.74	0.68
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.76	0.68
4:B:751:VAL:CG1	4:B:752:ALA:N	2.56	0.68
3:A:471:ASN:O	3:A:474:VAL:HG12	1.94	0.68
6:E:156:LEU:CD2	6:E:197:LYS:HB2	2.23	0.68
5:C:163:ILE:HD12	5:C:166:GLU:HB2	1.76	0.68
3:A:49:LYS:O	3:A:50:ILE:CG1	2.38	0.68
3:A:262:LEU:HG	3:A:328:ARG:NH2	2.09	0.68
3:A:535:THR:CG2	3:A:616:VAL:HA	2.23	0.68
3:A:858:ASN:ND2	3:A:858:ASN:C	2.46	0.68
5:C:92:CYS:SG	5:C:94:LYS:HB2	2.33	0.68
4:B:205:ILE:HG22	4:B:206:ASN:ND2	2.09	0.68
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.77	0.68
3:A:267:ALA:C	3:A:269:ILE:N	2.45	0.68
5:C:141:GLY:O	5:C:142:VAL:HB	1.91	0.68
3:A:901:LEU:O	3:A:902:LEU:C	2.31	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:350:GLN:O	4:B:352:ALA:N	2.27	0.68
3:A:852:TYR:CD2	3:A:1060:PRO:CB	2.77	0.68
3:A:1041:ALA:O	3:A:1044:TRP:N	2.23	0.68
3:A:401:GLY:H	3:A:435:HIS:CD2	2.10	0.68
3:A:765:VAL:HG21	3:A:800:VAL:HG11	1.74	0.68
3:A:809:THR:HB	3:A:810:PRO:HD2	1.74	0.68
9:I:75:CYS:SG	9:I:78:CYS:HB3	2.34	0.68
3:A:873:MET:HG2	3:A:957:PRO:HG3	1.74	0.68
3:A:1254:ALA:O	3:A:1255:GLU:HB2	1.91	0.68
4:B:847:ASP:HB3	5:C:167:HIS:CD2	2.28	0.68
4:B:994:TYR:HB2	4:B:999:MET:CE	2.23	0.68
5:C:39:ALA:HA	5:C:164:ALA:CB	2.24	0.68
4:B:781:PHE:O	4:B:782:LEU:HG	1.93	0.68
3:A:497:THR:HG23	4:B:1146:PHE:HD1	1.59	0.68
4:B:114:PRO:HG3	4:B:181:LEU:CD1	2.24	0.68
4:B:899:ILE:CD1	4:B:911:ILE:HG23	2.24	0.68
12:L:58:LYS:O	12:L:59:ALA:HB3	1.94	0.68
4:B:363:HIS:O	4:B:364:ILE:CB	2.42	0.68
3:A:858:ASN:ND2	3:A:860:LEU:H	1.92	0.68
3:A:444:PHE:HE2	3:A:470:LEU:HD23	1.56	0.68
3:A:1308:THR:HG22	3:A:1309:ASP:N	2.07	0.68
3:A:179:LEU:HD13	3:A:297:GLN:CG	2.24	0.68
3:A:780:VAL:O	3:A:782:ARG:HG2	1.94	0.68
3:A:219:PHE:O	3:A:222:LEU:O	2.12	0.68
4:B:256:VAL:HG11	4:B:382:ILE:HD13	1.73	0.68
3:A:575:LYS:HB3	3:A:612:ILE:HG12	1.76	0.68
11:K:32:VAL:HG23	11:K:74:ARG:CG	2.23	0.68
3:A:20:GLY:C	3:A:21:LEU:HD23	2.14	0.68
3:A:504:LEU:HD11	7:F:91:ALA:HB1	1.76	0.68
4:B:815:ARG:HG3	4:B:815:ARG:NH1	2.08	0.68
3:A:1121:GLU:O	3:A:1124:HIS:O	2.12	0.68
3:A:1095:THR:OG1	3:A:1113:THR:HB	1.94	0.68
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.29	0.68
3:A:1308:THR:HG22	3:A:1310:GLY:N	2.09	0.68
3:A:1339:LEU:HD13	6:E:147:HIS:HD2	1.59	0.68
3:A:40:THR:HG22	3:A:41:MET:CE	2.23	0.68
3:A:10:PRO:O	4:B:1193:GLN:HB3	1.94	0.68
8:H:93:TYR:CD2	8:H:145:ARG:HD3	2.29	0.68
4:B:369:GLY:O	4:B:370:PHE:CD1	2.47	0.68
3:A:710:LEU:HD12	3:A:710:LEU:H	1.59	0.68
4:B:34:ILE:H	4:B:34:ILE:HD13	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:918:ILE:O	4:B:933:SER:N	2.27	0.68
9:I:117:LYS:O	9:I:118:ARG:HG2	1.94	0.68
11:K:47:ARG:HH11	11:K:47:ARG:CG	2.07	0.68
3:A:356:ASP:HB2	3:A:469:ARG:NH1	2.09	0.68
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.29	0.67
3:A:30:ILE:HD11	4:B:1170:THR:OG1	1.94	0.67
3:A:211:PHE:O	3:A:213:HIS:N	2.27	0.67
3:A:534:LEU:O	3:A:539:THR:HG21	1.94	0.67
3:A:856:THR:HG22	3:A:856:THR:O	1.94	0.67
4:B:36:ALA:C	4:B:37:PHE:O	2.21	0.67
5:C:115:SER:CB	5:C:141:GLY:O	2.40	0.67
5:C:245:VAL:HA	5:C:248:ILE:HD12	1.76	0.67
3:A:868:TYR:CZ	3:A:1366:ARG:HD3	2.29	0.67
4:B:1024:ALA:HA	4:B:1027:ILE:CD1	2.23	0.67
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.30	0.67
5:C:32:SER:HA	5:C:35:ARG:HG3	1.74	0.67
3:A:913:LEU:HD11	3:A:981:LEU:O	1.95	0.67
4:B:817:LEU:N	4:B:818:PRO:CD	2.57	0.67
4:B:1156:ASP:HB3	4:B:1198:TYR:N	2.09	0.67
3:A:807:GLY:O	4:B:728:ARG:HD3	1.94	0.67
3:A:225:ASN:O	3:A:226:GLU:C	2.32	0.67
5:C:143:LEU:C	5:C:143:LEU:HD12	2.13	0.67
3:A:901:LEU:HG	3:A:926:GLN:NE2	1.99	0.67
8:H:47:PHE:CD2	8:H:95:TYR:HB2	2.29	0.67
6:E:57:MET:O	6:E:57:MET:HG2	1.95	0.67
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.76	0.67
5:C:145:CYS:HA	10:J:2:ILE:CD1	2.23	0.67
6:E:112:TYR:CZ	6:E:136:ASN:HB2	2.29	0.67
8:H:128:ASN:O	8:H:128:ASN:OD1	2.13	0.67
3:A:375:THR:OG1	3:A:434:ARG:N	2.27	0.67
3:A:1036:ARG:HG3	3:A:1036:ARG:HH11	1.60	0.67
4:B:597:MET:O	4:B:598:GLU:C	2.30	0.67
3:A:1193:LEU:HD12	3:A:1193:LEU:C	2.15	0.67
3:A:1136:SER:HB3	3:A:1206:ASP:OD2	1.95	0.67
4:B:641:GLU:O	4:B:643:ASP:N	2.28	0.67
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.01	0.67
3:A:1422:ARG:NH2	4:B:1220:ARG:CD	2.56	0.67
10:J:2:ILE:C	10:J:53:HIS:NE2	2.47	0.67
3:A:582:ILE:CG2	3:A:610:GLY:HA2	2.25	0.67
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.07	0.67
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:59:LEU:HD11	4:B:417:PHE:CE2	2.30	0.67
3:A:253:ASN:CG	3:A:254:GLU:N	2.47	0.67
5:C:74:SER:HB3	5:C:77:ILE:HG13	1.77	0.67
3:A:96:ILE:HG22	3:A:97:ALA:H	1.58	0.67
3:A:131:SER:O	3:A:134:ARG:HB3	1.93	0.67
3:A:535:THR:HG21	3:A:617:VAL:N	2.07	0.67
1:R:5:A:H2'	1:R:6:G:C8	2.30	0.67
3:A:1228:TRP:HA	3:A:1237:ILE:O	1.94	0.67
3:A:751:SER:HB2	4:B:1015:HIS:CE1	2.30	0.67
4:B:1104:HIS:CB	4:B:1122:ARG:HB2	2.24	0.67
5:C:18:VAL:CG2	5:C:240:VAL:CG1	2.73	0.67
3:A:889:SER:O	3:A:940:ARG:NH2	2.27	0.67
3:A:852:TYR:CD2	3:A:1060:PRO:HB2	2.29	0.67
4:B:1069:PHE:HA	4:B:1085:ILE:O	1.94	0.67
3:A:391:LEU:O	3:A:394:ASN:N	2.28	0.67
6:E:190:LEU:HD23	6:E:190:LEU:N	2.09	0.67
4:B:986:GLN:NE2	4:B:1016:ALA:HB1	2.09	0.67
3:A:289:ILE:O	3:A:291:GLU:N	2.28	0.67
4:B:1180:PHE:O	4:B:1181:GLU:O	2.12	0.67
6:E:156:LEU:HG	6:E:195:VAL:O	1.94	0.67
11:K:61:TYR:CD1	11:K:61:TYR:C	2.68	0.67
4:B:957:ASN:O	4:B:958:GLN:C	2.32	0.67
3:A:166:GLY:O	3:A:167:CYS:HB3	1.94	0.67
4:B:321:GLY:O	4:B:323:VAL:N	2.25	0.67
3:A:115:LEU:HD12	3:A:122:MET:CE	2.25	0.67
3:A:99:ILE:CA	3:A:102:VAL:HG23	2.24	0.67
3:A:401:GLY:C	3:A:435:HIS:CD2	2.68	0.67
3:A:1099:PRO:HG2	3:A:1100:ARG:H	1.59	0.67
5:C:186:LEU:HB3	5:C:188:HIS:HD2	1.60	0.67
8:H:128:ASN:OD1	8:H:131:ASN:ND2	2.28	0.67
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.30	0.67
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.30	0.67
5:C:226:ASP:O	5:C:227:THR:HB	1.95	0.67
7:F:111:LEU:H	7:F:111:LEU:HD13	1.59	0.67
3:A:267:ALA:O	3:A:269:ILE:N	2.28	0.66
5:C:240:VAL:O	5:C:243:VAL:N	2.28	0.66
3:A:892:ALA:HA	3:A:895:LYS:CB	2.13	0.66
4:B:376:PHE:CE2	4:B:569:TYR:HD2	2.13	0.66
6:E:79:TRP:N	6:E:107:THR:O	2.28	0.66
4:B:797:TYR:O	4:B:799:PRO:HD2	1.94	0.66
3:A:546:VAL:O	3:A:550:LEU:HD23	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1060:ARG:C	4:B:1062:HIS:H	1.99	0.66
3:A:689:LYS:HB3	3:A:721:PHE:CD1	2.30	0.66
3:A:783:THR:CG2	3:A:815:PHE:HE2	2.07	0.66
4:B:778:MET:CE	4:B:853:SER:HB3	2.25	0.66
4:B:1203:LEU:HD12	4:B:1207:LEU:HG	1.78	0.66
3:A:542:GLU:O	3:A:546:VAL:HG23	1.95	0.66
5:C:249:ASP:OD1	5:C:253:LYS:HE3	1.95	0.66
4:B:1120:GLU:O	4:B:1124:ARG:NH1	2.28	0.66
3:A:313:GLN:O	3:A:314:ALA:CB	2.44	0.66
4:B:1170:THR:CG2	4:B:1183:LYS:HZ1	2.08	0.66
4:B:352:ALA:C	4:B:354:ASP:H	1.97	0.66
10:J:53:HIS:HE1	10:J:55:ASP:OD1	1.79	0.66
3:A:185:TRP:CH2	3:A:200:ARG:HD3	2.30	0.66
8:H:76:THR:O	8:H:77:ARG:O	2.12	0.66
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.35	0.66
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.77	0.66
4:B:128:LEU:HB2	4:B:168:GLY:O	1.95	0.66
4:B:46:GLN:NE2	4:B:496:ARG:HG2	2.09	0.66
3:A:423:ASP:C	3:A:424:ILE:HG13	2.14	0.66
3:A:814:PHE:O	3:A:817:ALA:HB3	1.94	0.66
3:A:523:ILE:HG22	3:A:528:LEU:HB2	1.77	0.66
3:A:108:MET:N	3:A:108:MET:SD	2.68	0.66
3:A:1398:MET:HB2	3:A:1426:GLU:OE2	1.96	0.66
3:A:445:ASN:HB2	3:A:454:SER:O	1.96	0.66
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.28	0.66
3:A:261:ASP:HB3	3:A:323:LYS:CE	2.25	0.66
3:A:902:LEU:CD1	3:A:926:GLN:HG3	2.25	0.66
3:A:925:LEU:O	3:A:927:VAL:N	2.28	0.66
6:E:61:GLN:HG2	6:E:62:ALA:N	2.10	0.66
4:B:108:VAL:CG1	4:B:109:THR:H	2.04	0.66
3:A:582:ILE:HD11	3:A:629:LEU:HD11	1.76	0.66
3:A:364:VAL:HG12	3:A:458:HIS:HB3	1.77	0.66
4:B:227:LYS:HB2	4:B:395:GLN:OE1	1.96	0.66
3:A:990:VAL:HG21	3:A:1026:LEU:O	1.95	0.66
4:B:93:GLY:O	4:B:94:LYS:O	2.13	0.66
3:A:380:VAL:HG22	3:A:430:TRP:O	1.95	0.66
3:A:449:SER:OG	4:B:1134:GLU:OE2	2.14	0.66
3:A:601:LYS:HB3	3:A:603:ASN:OD1	1.95	0.66
3:A:1341:ILE:HG23	3:A:1342:GLU:N	2.10	0.66
3:A:736:ASN:O	3:A:737:LEU:C	2.34	0.66
11:K:53:ASP:OD1	11:K:56:VAL:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:743:VAL:O	3:A:747:VAL:HG23	1.96	0.66
3:A:614:PHE:CD1	3:A:614:PHE:C	2.69	0.66
3:A:849:MET:HG3	3:A:849:MET:O	1.95	0.66
9:I:119:THR:C	9:I:120:GLN:CG	2.64	0.66
3:A:1308:THR:HG21	3:A:1310:GLY:O	1.95	0.66
3:A:374:LEU:HB2	3:A:436:ILE:CD1	2.25	0.66
4:B:1149:GLU:HA	4:B:1153:GLU:OE2	1.96	0.66
4:B:449:ASN:OD1	4:B:451:LYS:HB3	1.96	0.66
3:A:1277:GLU:HG3	3:A:1278:ASN:HD22	1.58	0.66
4:B:1060:ARG:C	4:B:1062:HIS:N	2.48	0.66
3:A:838:GLN:OE1	3:A:838:GLN:O	2.14	0.66
4:B:662:MET:O	4:B:665:GLU:N	2.19	0.66
3:A:70:CYS:C	3:A:71:GLN:HG3	2.15	0.66
6:E:98:ILE:O	6:E:99:HIS:C	2.31	0.66
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.31	0.66
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.48	0.66
7:F:101:ILE:CD1	7:F:121:ALA:HB2	2.26	0.66
3:A:1172:LEU:N	3:A:1172:LEU:HD23	2.10	0.65
3:A:273:ASN:OD1	3:A:296:LEU:HD21	1.96	0.65
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	1.94	0.65
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.31	0.65
3:A:1436:ILE:O	3:A:1437:GLY:C	2.34	0.65
6:E:116:ILE:HG21	6:E:121:MET:HG2	1.78	0.65
7:F:101:ILE:HD13	7:F:117:PRO:O	1.97	0.65
6:E:168:TYR:C	6:E:169:ARG:CG	2.63	0.65
4:B:44:VAL:O	4:B:45:SER:C	2.33	0.65
3:A:650:GLN:O	3:A:654:ASN:HB2	1.97	0.65
4:B:199:MET:O	4:B:200:GLY:O	2.14	0.65
4:B:295:GLY:HA2	4:B:298:LEU:HG	1.78	0.65
4:B:46:GLN:HG3	4:B:47:GLN:N	2.11	0.65
4:B:383:ASN:HD22	4:B:384:ARG:HH11	1.44	0.65
8:H:102:TYR:N	8:H:102:TYR:CD2	2.64	0.65
3:A:1283:VAL:HG12	3:A:1284:MET:N	2.10	0.65
3:A:374:LEU:HB2	3:A:436:ILE:HD12	1.79	0.65
4:B:291:ILE:HD12	4:B:291:ILE:N	2.11	0.65
2:T:8:DT:H2'	2:T:9:DC:H6	1.61	0.65
3:A:993:LEU:HD11	3:A:997:LEU:HD21	1.77	0.65
8:H:77:ARG:HH11	8:H:77:ARG:HB2	1.59	0.65
3:A:1138:ILE:O	3:A:1276:VAL:HG23	1.97	0.65
11:K:63:VAL:O	11:K:63:VAL:HG23	1.96	0.65
4:B:957:ASN:O	4:B:959:ASP:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:645:LEU:O	3:A:649:ILE:HG13	1.96	0.65
3:A:568:PRO:CB	5:C:221:TYR:CE1	2.79	0.65
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.24	0.65
8:H:131:ASN:C	8:H:133:ASN:H	2.00	0.65
3:A:548:ASN:HD21	11:K:47:ARG:HE	1.44	0.65
6:E:178:ILE:HB	6:E:212:ARG:HD3	1.77	0.65
3:A:777:PHE:CE2	3:A:782:ARG:HA	2.31	0.65
3:A:40:THR:HG22	3:A:41:MET:HE3	1.78	0.65
3:A:606:LEU:HB2	3:A:614:PHE:CZ	2.32	0.65
2:T:11:DC:H2'	2:T:12:DG:H8	1.61	0.65
6:E:77:SER:HB3	6:E:105:PHE:HD2	1.61	0.65
11:K:22:ASP:HB3	11:K:23:PRO:HD2	1.79	0.65
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.10	0.65
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	2.11	0.65
4:B:471:LYS:O	4:B:472:ALA:C	2.35	0.65
4:B:428:ILE:C	4:B:430:ARG:H	1.99	0.65
8:H:93:TYR:CE2	8:H:145:ARG:HD3	2.31	0.65
4:B:1203:LEU:HD12	4:B:1203:LEU:C	2.17	0.65
3:A:1102:LYS:O	3:A:1106:ASN:ND2	2.30	0.65
8:H:89:LEU:HB2	8:H:91:ASP:CG	2.17	0.65
9:I:119:THR:C	9:I:120:GLN:HG2	2.17	0.65
4:B:392:ARG:O	4:B:393:LYS:HE3	1.97	0.65
3:A:265:LYS:CE	3:A:323:LYS:CG	2.74	0.65
4:B:882:THR:OG1	4:B:935:ARG:HG3	1.96	0.65
3:A:219:PHE:HE2	3:A:231:PRO:HD2	1.60	0.65
4:B:1072:MET:O	4:B:1081:LEU:HB2	1.96	0.65
11:K:12:LEU:H	11:K:12:LEU:CD1	2.09	0.65
5:C:137:LYS:HG2	5:C:138:GLU:N	2.11	0.65
4:B:637:LEU:HA	4:B:743:ILE:HD11	1.79	0.65
3:A:76:GLU:OE1	4:B:1159:ARG:NH1	2.28	0.65
4:B:352:ALA:O	4:B:356:LEU:HG	1.97	0.65
4:B:778:MET:CE	4:B:853:SER:CB	2.74	0.65
3:A:1154:TYR:HB2	3:A:1191:TRP:CZ3	2.32	0.65
5:C:74:SER:HA	5:C:77:ILE:HG12	1.77	0.65
3:A:997:LEU:N	3:A:997:LEU:HD23	2.10	0.65
6:E:102:GLU:O	6:E:104:ASN:N	2.30	0.65
3:A:756:ILE:HG22	3:A:757:ASN:N	2.10	0.65
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.31	0.65
4:B:1006:ILE:HG21	4:B:1087:PHE:HE2	1.61	0.65
3:A:51:GLY:HA2	3:A:56:PRO:HG2	1.79	0.65
3:A:279:LEU:O	3:A:282:ASN:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:94:LYS:HD3	4:B:95:ILE:O	1.96	0.65
3:A:505:CYS:SG	4:B:1141:HIS:HD2	2.20	0.65
3:A:475:THR:CG2	3:A:476:SER:N	2.60	0.65
3:A:169:ASN:ND2	3:A:169:ASN:N	2.11	0.65
8:H:3:ASN:OD1	8:H:4:THR:N	2.30	0.65
4:B:815:ARG:HH11	4:B:815:ARG:CG	2.09	0.65
3:A:1194:ARG:CZ	3:A:1237:ILE:HD13	2.27	0.64
4:B:62:ILE:CD1	4:B:418:LYS:HE2	2.26	0.64
3:A:96:ILE:CG2	3:A:97:ALA:N	2.59	0.64
3:A:718:VAL:HG12	3:A:722:LEU:HD11	1.78	0.64
4:B:556:THR:HG22	4:B:557:PHE:H	1.58	0.64
4:B:556:THR:CG2	4:B:557:PHE:N	2.59	0.64
3:A:1134:ILE:HA	3:A:1137:ALA:HB3	1.80	0.64
4:B:475:SER:C	4:B:477:ALA:H	2.01	0.64
4:B:211:VAL:O	4:B:480:SER:HA	1.97	0.64
3:A:51:GLY:HA2	3:A:56:PRO:CG	2.28	0.64
4:B:361:LEU:N	4:B:362:PRO:CD	2.60	0.64
4:B:589:VAL:HG12	4:B:590:HIS:N	2.11	0.64
5:C:57:VAL:HG21	10:J:57:ILE:HD11	1.78	0.64
2:T:4:DA:H2"	2:T:5:DT:C6	2.31	0.64
4:B:827:ILE:O	4:B:828:ALA:HB2	1.97	0.64
8:H:3:ASN:CG	8:H:4:THR:N	2.50	0.64
3:A:871:ASP:HB3	6:E:204:THR:HG23	1.79	0.64
4:B:435:THR:O	4:B:437:GLU:N	2.29	0.64
4:B:976:ILE:HD11	4:B:992:ILE:HD12	1.79	0.64
12:L:53:HIS:O	12:L:55:ILE:N	2.30	0.64
3:A:834:THR:HB	3:A:1077:THR:HG23	1.79	0.64
5:C:114:TYR:CD2	5:C:140:ASN:CB	2.80	0.64
3:A:419:LYS:HG3	3:A:420:ARG:HG3	1.77	0.64
3:A:1229:SER:HB3	3:A:1233:ASP:OD2	1.97	0.64
3:A:980:ASP:O	3:A:980:ASP:OD2	2.15	0.64
3:A:1166:ASP:O	3:A:1170:ILE:HG12	1.97	0.64
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	1.78	0.64
6:E:195:VAL:HG22	6:E:213:ILE:HD13	1.79	0.64
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.64
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.78	0.64
3:A:528:LEU:O	3:A:530:GLY:N	2.31	0.64
3:A:528:LEU:CA	3:A:531:ILE:HG22	2.24	0.64
3:A:567:LYS:CB	3:A:568:PRO:CD	2.69	0.64
1:R:8:G:O3'	4:B:776:GLN:NE2	2.31	0.64
3:A:541:ILE:CD1	3:A:574:GLY:HA2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:13:DA:H2"	2:T:14:DT:C5'	2.27	0.64
9:I:109:ILE:HD12	9:I:109:ILE:N	2.12	0.64
3:A:1193:LEU:HD11	3:A:1195:LEU:HD21	1.78	0.64
3:A:209:ASN:O	3:A:212:LYS:N	2.31	0.64
4:B:773:MET:O	4:B:776:GLN:N	2.31	0.64
4:B:1115:THR:HG22	4:B:1117:GLN:HG3	1.80	0.64
11:K:27:ALA:HB1	11:K:28:PRO:HD3	1.78	0.64
3:A:870:GLU:CB	6:E:204:THR:HG21	2.27	0.64
3:A:900:ASP:O	3:A:907:THR:HG23	1.98	0.64
9:I:15:TYR:CD1	9:I:15:TYR:N	2.65	0.64
4:B:1006:ILE:CG2	4:B:1007:VAL:N	2.61	0.64
4:B:1184:GLY:O	4:B:1185:CYS:C	2.36	0.64
3:A:913:LEU:CD1	3:A:914:GLU:N	2.39	0.64
4:B:431:TYR:CD1	4:B:447:ALA:HB2	2.32	0.64
4:B:550:ASP:OD1	4:B:551:PRO:CD	2.45	0.64
8:H:59:ILE:O	8:H:60:ALA:HB3	1.97	0.64
3:A:681:GLU:O	3:A:684:ALA:HB3	1.98	0.64
5:C:184:ASN:O	5:C:187:LYS:N	2.28	0.64
4:B:701:ILE:HG12	4:B:702:LEU:N	2.11	0.64
4:B:846:ILE:HG23	4:B:974:PRO:CG	2.22	0.64
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.27	0.64
3:A:1011:GLN:NE2	3:A:1015:VAL:HG21	2.12	0.64
4:B:93:GLY:O	4:B:94:LYS:C	2.36	0.64
4:B:984:HIS:ND1	4:B:984:HIS:N	2.45	0.64
5:C:93:ASP:OD1	5:C:122:SER:HB2	1.98	0.64
4:B:617:ARG:NE	4:B:619:ILE:HD13	2.13	0.64
4:B:995:ARG:HB3	4:B:997:GLU:OE2	1.98	0.64
10:J:32:GLU:CD	10:J:32:GLU:H	2.01	0.64
3:A:1141:THR:HG21	3:A:1205:LYS:HD2	1.78	0.64
3:A:1308:THR:HG22	3:A:1310:GLY:H	1.61	0.64
3:A:1331:SER:OG	3:A:1333:ILE:HG22	1.98	0.64
6:E:162:ARG:NH2	6:E:166:LYS:HZ3	1.94	0.64
5:C:41:ILE:HD11	5:C:172:PRO:HG3	1.79	0.64
4:B:60:GLN:OE1	4:B:94:LYS:HA	1.97	0.64
3:A:13:THR:HB	3:A:15:LYS:HZ2	1.59	0.64
4:B:1084:GLN:NE2	5:C:192:TRP:N	2.45	0.64
4:B:485:ARG:HH11	4:B:485:ARG:HG3	1.62	0.64
3:A:893:PHE:CD2	3:A:893:PHE:C	2.70	0.64
6:E:211:TYR:CD1	6:E:211:TYR:N	2.65	0.64
3:A:780:VAL:HG23	4:B:699:GLU:OE1	1.97	0.64
11:K:7:PHE:C	11:K:9:LEU:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:380:VAL:CG2	3:A:430:TRP:O	2.45	0.64
3:A:590:ARG:HH21	3:A:621:THR:HA	1.63	0.64
4:B:230:ALA:HB3	4:B:231:PRO:CD	2.25	0.64
9:I:55:THR:HG23	9:I:58:VAL:HG23	1.78	0.64
6:E:102:GLU:C	6:E:104:ASN:H	2.02	0.64
4:B:616:ILE:HD12	4:B:616:ILE:N	2.12	0.64
4:B:1103:ILE:H	4:B:1103:ILE:CD1	1.93	0.63
10:J:10:CYS:SG	10:J:43:ARG:NE	2.71	0.63
3:A:76:GLU:O	3:A:78:PRO:HD3	1.98	0.63
6:E:55:ARG:O	6:E:58:MET:HB2	1.97	0.63
4:B:355:ILE:C	4:B:356:LEU:HD23	2.18	0.63
8:H:12:VAL:HA	8:H:28:ALA:CB	2.29	0.63
9:I:27:PHE:O	9:I:28:GLU:HB3	1.98	0.63
9:I:29:CYS:SG	9:I:32:CYS:N	2.68	0.63
3:A:1410:PHE:O	3:A:1413:GLY:N	2.32	0.63
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	1.98	0.63
3:A:855:THR:HG23	3:A:857:ARG:HG2	1.80	0.63
3:A:352:VAL:CG1	3:A:353:ILE:N	2.61	0.63
3:A:58:LEU:HD21	3:A:243:PRO:HB3	1.77	0.63
3:A:70:CYS:O	3:A:71:GLN:OE1	2.16	0.63
8:H:84:ALA:C	8:H:86:ASP:N	2.48	0.63
3:A:123:ARG:O	3:A:124:GLN:C	2.36	0.63
9:I:15:TYR:HB3	9:I:16:PRO:HD3	1.77	0.63
3:A:8:SER:HG	4:B:1180:PHE:HE1	1.46	0.63
4:B:628:THR:HG22	4:B:628:THR:O	1.97	0.63
4:B:256:VAL:O	4:B:385:LEU:HD13	1.98	0.63
6:E:65:THR:C	6:E:67:GLU:N	2.52	0.63
3:A:1219:THR:CG2	3:A:1271:ILE:HD11	2.29	0.63
3:A:1308:THR:CG2	3:A:1309:ASP:N	2.61	0.63
3:A:1341:ILE:CG2	3:A:1342:GLU:N	2.61	0.63
3:A:777:PHE:HD2	3:A:782:ARG:C	2.02	0.63
4:B:640:VAL:O	4:B:641:GLU:C	2.37	0.63
4:B:957:ASN:ND2	4:B:958:GLN:N	2.45	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.45	0.63
3:A:1434:ALA:CB	3:A:1436:ILE:HD12	2.24	0.63
5:C:74:SER:O	5:C:77:ILE:HB	1.98	0.63
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.18	0.63
3:A:1105:LEU:HB3	3:A:1384:VAL:HG21	1.80	0.63
2:T:11:DC:H2''	2:T:12:DG:H5'	1.80	0.63
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.64	0.63
3:A:265:LYS:HZ1	3:A:322:VAL:HG11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:HG22	8:H:59:ILE:N	2.13	0.63
3:A:95:PHE:CD1	3:A:234:MET:HG2	2.33	0.63
3:A:90:VAL:CG1	3:A:297:GLN:HE21	2.07	0.63
3:A:785:PRO:HG3	4:B:698:GLU:HG2	1.81	0.63
4:B:34:ILE:HD12	4:B:542:MET:HE1	1.80	0.63
4:B:843:GLN:HA	4:B:846:ILE:CD1	2.28	0.63
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.99	0.63
5:C:77:ILE:HD13	5:C:129:ILE:HD11	1.80	0.63
3:A:96:ILE:HG21	3:A:176:LYS:HE3	1.79	0.63
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.27	0.63
3:A:605:MET:CE	3:A:605:MET:HA	2.28	0.63
6:E:187:TYR:O	6:E:187:TYR:CD2	2.51	0.63
6:E:204:THR:HG22	6:E:205:SER:N	2.14	0.63
11:K:47:ARG:HH11	11:K:47:ARG:C	2.02	0.63
4:B:219:ALA:HB3	4:B:222:ILE:HD11	1.81	0.63
3:A:1136:SER:CB	3:A:1206:ASP:OD2	2.47	0.63
4:B:575:PRO:C	4:B:577:ALA:H	2.02	0.63
4:B:585:VAL:HG12	4:B:587:HIS:CD2	2.33	0.63
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.33	0.63
4:B:280:ILE:HG21	4:B:285:ILE:CG1	2.24	0.63
8:H:126:GLU:C	8:H:130:ARG:NH1	2.52	0.63
4:B:52:ASN:O	4:B:56:ASP:HB2	1.98	0.63
3:A:308:ILE:H	3:A:308:ILE:HD12	1.62	0.63
3:A:30:ILE:HG13	4:B:1170:THR:HG23	1.81	0.63
4:B:900:ALA:O	4:B:903:VAL:HG23	1.98	0.63
4:B:377:PHE:O	4:B:380:TYR:N	2.31	0.63
5:C:148:ARG:H	5:C:151:GLN:HG3	1.64	0.63
4:B:546:SER:HA	4:B:612:GLU:OE2	1.99	0.63
4:B:597:MET:O	4:B:600:LEU:N	2.32	0.63
2:T:13:DA:H2"	2:T:14:DT:H5'	1.79	0.63
4:B:519:TRP:C	4:B:519:TRP:CD1	2.72	0.63
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.34	0.63
11:K:7:PHE:O	11:K:9:LEU:N	2.32	0.63
4:B:65:GLU:C	4:B:67:SER:H	1.99	0.63
6:E:131:THR:HG22	6:E:132:ILE:N	2.12	0.63
5:C:43:THR:CG2	5:C:44:LEU:N	2.61	0.63
9:I:101:PHE:N	9:I:101:PHE:CD1	2.66	0.63
3:A:518:LYS:HG3	3:A:519:PRO:O	1.98	0.63
3:A:706:HIS:HD2	3:A:1282:VAL:O	1.82	0.62
4:B:34:ILE:HD13	4:B:34:ILE:N	2.14	0.62
4:B:634:TYR:O	4:B:635:ARG:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:641:GLU:C	4:B:643:ASP:H	2.01	0.62
4:B:637:LEU:HD13	4:B:740:HIS:HB2	1.81	0.62
3:A:68:GLN:C	3:A:70:CYS:N	2.50	0.62
9:I:8:ARG:O	9:I:9:ASP:C	2.37	0.62
4:B:485:ARG:HH11	4:B:485:ARG:CG	2.11	0.62
3:A:1057:VAL:CG1	3:A:1058:VAL:N	2.62	0.62
3:A:265:LYS:CE	3:A:323:LYS:HG3	2.27	0.62
3:A:914:GLU:C	3:A:916:GLY:H	2.02	0.62
6:E:124:VAL:HG22	6:E:132:ILE:HG22	1.80	0.62
4:B:801:LYS:H	10:J:52:THR:CG2	2.11	0.62
3:A:852:TYR:HH	3:A:1441:PHE:HD2	1.46	0.62
3:A:1394:THR:CG2	3:A:1398:MET:HE3	2.29	0.62
3:A:445:ASN:HD22	3:A:446:ARG:H	1.45	0.62
6:E:161:LYS:O	6:E:162:ARG:C	2.37	0.62
3:A:904:THR:HG22	3:A:905:ASP:H	1.64	0.62
4:B:329:THR:HG22	4:B:332:ASP:OD2	1.99	0.62
3:A:476:SER:O	3:A:479:ASN:N	2.32	0.62
4:B:1059:LEU:HD11	4:B:1064:TYR:HB2	1.81	0.62
4:B:1192:TYR:CE2	4:B:1218:THR:HG21	2.34	0.62
4:B:227:LYS:CB	4:B:395:GLN:OE1	2.47	0.62
3:A:375:THR:HA	3:A:434:ARG:O	1.98	0.62
6:E:7:ARG:C	6:E:9:ILE:N	2.50	0.62
5:C:262:LEU:HD21	11:K:19:LEU:HD12	1.81	0.62
4:B:35:SER:O	4:B:37:PHE:O	2.18	0.62
4:B:471:LYS:CG	4:B:472:ALA:N	2.49	0.62
5:C:134:ILE:CD1	5:C:141:GLY:CA	2.70	0.62
3:A:793:SER:CB	3:A:794:PRO:HD2	2.25	0.62
7:F:123:LYS:O	7:F:123:LYS:HG2	1.98	0.62
12:L:42:ARG:O	12:L:43:THR:HB	1.98	0.62
4:B:492:LEU:HB3	4:B:751:VAL:HG21	1.79	0.62
3:A:272:ALA:HB3	3:A:296:LEU:HD12	1.82	0.62
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.29	0.62
4:B:957:ASN:ND2	4:B:958:GLN:HB2	2.14	0.62
4:B:129:PHE:HE2	4:B:166:PHE:HB3	1.63	0.62
4:B:287:ARG:HA	4:B:291:ILE:O	1.99	0.62
8:H:116:TYR:HB2	8:H:123:MET:CB	2.25	0.62
9:I:7:CYS:C	9:I:8:ARG:O	2.34	0.62
3:A:455:MET:C	3:A:456:MET:HG2	2.19	0.62
4:B:1084:GLN:HE22	5:C:191:TYR:C	2.03	0.62
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.24	0.62
2:T:11:DC:H2'	2:T:12:DG:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:58:LYS:O	12:L:59:ALA:CB	2.47	0.62
3:A:622:VAL:HA	3:A:630:ILE:HD11	1.80	0.62
11:K:51:LEU:HD12	11:K:59:ALA:HB3	1.79	0.62
4:B:1096:ARG:HH11	4:B:1096:ARG:CG	2.12	0.62
2:T:8:DT:H2''	2:T:9:DC:O5'	1.98	0.62
3:A:98:LYS:O	3:A:101:LYS:N	2.32	0.62
3:A:996:ASN:HA	3:A:998:LEU:HD23	1.81	0.62
4:B:435:THR:O	4:B:436:VAL:HG23	2.00	0.62
3:A:1057:VAL:HG12	3:A:1058:VAL:N	2.13	0.62
3:A:1336:MET:HE3	3:A:1381:LEU:HG	1.82	0.62
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.14	0.62
6:E:211:TYR:HD1	6:E:211:TYR:N	1.97	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.64	0.62
4:B:1033:LYS:HB2	4:B:1089:PRO:HD2	1.81	0.62
11:K:40:HIS:HE1	11:K:63:VAL:HG13	1.62	0.62
4:B:1184:GLY:O	4:B:1186:ASP:OD2	2.17	0.62
3:A:7:SER:HB2	4:B:1193:GLN:NE2	2.11	0.62
3:A:897:TYR:HD1	3:A:897:TYR:N	1.97	0.62
4:B:449:ASN:OD1	4:B:451:LYS:HD2	1.99	0.62
4:B:563:MET:HE2	4:B:588:GLY:HA3	1.82	0.62
3:A:27:VAL:HG11	3:A:238:CYS:SG	2.39	0.62
2:T:4:DA:H2'	2:T:5:DT:C7	2.29	0.62
3:A:129:LYS:O	3:A:130:ASP:CB	2.48	0.62
4:B:333:PHE:O	4:B:333:PHE:CD1	2.52	0.62
3:A:89:PRO:O	3:A:204:THR:CG2	2.38	0.62
4:B:739:THR:HG1	4:B:740:HIS:CE1	2.18	0.62
3:A:265:LYS:NZ	3:A:322:VAL:CB	2.62	0.62
3:A:531:ILE:CD1	3:A:622:VAL:HG21	2.29	0.62
3:A:567:LYS:HD3	8:H:95:TYR:CG	2.34	0.62
3:A:114:LEU:C	3:A:115:LEU:HD23	2.19	0.62
9:I:10:CYS:CB	9:I:31:THR:CG2	2.70	0.62
9:I:103:CYS:SG	9:I:104:LEU:N	2.73	0.62
3:A:768:GLN:CG	3:A:816:HIS:HA	2.30	0.62
3:A:267:ALA:O	3:A:271:LYS:N	2.32	0.62
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.29	0.62
4:B:773:MET:O	4:B:775:LYS:N	2.33	0.62
7:F:81:THR:OG1	7:F:144:GLU:OE1	2.18	0.62
6:E:118:PRO:O	6:E:122:LYS:HD2	1.99	0.62
4:B:1196:ILE:HB	4:B:1197:PRO:CD	2.29	0.62
4:B:118:ARG:HH22	4:B:194:GLU:CD	2.03	0.62
4:B:638:PHE:CD2	4:B:653:VAL:HG21	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:291:ILE:HG22	4:B:297:ILE:CD1	2.29	0.62
8:H:42:ILE:HD12	8:H:95:TYR:CE2	2.35	0.62
3:A:587:HIS:CE1	3:A:969:GLN:HG2	2.35	0.62
4:B:313:MET:CG	4:B:390:LEU:HD21	2.28	0.62
5:C:136:ASP:OD2	5:C:140:ASN:O	2.18	0.62
4:B:1191:ILE:HG23	4:B:1192:TYR:N	2.15	0.62
8:H:2:SER:O	8:H:3:ASN:HB2	1.99	0.62
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.82	0.61
3:A:320:ARG:NH2	4:B:471:LYS:HB3	2.06	0.61
4:B:166:PHE:HD2	4:B:166:PHE:C	2.03	0.61
4:B:1056:SER:HB3	4:B:1066:SER:O	2.00	0.61
3:A:1389:PHE:CE1	3:A:1390:ASN:OD1	2.53	0.61
6:E:89:GLY:HA3	6:E:117:THR:OG1	2.00	0.61
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.99	0.61
4:B:36:ALA:O	4:B:37:PHE:O	2.17	0.61
3:A:897:TYR:HD2	3:A:936:LEU:CD1	2.11	0.61
3:A:598:LEU:HD13	8:H:25:ARG:HH12	1.65	0.61
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.35	0.61
3:A:134:ARG:O	3:A:137:ALA:HB3	2.00	0.61
3:A:668:ASP:HB3	3:A:743:VAL:HG23	1.82	0.61
4:B:314:LEU:C	4:B:316:PRO:HD2	2.21	0.61
3:A:693:VAL:HG13	3:A:702:LEU:HD21	1.81	0.61
3:A:1168:GLU:C	3:A:1170:ILE:H	2.03	0.61
4:B:638:PHE:O	4:B:740:HIS:CB	2.48	0.61
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.65	0.61
3:A:588:LEU:HD12	3:A:589:GLN:N	2.14	0.61
4:B:258:LEU:HD13	4:B:269:ILE:HG12	1.82	0.61
5:C:80:LEU:CD1	5:C:95:CYS:HA	2.30	0.61
8:H:79:TRP:C	8:H:80:ARG:O	2.32	0.61
3:A:1140:HIS:HB2	3:A:1276:VAL:O	1.99	0.61
3:A:1313:LEU:O	3:A:1315:GLU:N	2.33	0.61
3:A:1338:VAL:HG12	3:A:1339:LEU:N	2.15	0.61
3:A:321:PRO:HG2	3:A:322:VAL:N	2.15	0.61
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.82	0.61
3:A:896:ARG:HD2	3:A:897:TYR:CE1	2.35	0.61
4:B:420:LEU:O	4:B:423:LYS:N	2.34	0.61
4:B:778:MET:HE3	4:B:853:SER:CB	2.30	0.61
10:J:3:VAL:HA	10:J:53:HIS:CG	2.35	0.61
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.66	0.61
3:A:577:ILE:O	3:A:580:VAL:N	2.29	0.61
3:A:605:MET:HE2	3:A:606:LEU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1105:LEU:HB3	3:A:1384:VAL:CG2	2.31	0.61
3:A:33:ALA:CB	3:A:82:GLY:HA2	2.29	0.61
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.30	0.61
3:A:1193:LEU:HD11	3:A:1195:LEU:CD2	2.31	0.61
3:A:899:VAL:HG21	3:A:1029:ARG:HG2	1.83	0.61
4:B:449:ASN:O	4:B:450:ALA:C	2.39	0.61
3:A:645:LEU:O	3:A:645:LEU:HD12	2.01	0.61
4:B:326:ASP:OD1	4:B:329:THR:OG1	2.18	0.61
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.81	0.61
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.68	0.61
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.46	0.61
3:A:1426:GLU:HA	3:A:1429:ILE:HD12	1.83	0.61
6:E:113:GLN:CA	6:E:137:GLU:HG3	2.28	0.61
8:H:112:ILE:O	8:H:126:GLU:HA	2.00	0.61
4:B:681:TRP:O	4:B:684:LEU:HB2	2.01	0.61
6:E:2:ASP:O	6:E:3:GLN:HB3	1.99	0.61
3:A:18:GLN:HE21	3:A:1418:LEU:CD1	2.13	0.61
3:A:492:PRO:O	3:A:493:GLN:NE2	2.33	0.61
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.35	0.61
8:H:47:PHE:HD2	8:H:95:TYR:CD1	2.19	0.61
6:E:28:TYR:HE1	6:E:78:LEU:CD1	2.04	0.61
4:B:1096:ARG:NH1	4:B:1096:ARG:HG2	2.16	0.61
6:E:114:ASN:O	6:E:115:ASN:HB3	2.00	0.61
3:A:100:LYS:NZ	3:A:100:LYS:HB3	2.15	0.61
4:B:40:GLU:OE1	4:B:682:SER:HB2	2.01	0.61
4:B:248:SER:O	4:B:249:ARG:HB2	2.00	0.61
6:E:7:ARG:O	6:E:9:ILE:N	2.34	0.61
3:A:68:GLN:NE2	3:A:70:CYS:HB3	2.16	0.61
4:B:427:ASP:O	4:B:430:ARG:HB2	2.00	0.61
3:A:254:GLU:O	4:B:918:ILE:HG13	2.00	0.61
3:A:255:SER:CB	4:B:918:ILE:HG23	2.30	0.61
8:H:142:LEU:HD12	8:H:143:LEU:H	1.64	0.61
8:H:26:ILE:O	8:H:39:THR:HA	1.99	0.61
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	2.01	0.61
4:B:869:SER:O	4:B:870:ILE:HG13	2.00	0.61
3:A:276:LEU:HD11	3:A:292:ALA:O	2.01	0.61
3:A:1209:MET:HB2	3:A:1231:ASP:OD2	2.01	0.61
3:A:1339:LEU:CD1	6:E:147:HIS:CD2	2.84	0.61
6:E:178:ILE:CD1	6:E:185:ALA:HB2	2.31	0.61
3:A:367:PRO:HB3	3:A:465:TYR:O	2.01	0.61
4:B:431:TYR:CD1	4:B:447:ALA:CB	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:797:TYR:C	4:B:799:PRO:HD2	2.20	0.61
5:C:63:ILE:O	5:C:64:ALA:C	2.39	0.61
3:A:332:LYS:H	3:A:337:ARG:CB	2.13	0.61
6:E:116:ILE:O	6:E:118:PRO:CD	2.48	0.61
7:F:111:LEU:N	7:F:111:LEU:CD1	2.64	0.61
7:F:127:GLU:O	7:F:129:LYS:N	2.33	0.61
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.82	0.61
4:B:977:GLY:C	4:B:1099:VAL:CG2	2.68	0.61
12:L:45:ALA:O	12:L:46:VAL:CG2	2.49	0.61
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.83	0.61
3:A:901:LEU:N	3:A:926:GLN:NE2	2.48	0.61
3:A:902:LEU:O	3:A:903:ASN:CB	2.48	0.61
6:E:58:MET:O	6:E:60:PHE:N	2.34	0.61
7:F:89:GLU:O	7:F:93:ILE:HD13	2.01	0.61
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.48	0.61
3:A:744:LYS:HG2	3:A:748:MET:HE2	1.83	0.61
4:B:233:PRO:HG2	4:B:234:ILE:HD13	1.82	0.61
3:A:805:LEU:O	3:A:805:LEU:HD12	2.00	0.61
4:B:248:SER:HG	4:B:250:PHE:HD2	1.48	0.61
8:H:76:THR:HG22	8:H:76:THR:O	2.00	0.61
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.31	0.60
3:A:445:ASN:HB3	3:A:455:MET:HE2	1.83	0.60
4:B:1065:GLN:NE2	4:B:1067:ARG:H	1.98	0.60
3:A:918:GLU:O	3:A:919:ILE:HD13	2.00	0.60
3:A:1017:LEU:HB2	6:E:205:SER:CA	2.30	0.60
3:A:964:ILE:CD1	3:A:1037:LEU:HD21	2.31	0.60
4:B:604:ARG:NH2	4:B:614:SER:HA	2.15	0.60
4:B:704:ALA:HB3	4:B:741:CYS:HB2	1.82	0.60
10:J:8:PHE:H	10:J:49:MET:CE	2.14	0.60
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.83	0.60
8:H:25:ARG:O	8:H:26:ILE:HD12	2.01	0.60
3:A:208:LEU:O	3:A:209:ASN:C	2.39	0.60
4:B:797:TYR:HB3	4:B:798:TYR:HD1	1.63	0.60
3:A:92:HIS:HB2	3:A:236:LEU:HD11	1.82	0.60
3:A:714:PHE:O	3:A:718:VAL:HG23	2.01	0.60
3:A:1386:ARG:HA	3:A:1390:ASN:HB2	1.82	0.60
5:C:69:LEU:O	10:J:6:ARG:NH1	2.34	0.60
6:E:173:SER:O	6:E:175:LEU:N	2.34	0.60
3:A:90:VAL:HG12	3:A:297:GLN:CD	2.21	0.60
4:B:22:SER:O	4:B:23:ALA:O	2.19	0.60
5:C:167:HIS:CE1	12:L:70:ARG:HA	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:5:GLY:O	5:C:7:GLN:CG	2.48	0.60
4:B:273:LEU:HB2	4:B:276:ILE:CD1	2.30	0.60
3:A:1052:GLN:C	3:A:1053:PHE:O	2.35	0.60
3:A:185:TRP:O	3:A:186:LYS:CB	2.48	0.60
4:B:322:PHE:CE2	9:I:30:ARG:HD2	2.36	0.60
7:F:128:LYS:NZ	7:F:149:GLU:O	2.29	0.60
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.83	0.60
6:E:162:ARG:HH21	6:E:166:LYS:NZ	1.92	0.60
4:B:701:ILE:CB	4:B:740:HIS:CE1	2.74	0.60
3:A:321:PRO:HG2	3:A:322:VAL:H	1.65	0.60
4:B:994:TYR:HB2	4:B:999:MET:HE1	1.83	0.60
4:B:992:ILE:HD11	11:K:67:PHE:HE2	1.65	0.60
3:A:898:ARG:HA	3:A:933:TYR:HD1	1.64	0.60
3:A:380:VAL:HB	3:A:428:TYR:HA	1.83	0.60
8:H:96:VAL:HG22	8:H:143:LEU:HA	1.83	0.60
6:E:135:PHE:HB3	6:E:140:LEU:CD1	2.24	0.60
3:A:1051:ALA:O	3:A:1054:LEU:HB2	2.01	0.60
6:E:36:GLU:O	6:E:38:PRO:HD3	2.01	0.60
9:I:52:ILE:HG13	9:I:52:ILE:O	2.01	0.60
8:H:49:VAL:CG1	8:H:50:ALA:N	2.64	0.60
6:E:178:ILE:CG1	6:E:179:GLN:N	2.64	0.60
8:H:15:VAL:CG1	8:H:15:VAL:O	2.49	0.60
5:C:116:LYS:HB2	5:C:140:ASN:HA	1.84	0.60
3:A:1168:GLU:HB3	3:A:1169:ILE:HD12	1.83	0.60
3:A:853:ASP:OD1	3:A:853:ASP:O	2.19	0.60
4:B:461:LEU:CD1	4:B:466:TRP:CH2	2.85	0.60
4:B:976:ILE:HG22	4:B:977:GLY:N	2.16	0.60
5:C:22:LEU:CD2	5:C:25:VAL:CG2	2.70	0.60
3:A:527:THR:O	3:A:531:ILE:N	2.35	0.60
4:B:293:PRO:O	4:B:295:GLY:N	2.33	0.60
3:A:608:ILE:O	3:A:611:GLN:HB2	2.02	0.60
4:B:1067:ARG:O	4:B:1086:PHE:HE1	1.83	0.60
3:A:1349:TYR:HB2	3:A:1372:VAL:HG21	1.84	0.60
4:B:593:PRO:HG2	4:B:617:ARG:NH1	2.16	0.60
3:A:1107:VAL:HG11	3:A:1381:LEU:HB3	1.84	0.60
4:B:461:LEU:HD12	4:B:466:TRP:CZ3	2.35	0.60
3:A:351:THR:HG22	3:A:352:VAL:N	2.09	0.60
3:A:898:ARG:CB	3:A:933:TYR:CE1	2.83	0.60
3:A:596:THR:O	3:A:598:LEU:N	2.35	0.60
11:K:49:GLU:CB	11:K:94:ILE:HD11	2.31	0.60
3:A:886:ILE:HD11	3:A:943:LEU:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1154:TYR:HE1	9:I:18:GLU:CG	2.14	0.60
3:A:1067:LEU:O	3:A:1067:LEU:HG	1.97	0.60
4:B:806:THR:H	4:B:809:MET:HE3	1.65	0.60
3:A:1293:SER:OG	3:A:1295:THR:HG23	2.01	0.60
4:B:174:LEU:HD12	4:B:179:CYS:HG	1.66	0.60
3:A:168:GLY:C	3:A:169:ASN:O	2.39	0.60
3:A:566:ILE:O	3:A:567:LYS:O	2.19	0.60
5:C:145:CYS:SG	5:C:146:LYS:N	2.74	0.60
3:A:1444:MET:HB3	3:A:1445:ILE:HD12	1.83	0.60
5:C:29:MET:HB2	11:K:45:LEU:HD11	1.84	0.60
3:A:1120:LEU:CD2	3:A:1125:ALA:O	2.49	0.60
3:A:419:LYS:NZ	3:A:419:LYS:HB3	2.16	0.60
4:B:723:VAL:O	4:B:725:PRO:N	2.35	0.60
4:B:802:PRO:HB3	4:B:1091:TYR:CD1	2.36	0.60
4:B:863:GLU:OE2	4:B:873:THR:HA	2.01	0.60
5:C:244:VAL:HG21	11:K:105:PHE:CZ	2.36	0.60
3:A:304:MET:HG3	4:B:1210:MET:HG3	1.84	0.60
4:B:64:CYS:O	4:B:65:GLU:CB	2.48	0.60
3:A:380:VAL:HG23	3:A:430:TRP:H	1.61	0.60
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.17	0.60
3:A:1339:LEU:CD1	6:E:147:HIS:HD2	2.14	0.60
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.02	0.60
4:B:1170:THR:CG2	4:B:1183:LYS:NZ	2.64	0.60
3:A:381:THR:O	3:A:384:ASN:N	2.34	0.60
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.31	0.60
6:E:78:LEU:HD12	6:E:107:THR:HG21	1.84	0.60
6:E:61:GLN:CG	6:E:62:ALA:N	2.64	0.60
3:A:13:THR:HB	3:A:15:LYS:HZ1	1.65	0.60
3:A:809:THR:HB	3:A:810:PRO:CD	2.31	0.60
3:A:921:GLY:O	3:A:922:ASP:O	2.18	0.60
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.17	0.60
3:A:304:MET:CG	4:B:1210:MET:HG3	2.31	0.59
4:B:325:GLN:NE2	9:I:12:ASN:OD1	2.34	0.59
8:H:25:ARG:HA	8:H:40:LEU:O	2.02	0.59
7:F:97:ARG:NE	7:F:124:GLU:OE2	2.35	0.59
9:I:50:THR:HG22	9:I:52:ILE:HG22	1.81	0.59
4:B:947:GLY:C	4:B:948:ILE:HG13	2.21	0.59
3:A:1283:VAL:O	3:A:1306:LEU:HA	2.01	0.59
4:B:408:LEU:O	4:B:412:LEU:HD12	2.01	0.59
3:A:135:PHE:HD1	3:A:222:LEU:HB2	1.67	0.59
4:B:801:LYS:H	10:J:52:THR:HG22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:CE1	10:J:55:ASP:OD1	2.54	0.59
4:B:1202:LEU:HD13	4:B:1206:GLU:OE2	2.02	0.59
3:A:31:SER:CB	3:A:83:HIS:HB3	2.32	0.59
11:K:6:ARG:O	11:K:8:GLU:N	2.36	0.59
4:B:1170:THR:O	4:B:1170:THR:HG22	2.03	0.59
3:A:648:ASN:OD1	3:A:648:ASN:N	2.34	0.59
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.84	0.59
3:A:472:LEU:HD11	4:B:835:GLN:HE22	1.66	0.59
6:E:136:ASN:C	6:E:136:ASN:OD1	2.40	0.59
3:A:993:LEU:CD1	3:A:997:LEU:HD21	2.32	0.59
4:B:547:VAL:N	4:B:612:GLU:OE2	2.36	0.59
4:B:20:ASP:N	4:B:655:LYS:HZ3	2.00	0.59
3:A:91:PHE:N	3:A:297:GLN:HE22	2.00	0.59
5:C:4:GLU:HG3	5:C:5:GLY:N	2.17	0.59
8:H:58:THR:HB	8:H:143:LEU:HD12	1.83	0.59
3:A:211:PHE:C	3:A:213:HIS:N	2.54	0.59
7:F:135:ARG:O	7:F:135:ARG:HG2	2.02	0.59
3:A:331:GLY:O	3:A:332:LYS:HB3	2.02	0.59
3:A:666:ILE:O	3:A:667:GLY:C	2.41	0.59
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.98	0.59
7:F:97:ARG:HD3	7:F:100:GLN:OE1	2.02	0.59
3:A:493:GLN:HE21	3:A:493:GLN:N	2.01	0.59
3:A:206:GLU:O	3:A:209:ASN:HB2	2.02	0.59
6:E:81:GLU:HB3	6:E:96:PHE:HE1	1.66	0.59
3:A:1441:PHE:HZ	7:F:88:TYR:O	1.84	0.59
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.85	0.59
3:A:150:THR:O	3:A:151:ASP:OD2	2.21	0.59
9:I:75:CYS:HB3	9:I:103:CYS:HB2	1.85	0.59
3:A:1120:LEU:O	3:A:1323:ASP:CB	2.50	0.59
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.03	0.59
4:B:53:GLN:HG3	4:B:53:GLN:O	2.03	0.59
3:A:494:SER:O	3:A:498:ARG:HG3	2.03	0.59
4:B:851:PHE:O	4:B:974:PRO:HD3	2.01	0.59
5:C:16:ASP:HA	5:C:240:VAL:HG22	1.85	0.59
3:A:49:LYS:NZ	3:A:60:SER:HA	2.18	0.59
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.84	0.59
3:A:1011:GLN:HE22	3:A:1015:VAL:HG21	1.67	0.59
3:A:904:THR:O	3:A:905:ASP:C	2.40	0.59
4:B:352:ALA:C	4:B:354:ASP:N	2.55	0.59
3:A:23:SER:HB2	3:A:25:GLU:HB2	1.84	0.59
3:A:1120:LEU:O	3:A:1323:ASP:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:744:HIS:CG	4:B:745:PRO:HD2	2.38	0.59
5:C:241:ASP:CG	5:C:242:GLN:N	2.54	0.59
12:L:47:ARG:HG3	12:L:52:GLY:O	2.02	0.59
4:B:300:HIS:HE1	4:B:376:PHE:CE1	2.20	0.59
5:C:146:LYS:NZ	10:J:58:GLU:OE2	2.30	0.59
7:F:81:THR:O	7:F:82:THR:C	2.40	0.59
3:A:541:ILE:HD11	3:A:574:GLY:HA2	1.83	0.59
3:A:997:LEU:O	3:A:998:LEU:O	2.20	0.59
5:C:116:LYS:HE2	5:C:117:ASP:OD1	2.03	0.59
5:C:92:CYS:SG	5:C:94:LYS:HB3	2.42	0.59
3:A:495:GLU:HA	3:A:498:ARG:HG3	1.85	0.59
11:K:63:VAL:O	11:K:63:VAL:CG2	2.50	0.59
3:A:878:ILE:HG22	3:A:879:GLU:N	2.17	0.59
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.78	0.59
4:B:431:TYR:CZ	4:B:447:ALA:HB2	2.37	0.59
8:H:32:THR:HG22	8:H:33:GLN:H	1.68	0.59
3:A:99:ILE:HG12	3:A:234:MET:SD	2.43	0.59
3:A:1344:GLY:O	3:A:1345:ARG:C	2.39	0.59
6:E:83:CYS:SG	6:E:85:GLU:HB2	2.43	0.59
3:A:89:PRO:C	3:A:204:THR:HG21	2.22	0.59
3:A:302:THR:HA	3:A:305:ASP:O	2.03	0.59
4:B:1172:ILE:O	4:B:1172:ILE:HG22	2.02	0.59
4:B:816:GLU:N	4:B:816:GLU:CD	2.56	0.59
3:A:834:THR:CB	3:A:1077:THR:HG23	2.33	0.59
3:A:576:GLN:O	3:A:579:SER:HB2	2.02	0.59
3:A:14:VAL:HG23	3:A:1432:GLN:NE2	2.18	0.59
4:B:805:THR:HA	4:B:809:MET:HE1	1.84	0.59
12:L:34:CYS:O	12:L:35:SER:HB2	2.03	0.59
3:A:715:GLU:O	3:A:719:VAL:HG23	2.02	0.59
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.84	0.59
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.84	0.59
4:B:642:ASP:N	4:B:642:ASP:OD1	2.36	0.59
4:B:461:LEU:CD1	4:B:466:TRP:HH2	2.16	0.59
3:A:306:ASN:HD21	3:A:324:SER:HB3	1.68	0.59
12:L:53:HIS:O	12:L:55:ILE:HG12	2.03	0.59
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.84	0.59
6:E:20:LYS:HE2	6:E:60:PHE:CZ	2.36	0.59
4:B:276:ILE:HG22	4:B:277:LYS:N	2.18	0.59
4:B:286:PHE:HB3	4:B:297:ILE:CD1	2.33	0.59
6:E:94:LYS:HE2	6:E:98:ILE:HG12	1.84	0.59
3:A:1156:PRO:CD	3:A:1157:ASP:H	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:VAL:CG2	3:A:301:ALA:HA	2.33	0.59
5:C:226:ASP:O	5:C:227:THR:CB	2.47	0.59
4:B:1067:ARG:O	4:B:1086:PHE:CE1	2.56	0.59
11:K:22:ASP:HB3	11:K:23:PRO:CD	2.33	0.59
4:B:578:THR:OG1	4:B:593:PRO:HG3	2.03	0.59
3:A:1009:ASN:O	3:A:1013:ASP:OD2	2.21	0.59
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.38	0.58
6:E:109:ILE:HG22	6:E:109:ILE:O	2.02	0.58
3:A:384:ASN:OD1	3:A:385:ILE:N	2.36	0.58
7:F:83:PRO:CD	7:F:84:TYR:H	2.15	0.58
3:A:101:LYS:HA	3:A:139:TRP:HE1	1.66	0.58
3:A:668:ASP:CG	3:A:742:ASN:HD22	2.04	0.58
4:B:278:GLN:HG2	4:B:279:ASP:N	2.14	0.58
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.03	0.58
3:A:416:ARG:HG3	3:A:417:TYR:CE2	2.38	0.58
2:T:11:DC:H2"	2:T:12:DG:C5'	2.33	0.58
3:A:1208:THR:HB	3:A:1211:GLN:HB2	1.83	0.58
3:A:7:SER:HB3	4:B:1193:GLN:CD	2.24	0.58
3:A:381:THR:O	3:A:382:PRO:C	2.42	0.58
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.86	0.58
8:H:58:THR:O	8:H:59:ILE:HD13	2.03	0.58
3:A:635:ARG:NH2	3:A:877:HIS:HA	2.16	0.58
9:I:4:PHE:CE1	9:I:13:MET:HE3	2.38	0.58
4:B:650:GLU:HG3	4:B:651:LEU:H	1.67	0.58
3:A:322:VAL:O	3:A:323:LYS:CD	2.52	0.58
3:A:933:TYR:O	3:A:937:VAL:HG23	2.03	0.58
4:B:166:PHE:HD2	4:B:166:PHE:O	1.86	0.58
6:E:81:GLU:HB3	6:E:96:PHE:CE1	2.38	0.58
10:J:21:TYR:CE1	10:J:25:LEU:HD21	2.38	0.58
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.38	0.58
3:A:963:ILE:CG2	3:A:1045:VAL:HG13	2.33	0.58
3:A:1198:ASP:OD1	3:A:1199:ARG:N	2.37	0.58
4:B:789:MET:HE3	4:B:965:LYS:HB3	1.86	0.58
3:A:436:ILE:HD11	3:A:491:VAL:HG21	1.86	0.58
3:A:1364:ASN:HD22	3:A:1366:ARG:HG2	1.64	0.58
3:A:567:LYS:NZ	8:H:95:TYR:CZ	2.64	0.58
3:A:112:LYS:HG2	3:A:113:LEU:H	1.68	0.58
6:E:86:PRO:O	6:E:114:ASN:HB2	2.03	0.58
3:A:244:PRO:HG2	3:A:245:PRO:HD2	1.83	0.58
3:A:356:ASP:HB2	3:A:469:ARG:HH11	1.68	0.58
4:B:411:PRO:HA	4:B:414:ALA:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.04	0.58
3:A:1342:GLU:CG	6:E:212:ARG:HH12	2.16	0.58
3:A:294:SER:O	3:A:298:PHE:HB3	2.04	0.58
3:A:777:PHE:CD2	3:A:782:ARG:C	2.77	0.58
5:C:146:LYS:O	5:C:147:LEU:HD23	2.03	0.58
5:C:66:ARG:CZ	10:J:2:ILE:CG2	2.82	0.58
2:T:5:DT:C2'	2:T:6:DC:H5'	2.28	0.58
6:E:121:MET:C	6:E:123:LEU:H	2.07	0.58
4:B:787:VAL:HG12	4:B:787:VAL:O	2.02	0.58
3:A:321:PRO:C	3:A:322:VAL:HG22	2.22	0.58
3:A:751:SER:CB	4:B:1015:HIS:HE1	2.16	0.58
3:A:35:ILE:O	3:A:270:LEU:HD11	2.03	0.58
3:A:58:LEU:HD23	3:A:80:HIS:O	2.01	0.58
4:B:912:ILE:HD11	4:B:966:VAL:HG21	1.86	0.58
3:A:929:LEU:N	3:A:929:LEU:HD23	2.18	0.58
4:B:282:ILE:HG13	4:B:283:VAL:N	2.19	0.58
4:B:1219:ASP:O	4:B:1220:ARG:C	2.42	0.58
3:A:335:ARG:O	3:A:336:ILE:C	2.41	0.58
3:A:541:ILE:HG22	3:A:546:VAL:CG2	2.33	0.58
4:B:1080:LYS:HG3	5:C:180:TYR:CE2	2.38	0.58
3:A:376:TYR:CD2	3:A:376:TYR:C	2.76	0.58
4:B:635:ARG:NH2	4:B:698:GLU:OE2	2.37	0.58
11:K:7:PHE:C	11:K:9:LEU:N	2.55	0.58
3:A:528:LEU:HD13	3:A:531:ILE:CG2	2.34	0.58
1:R:9:G:H4'	4:B:1097:HIS:CD2	2.39	0.58
6:E:65:THR:OG1	6:E:68:SER:N	2.31	0.58
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.69	0.58
3:A:614:PHE:CD1	3:A:614:PHE:O	2.56	0.58
9:I:96:SER:CB	9:I:98:VAL:HG23	2.34	0.58
9:I:98:VAL:HG12	9:I:99:LEU:N	2.19	0.58
4:B:230:ALA:N	4:B:231:PRO:CD	2.65	0.58
3:A:444:PHE:HE2	3:A:470:LEU:CD2	2.16	0.58
3:A:496:GLU:O	3:A:499:ALA:N	2.35	0.58
4:B:273:LEU:O	4:B:274:PRO:O	2.22	0.58
3:A:1292:PRO:HD3	3:A:1298:TYR:CE2	2.39	0.58
4:B:236:HIS:HD2	4:B:389:ALA:CB	2.15	0.58
10:J:1:MET:N	10:J:56:LEU:N	2.52	0.58
3:A:1074:GLU:O	3:A:1078:GLN:HG2	2.04	0.58
3:A:709:THR:HB	3:A:712:GLU:HG3	1.86	0.58
7:F:109:VAL:CG2	7:F:124:GLU:HG3	2.34	0.58
6:E:204:THR:CG2	6:E:205:SER:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:HG2	11:K:47:ARG:O	2.02	0.58
4:B:760:ASP:N	4:B:760:ASP:OD1	2.30	0.58
3:A:1273:LEU:O	3:A:1274:ARG:CB	2.50	0.58
3:A:908:LEU:CD1	3:A:983:ILE:HD11	2.27	0.58
4:B:362:PRO:C	4:B:363:HIS:O	2.40	0.58
4:B:189:LEU:O	4:B:190:TYR:C	2.40	0.58
3:A:71:GLN:C	3:A:73:GLY:H	1.97	0.58
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.37	0.58
3:A:834:THR:O	3:A:837:ILE:HB	2.03	0.58
3:A:657:LEU:O	3:A:658:LEU:C	2.42	0.58
3:A:743:VAL:HG11	3:A:758:ILE:CD1	2.34	0.58
3:A:432:VAL:O	3:A:433:GLU:C	2.42	0.58
5:C:11:ARG:HG3	5:C:19:ASP:O	2.04	0.58
3:A:482:PHE:O	4:B:989:THR:HG23	2.04	0.58
4:B:263:GLY:O	4:B:264:SER:C	2.40	0.58
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.67	0.57
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.33	0.57
3:A:68:GLN:NE2	3:A:80:HIS:CE1	2.72	0.57
5:C:56:THR:HG22	5:C:57:VAL:H	1.69	0.57
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.86	0.57
3:A:1150:SER:HB2	3:A:1195:LEU:HD22	1.86	0.57
6:E:161:LYS:O	6:E:164:LEU:N	2.38	0.57
5:C:133:ILE:HD11	5:C:237:SER:CA	2.33	0.57
3:A:57:ARG:O	3:A:68:GLN:HG3	2.04	0.57
3:A:1039:LYS:HG3	3:A:1040:GLN:N	2.18	0.57
3:A:898:ARG:CB	3:A:933:TYR:HE1	2.16	0.57
5:C:4:GLU:CG	5:C:5:GLY:H	2.14	0.57
3:A:530:GLY:HA2	3:A:533:LYS:H	1.69	0.57
4:B:282:ILE:HG13	4:B:283:VAL:H	1.67	0.57
9:I:33:SER:C	9:I:34:TYR:O	2.40	0.57
6:E:75:MET:CG	6:E:76:GLY:N	2.67	0.57
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.39	0.57
3:A:387:ARG:O	3:A:391:LEU:HD23	2.04	0.57
3:A:33:ALA:C	3:A:34:LYS:HG3	2.23	0.57
3:A:103:CYS:O	3:A:105:CYS:N	2.37	0.57
3:A:8:SER:OG	4:B:1180:PHE:HE1	1.87	0.57
3:A:845:LEU:O	3:A:848:ILE:HG12	2.04	0.57
3:A:148:CYS:HB3	3:A:167:CYS:O	2.05	0.57
11:K:50:LEU:O	11:K:56:VAL:HG11	2.05	0.57
7:F:75:PRO:C	7:F:77:ASP:N	2.55	0.57
3:A:1042:PHE:CE2	3:A:1046:LEU:CD1	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.04	0.57
4:B:616:ILE:H	4:B:616:ILE:HD12	1.69	0.57
3:A:1368:MET:O	3:A:1371:LEU:HB3	2.04	0.57
6:E:164:LEU:HD22	6:E:211:TYR:HD2	1.69	0.57
3:A:300:VAL:O	3:A:300:VAL:HG12	2.02	0.57
4:B:114:PRO:O	4:B:115:GLN:C	2.40	0.57
3:A:897:TYR:CD1	3:A:897:TYR:N	2.70	0.57
6:E:40:GLU:O	6:E:43:LYS:HB3	2.04	0.57
3:A:1376:THR:HG23	3:A:1376:THR:O	2.03	0.57
12:L:60:ARG:HD2	12:L:61:THR:H	1.70	0.57
3:A:979:SER:OG	3:A:981:LEU:HD12	2.04	0.57
4:B:423:LYS:HZ3	4:B:423:LYS:HB2	1.69	0.57
3:A:564:ALA:O	8:H:97:MET:HB3	2.04	0.57
6:E:97:VAL:HG13	6:E:127:ILE:HG21	1.86	0.57
4:B:1219:ASP:O	4:B:1221:SER:N	2.37	0.57
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.86	0.57
3:A:1256:GLU:O	3:A:1259:MET:N	2.37	0.57
5:C:73:GLN:HG3	5:C:74:SER:N	2.18	0.57
6:E:88:VAL:O	6:E:116:ILE:HA	2.05	0.57
11:K:70:ARG:O	11:K:71:PHE:HB3	2.02	0.57
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.19	0.57
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.18	0.57
3:A:1007:ILE:O	3:A:1010:ALA:HB3	2.04	0.57
4:B:205:ILE:CG2	4:B:206:ASN:ND2	2.67	0.57
3:A:116:ASP:C	3:A:118:HIS:N	2.58	0.57
3:A:1195:LEU:HD11	3:A:1267:MET:CE	2.34	0.57
3:A:705:LYS:O	3:A:706:HIS:C	2.41	0.57
4:B:1006:ILE:CD1	10:J:45:CYS:SG	2.93	0.57
5:C:36:VAL:HG23	11:K:41:THR:CG2	2.29	0.57
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
4:B:1173:ALA:C	4:B:1175:LEU:H	2.07	0.57
4:B:952:VAL:HB	12:L:58:LYS:HB2	1.86	0.57
11:K:100:ALA:O	11:K:103:THR:HB	2.04	0.57
3:A:115:LEU:CD1	3:A:142:CYS:HB3	2.34	0.57
6:E:127:ILE:H	6:E:127:ILE:HD13	1.70	0.57
3:A:1154:TYR:HD1	3:A:1191:TRP:CH2	2.21	0.57
5:C:26:ASP:O	5:C:27:LEU:C	2.42	0.57
3:A:582:ILE:CD1	3:A:629:LEU:HD11	2.34	0.57
3:A:808:LEU:O	4:B:728:ARG:NH1	2.37	0.57
10:J:32:GLU:CD	10:J:32:GLU:N	2.58	0.57
3:A:18:GLN:HB3	4:B:1215:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.86	0.57
4:B:33:VAL:O	4:B:36:ALA:HB3	2.05	0.57
4:B:744:HIS:O	4:B:747:MET:HG2	2.04	0.57
4:B:913:GLY:HA2	4:B:938:SER:CB	2.35	0.57
3:A:224:PHE:CZ	3:A:231:PRO:HG3	2.39	0.57
7:F:82:THR:HG22	7:F:83:PRO:HD2	1.87	0.57
3:A:609:ASP:O	3:A:610:GLY:C	2.40	0.57
3:A:130:ASP:O	3:A:132:LYS:N	2.38	0.57
4:B:754:SER:O	4:B:806:THR:HG21	2.04	0.57
3:A:22:PHE:HB2	4:B:1211:ASN:OD1	2.04	0.57
3:A:442:VAL:O	3:A:457:ALA:HA	2.04	0.57
4:B:48:LEU:O	4:B:49:ASP:C	2.42	0.57
6:E:161:LYS:HD2	6:E:195:VAL:HG23	1.85	0.57
4:B:839:MET:HG3	4:B:1010:LEU:HD11	1.87	0.57
5:C:133:ILE:HD13	5:C:236:GLY:C	2.25	0.57
4:B:361:LEU:O	4:B:363:HIS:O	2.23	0.57
2:T:5:DT:H1'	3:A:448:PRO:HB3	1.87	0.57
3:A:1349:TYR:HD2	3:A:1350:LYS:N	2.02	0.57
3:A:247:ARG:HG3	3:A:247:ARG:O	2.05	0.57
3:A:1035:TYR:O	3:A:1037:LEU:N	2.37	0.57
3:A:356:ASP:OD1	3:A:356:ASP:C	2.43	0.57
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.40	0.57
4:B:644:GLU:CG	4:B:654:ARG:HH22	2.18	0.57
4:B:708:GLU:CG	4:B:709:ASP:H	2.04	0.57
4:B:350:GLN:O	4:B:351:TYR:C	2.43	0.57
3:A:546:VAL:O	3:A:550:LEU:CD2	2.53	0.57
3:A:599:SER:C	3:A:601:LYS:H	2.08	0.57
3:A:540:PHE:HD2	3:A:572:TRP:O	1.87	0.57
6:E:164:LEU:HD22	6:E:211:TYR:CD2	2.40	0.57
4:B:28:GLU:O	4:B:30:SER:N	2.37	0.57
3:A:35:ILE:O	3:A:35:ILE:HG22	2.05	0.57
3:A:255:SER:HB3	4:B:918:ILE:CG2	2.35	0.57
4:B:797:TYR:HB3	4:B:798:TYR:CE1	2.40	0.57
4:B:798:TYR:HH	5:C:62:PHE:HE2	1.51	0.57
2:T:6:DC:H4'	3:A:447:GLN:CD	2.25	0.57
3:A:403:LYS:HB2	3:A:404:TYR:HD1	1.67	0.57
3:A:348:SER:HB2	4:B:1128:LEU:HD12	1.86	0.57
3:A:1391:ARG:HG2	3:A:1391:ARG:HH11	1.70	0.57
3:A:1116:LEU:CD2	3:A:1311:VAL:HA	2.35	0.56
3:A:1238:ILE:HG22	3:A:1240:CYS:SG	2.45	0.56
3:A:55:ASP:O	3:A:58:LEU:N	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:47:ARG:HH21	3:A:255:SER:HA	1.70	0.56
11:K:56:VAL:HA	11:K:77:THR:HG22	1.87	0.56
4:B:798:TYR:CD1	4:B:798:TYR:N	2.71	0.56
7:F:147:SER:OG	7:F:150:GLU:CG	2.48	0.56
8:H:36:CYS:CB	8:H:130:ARG:HH22	2.17	0.56
3:A:591:PHE:CD2	3:A:595:THR:HG22	2.40	0.56
4:B:1074:ASN:C	4:B:1074:ASN:OD1	2.42	0.56
3:A:857:ARG:HB3	3:A:863:VAL:HA	1.86	0.56
4:B:64:CYS:O	4:B:65:GLU:HB3	2.04	0.56
4:B:365:THR:CG2	4:B:366:GLN:N	2.68	0.56
4:B:361:LEU:CD2	4:B:377:PHE:HD2	2.18	0.56
3:A:115:LEU:HB2	3:A:122:MET:CE	2.35	0.56
4:B:800:GLN:CG	10:J:52:THR:CG2	2.82	0.56
4:B:778:MET:HE1	4:B:853:SER:CB	2.35	0.56
3:A:31:SER:HB2	3:A:83:HIS:HB3	1.87	0.56
3:A:765:VAL:CG2	3:A:800:VAL:CG1	2.83	0.56
8:H:129:TYR:N	8:H:129:TYR:CD2	2.73	0.56
4:B:666:TYR:O	4:B:668:ASP:N	2.33	0.56
3:A:18:GLN:HB3	4:B:1215:ARG:HB2	1.86	0.56
3:A:726:ARG:HG2	3:A:727:ASP:N	2.19	0.56
3:A:706:HIS:CD2	3:A:1282:VAL:O	2.58	0.56
4:B:640:VAL:CG2	4:B:740:HIS:CA	2.82	0.56
3:A:67:CYS:O	3:A:70:CYS:CB	2.32	0.56
4:B:954:VAL:HG21	12:L:29:TYR:HE2	1.69	0.56
3:A:925:LEU:O	3:A:928:LEU:N	2.39	0.56
3:A:522:GLY:O	3:A:523:ILE:HD12	2.05	0.56
3:A:531:ILE:HD12	3:A:649:ILE:CG2	2.35	0.56
3:A:565:ILE:HG12	3:A:567:LYS:NZ	2.20	0.56
3:A:106:VAL:C	3:A:114:LEU:HD21	2.25	0.56
3:A:135:PHE:HD1	3:A:222:LEU:CB	2.19	0.56
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.36	0.56
3:A:668:ASP:OD2	3:A:742:ASN:ND2	2.32	0.56
3:A:1347:ALA:O	3:A:1348:LEU:C	2.38	0.56
3:A:635:ARG:CZ	3:A:877:HIS:ND1	2.68	0.56
4:B:121:ASN:H	4:B:121:ASN:HD22	1.53	0.56
3:A:18:GLN:NE2	3:A:1418:LEU:HB2	2.20	0.56
4:B:461:LEU:HD11	4:B:466:TRP:HH2	1.71	0.56
4:B:412:LEU:HB3	4:B:466:TRP:NE1	2.19	0.56
4:B:466:TRP:HB2	4:B:479:VAL:CG2	2.36	0.56
3:A:67:CYS:O	3:A:68:GLN:NE2	2.38	0.56
4:B:175:ARG:NH1	4:B:175:ARG:CG	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:947:PHE:CD2	3:A:954:TRP:CE2	2.94	0.56
3:A:1049:ILE:O	3:A:1050:GLU:C	2.43	0.56
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.56
4:B:252:SER:O	4:B:252:SER:OG	2.20	0.56
3:A:1137:ALA:C	3:A:1138:ILE:HD13	2.25	0.56
4:B:689:LEU:O	4:B:690:VAL:HG23	2.04	0.56
3:A:443:LEU:HD12	4:B:1146:PHE:CZ	2.41	0.56
5:C:36:VAL:CG2	11:K:41:THR:HG21	2.32	0.56
4:B:893:LEU:HD21	4:B:913:GLY:H	1.71	0.56
6:E:46:TYR:CD2	6:E:58:MET:HE3	2.41	0.56
4:B:454:THR:HG22	4:B:454:THR:O	2.05	0.56
11:K:33:ILE:CD1	11:K:87:LEU:HD22	2.36	0.56
6:E:27:GLY:O	6:E:28:TYR:CD2	2.59	0.56
4:B:1131:GLY:O	4:B:1132:GLU:C	2.43	0.56
3:A:1355:VAL:O	3:A:1358:SER:OG	2.23	0.56
5:C:169:LYS:NZ	12:L:69:ALA:O	2.38	0.56
7:F:111:LEU:H	7:F:111:LEU:CD1	2.19	0.56
3:A:1116:LEU:HD13	3:A:1329:THR:OG1	2.05	0.56
4:B:642:ASP:HA	4:B:649:LYS:HA	1.87	0.56
4:B:476:ARG:O	4:B:478:GLY:N	2.39	0.56
3:A:303:TYR:O	3:A:325:ILE:HG13	2.06	0.56
3:A:901:LEU:HD23	3:A:907:THR:HG22	1.83	0.56
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.88	0.56
8:H:47:PHE:CD2	8:H:95:TYR:CB	2.89	0.56
5:C:77:ILE:HA	5:C:129:ILE:HD11	1.87	0.56
4:B:792:MET:HA	4:B:856:PHE:O	2.05	0.56
3:A:1322:ILE:HD13	3:A:1322:ILE:H	1.70	0.56
3:A:18:GLN:CB	4:B:1215:ARG:HB2	2.35	0.56
3:A:18:GLN:HG3	3:A:228:PHE:CE1	2.40	0.56
6:E:182:ASP:O	6:E:185:ALA:N	2.38	0.56
3:A:1340:GLY:N	6:E:183:PRO:HG2	2.20	0.56
3:A:265:LYS:HZ2	3:A:322:VAL:CB	2.19	0.56
5:C:244:VAL:CG2	5:C:245:VAL:N	2.69	0.56
4:B:1182:CYS:O	4:B:1182:CYS:SG	2.63	0.56
3:A:924:LYS:O	3:A:927:VAL:HG12	2.06	0.56
4:B:169:ARG:N	4:B:454:THR:OG1	2.39	0.56
3:A:531:ILE:HD12	3:A:649:ILE:HG21	1.87	0.56
7:F:72:LYS:O	7:F:73:ALA:CB	2.54	0.56
5:C:58:LEU:CD2	10:J:57:ILE:HD13	2.35	0.56
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.68	0.56
4:B:1202:LEU:O	4:B:1205:GLN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HB2	8:H:125:LEU:CD1	2.36	0.56
3:A:805:LEU:O	4:B:761:HIS:ND1	2.38	0.56
3:A:804:TYR:CE2	4:B:763:GLN:HA	2.40	0.56
3:A:289:ILE:HG22	3:A:290:GLU:N	2.21	0.56
4:B:560:GLU:O	4:B:561:TRP:CD1	2.58	0.56
3:A:463:ILE:CB	3:A:464:PRO:HD2	2.30	0.56
5:C:241:ASP:CG	5:C:242:GLN:H	2.08	0.56
3:A:868:TYR:CE1	3:A:1064:VAL:CG2	2.89	0.56
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.87	0.56
9:I:96:SER:C	9:I:98:VAL:H	2.08	0.56
7:F:111:LEU:C	7:F:113:GLY:N	2.54	0.56
4:B:1017:ILE:H	4:B:1018:PRO:CD	2.19	0.56
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.71	0.56
4:B:469:GLN:HG3	4:B:470:LYS:H	1.70	0.56
5:C:22:LEU:HD23	5:C:25:VAL:HG21	1.84	0.56
4:B:236:HIS:CD2	4:B:389:ALA:CB	2.88	0.56
3:A:1001:ARG:HD2	7:F:80:ALA:O	2.05	0.56
3:A:765:VAL:HG23	3:A:800:VAL:HB	1.87	0.56
3:A:1132:LYS:O	3:A:1133:LEU:C	2.44	0.56
3:A:1170:ILE:O	3:A:1171:GLN:C	2.44	0.56
4:B:519:TRP:CH2	4:B:705:MET:HE1	2.40	0.56
5:C:243:VAL:O	5:C:244:VAL:C	2.43	0.56
3:A:531:ILE:CD1	3:A:622:VAL:HG11	2.34	0.56
4:B:298:LEU:N	4:B:298:LEU:HD23	2.20	0.56
4:B:323:VAL:HG12	4:B:323:VAL:O	2.06	0.56
4:B:773:MET:C	4:B:775:LYS:H	2.09	0.56
6:E:63:ASN:HB3	6:E:64:PRO:HD2	1.88	0.56
3:A:1394:THR:HG21	3:A:1398:MET:HE3	1.87	0.56
11:K:32:VAL:CG2	11:K:74:ARG:HG3	2.32	0.56
3:A:346:ASP:HB2	4:B:1154:ALA:HB1	1.88	0.56
4:B:70:ILE:HG22	4:B:70:ILE:O	2.06	0.56
3:A:1325:THR:HG22	3:A:1326:ARG:HG3	1.87	0.55
3:A:496:GLU:O	3:A:499:ALA:HB3	2.06	0.55
3:A:841:LEU:O	3:A:845:LEU:HG	2.05	0.55
4:B:361:LEU:HD23	4:B:377:PHE:HD2	1.70	0.55
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.64	0.55
5:C:74:SER:CA	5:C:77:ILE:HG12	2.35	0.55
3:A:711:ARG:HH12	9:I:95:THR:HB	1.70	0.55
3:A:1389:PHE:C	3:A:1389:PHE:CD1	2.78	0.55
8:H:99:GLY:O	8:H:138:GLU:O	2.24	0.55
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:164:LEU:CD1	6:E:211:TYR:CE2	2.88	0.55
4:B:899:ILE:CD1	4:B:911:ILE:HG12	2.30	0.55
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.41	0.55
3:A:709:THR:HB	3:A:712:GLU:H	1.71	0.55
4:B:130:VAL:HG12	4:B:132:VAL:CG2	2.33	0.55
6:E:187:TYR:HD2	6:E:188:LEU:CD2	2.17	0.55
3:A:247:ARG:NH1	3:A:263:THR:HG23	2.19	0.55
3:A:1117:THR:N	3:A:1328:TYR:O	2.35	0.55
4:B:653:VAL:O	4:B:654:ARG:CD	2.55	0.55
4:B:1159:ARG:NE	4:B:1193:GLN:HG3	2.21	0.55
4:B:286:PHE:HB3	4:B:297:ILE:HD11	1.88	0.55
4:B:365:THR:HG23	4:B:367:LEU:N	2.19	0.55
6:E:100:ILE:HG22	6:E:101:GLN:N	2.21	0.55
4:B:778:MET:O	4:B:819:ALA:HB1	2.07	0.55
7:F:133:VAL:HG23	7:F:147:SER:HA	1.88	0.55
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.40	0.55
5:C:258:ILE:HD11	11:K:42:LEU:CD2	2.29	0.55
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.15	0.55
3:A:690:VAL:CG2	3:A:718:VAL:HG13	2.36	0.55
3:A:1100:ARG:CZ	3:A:1104:ILE:HD11	2.37	0.55
4:B:130:VAL:CG1	4:B:132:VAL:HG23	2.31	0.55
3:A:1319:VAL:CG1	3:A:1320:PRO:CD	2.84	0.55
3:A:873:MET:HG2	3:A:957:PRO:HG2	1.88	0.55
8:H:102:TYR:N	8:H:102:TYR:HD2	2.05	0.55
4:B:613:VAL:HG12	4:B:627:PHE:O	2.06	0.55
4:B:627:PHE:HB3	4:B:632:ARG:HH11	1.70	0.55
3:A:733:ALA:C	3:A:735:VAL:N	2.57	0.55
3:A:397:ASN:N	3:A:397:ASN:OD1	2.39	0.55
4:B:26:THR:O	4:B:29:ASP:HB2	2.07	0.55
3:A:494:SER:N	4:B:1149:GLU:OE2	2.39	0.55
3:A:40:THR:C	3:A:41:MET:HG3	2.26	0.55
4:B:911:ILE:CD1	4:B:941:LEU:HD23	2.36	0.55
3:A:909:ASP:CG	3:A:910:PRO:CD	2.75	0.55
3:A:407:ARG:HD3	3:A:413:ILE:HD13	1.87	0.55
3:A:115:LEU:HD12	3:A:122:MET:HE2	1.89	0.55
4:B:1203:LEU:HD11	4:B:1207:LEU:HG	1.88	0.55
3:A:1044:TRP:O	3:A:1045:VAL:C	2.44	0.55
3:A:152:VAL:HG12	3:A:153:PRO:N	2.22	0.55
5:C:8:VAL:HA	5:C:21:ILE:O	2.06	0.55
9:I:62:ILE:CG2	9:I:63:GLY:N	2.69	0.55
11:K:88:LYS:O	11:K:89:ASN:C	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1127:ASP:C	3:A:1129:GLU:N	2.60	0.55
3:A:267:ALA:C	3:A:269:ILE:H	2.09	0.55
4:B:203:PHE:CD1	4:B:461:LEU:HD21	2.41	0.55
4:B:976:ILE:O	4:B:990:ILE:HB	2.07	0.55
8:H:12:VAL:HG13	8:H:26:ILE:HG23	1.88	0.55
3:A:1256:GLU:C	3:A:1258:HIS:H	2.10	0.55
3:A:1100:ARG:O	3:A:1101:LEU:C	2.44	0.55
5:C:80:LEU:HD11	5:C:95:CYS:HA	1.88	0.55
10:J:34:THR:O	10:J:35:ALA:C	2.43	0.55
4:B:658:ILE:O	4:B:661:LEU:HB2	2.07	0.55
5:C:172:PRO:CD	5:C:173:ALA:N	2.69	0.55
4:B:897:GLY:O	4:B:898:LEU:HD23	2.06	0.55
4:B:900:ALA:HB1	12:L:61:THR:OG1	2.06	0.55
6:E:75:MET:HG2	6:E:76:GLY:N	2.21	0.55
4:B:1208:MET:HA	4:B:1212:ILE:O	2.07	0.55
3:A:1349:TYR:CD2	3:A:1349:TYR:C	2.79	0.55
9:I:103:CYS:C	9:I:104:LEU:HD23	2.27	0.55
4:B:1017:ILE:H	4:B:1018:PRO:HD2	1.71	0.55
4:B:665:GLU:O	4:B:668:ASP:HB2	2.07	0.55
4:B:766:ARG:O	4:B:769:TYR:N	2.38	0.55
9:I:83:ASN:N	9:I:83:ASN:ND2	2.55	0.55
4:B:349:ILE:O	4:B:350:GLN:C	2.45	0.55
11:K:21:ILE:HG13	11:K:33:ILE:HG23	1.89	0.55
3:A:832:ALA:O	3:A:833:GLU:C	2.45	0.55
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.70	0.55
3:A:607:ILE:CG1	3:A:612:ILE:HA	2.37	0.55
3:A:963:ILE:HG22	3:A:1045:VAL:HG13	1.89	0.55
4:B:234:ILE:CD1	4:B:234:ILE:H	2.12	0.55
8:H:88:SER:C	8:H:89:LEU:HG	2.27	0.55
3:A:1338:VAL:HG12	3:A:1339:LEU:HG	1.88	0.55
3:A:1342:GLU:CG	6:E:212:ARG:NH1	2.69	0.55
4:B:110:HIS:CD2	4:B:111:ALA:H	2.25	0.55
3:A:642:CYS:O	3:A:645:LEU:HB3	2.06	0.55
4:B:795:ILE:N	4:B:795:ILE:HD12	2.21	0.55
4:B:1106:ARG:NH2	4:B:1109:GLY:N	2.54	0.55
3:A:614:PHE:HD1	3:A:614:PHE:C	2.09	0.55
4:B:170:LEU:HD12	4:B:171:PRO:HD2	1.88	0.55
4:B:760:ASP:O	4:B:762:ASN:N	2.36	0.55
4:B:400:HIS:CE1	4:B:517:THR:HG21	2.42	0.55
4:B:449:ASN:O	4:B:451:LYS:N	2.40	0.55
4:B:69:LEU:HD22	4:B:429:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.89	0.55
3:A:24:PRO:CB	3:A:237:THR:HG21	2.37	0.55
4:B:778:MET:HE1	4:B:853:SER:HB3	1.89	0.55
3:A:574:GLY:O	3:A:575:LYS:C	2.44	0.55
5:C:47:ASP:O	5:C:48:SER:HB2	2.06	0.55
3:A:179:LEU:CD1	3:A:297:GLN:CG	2.81	0.55
3:A:7:SER:HA	4:B:1175:LEU:HD21	1.89	0.55
4:B:114:PRO:HG2	4:B:181:LEU:HD11	1.88	0.55
4:B:446:LEU:O	4:B:446:LEU:HD23	2.07	0.55
3:A:569:LYS:HD2	5:C:221:TYR:O	2.06	0.55
3:A:335:ARG:HH11	4:B:1202:LEU:HD12	1.72	0.55
8:H:36:CYS:HB2	8:H:126:GLU:O	2.06	0.55
9:I:59:VAL:O	9:I:60:GLN:C	2.45	0.55
3:A:474:VAL:HG22	3:A:474:VAL:O	2.07	0.55
4:B:22:SER:O	4:B:654:ARG:HD2	2.07	0.54
4:B:640:VAL:CG2	4:B:740:HIS:N	2.70	0.54
4:B:1076:HIS:CG	11:K:40:HIS:HD2	2.24	0.54
4:B:975:GLN:HG2	4:B:976:ILE:H	1.71	0.54
5:C:240:VAL:O	5:C:241:ASP:C	2.45	0.54
3:A:300:VAL:O	3:A:304:MET:HE2	2.06	0.54
4:B:899:ILE:HD11	4:B:911:ILE:CB	2.37	0.54
3:A:845:LEU:HB3	3:A:1065:GLY:O	2.07	0.54
3:A:639:PRO:HG2	3:A:640:GLN:H	1.72	0.54
4:B:356:LEU:CD2	4:B:356:LEU:N	2.66	0.54
5:C:43:THR:HG23	5:C:44:LEU:H	1.72	0.54
4:B:118:ARG:HA	4:B:207:GLY:HA2	1.89	0.54
3:A:559:VAL:O	3:A:560:ILE:C	2.44	0.54
4:B:223:VAL:O	4:B:223:VAL:CG1	2.54	0.54
4:B:1008:PRO:HG2	4:B:1011:ILE:HD11	1.89	0.54
3:A:879:GLU:O	3:A:881:GLN:HG3	2.07	0.54
3:A:679:ILE:CG2	3:A:729:ALA:HB1	2.32	0.54
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.43	0.54
3:A:886:ILE:HG22	3:A:887:GLY:N	2.22	0.54
2:T:8:DT:H2'	2:T:9:DC:C6	2.41	0.54
11:K:32:VAL:O	11:K:32:VAL:CG1	2.55	0.54
9:I:59:VAL:O	9:I:61:ASP:N	2.40	0.54
4:B:43:LEU:HD11	4:B:811:TYR:O	2.08	0.54
3:A:1224:LEU:HD11	3:A:1240:CYS:CB	2.37	0.54
3:A:273:ASN:CA	3:A:296:LEU:HD11	2.37	0.54
4:B:178:ASN:O	4:B:179:CYS:C	2.45	0.54
4:B:900:ALA:CB	12:L:61:THR:OG1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:81:PRO:CB	8:H:82:PRO:CD	2.71	0.54
3:A:427:GLN:O	3:A:428:TYR:C	2.46	0.54
8:H:58:THR:HB	8:H:143:LEU:CD1	2.37	0.54
5:C:58:LEU:HD21	10:J:57:ILE:CD1	2.33	0.54
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.47	0.54
6:E:190:LEU:CD2	6:E:190:LEU:N	2.69	0.54
8:H:61:SER:HB3	8:H:139:ASN:HB3	1.90	0.54
8:H:4:THR:HG22	8:H:5:LEU:N	2.23	0.54
3:A:261:ASP:HB3	3:A:323:LYS:HE3	1.88	0.54
4:B:174:LEU:HD22	4:B:204:ILE:CD1	2.14	0.54
4:B:893:LEU:CD2	4:B:913:GLY:H	2.21	0.54
4:B:423:LYS:HA	4:B:426:LYS:HZ1	1.72	0.54
3:A:640:GLN:O	3:A:643:ALA:HB3	2.07	0.54
9:I:32:CYS:O	9:I:33:SER:OG	2.23	0.54
4:B:1064:TYR:N	4:B:1064:TYR:CD1	2.75	0.54
7:F:123:LYS:CG	7:F:123:LYS:O	2.55	0.54
3:A:181:LEU:O	3:A:202:LEU:HD12	2.08	0.54
4:B:34:ILE:CD1	4:B:34:ILE:N	2.71	0.54
5:C:242:GLN:HE21	5:C:246:ARG:NE	2.00	0.54
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.42	0.54
2:T:1:DA:C2'	2:T:2:DC:O5'	2.44	0.54
3:A:909:ASP:OD2	3:A:910:PRO:HD3	2.07	0.54
5:C:6:PRO:HG2	11:K:97:LYS:HB3	1.89	0.54
4:B:589:VAL:CG1	4:B:590:HIS:N	2.70	0.54
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.73	0.54
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.89	0.54
3:A:1291:VAL:CG1	3:A:1292:PRO:CD	2.84	0.54
3:A:1436:ILE:CD1	4:B:1139:ILE:HG23	2.38	0.54
3:A:658:LEU:HD12	3:A:658:LEU:C	2.28	0.54
4:B:230:ALA:CB	4:B:231:PRO:CD	2.83	0.54
3:A:918:GLU:O	3:A:918:GLU:OE1	2.25	0.54
3:A:417:TYR:O	3:A:418:SER:CB	2.56	0.54
3:A:756:ILE:O	3:A:759:ALA:HB3	2.08	0.54
6:E:90:VAL:H	6:E:120:ALA:HB2	1.72	0.54
4:B:871:THR:O	4:B:872:GLU:C	2.46	0.54
3:A:283:GLY:O	3:A:285:PRO:HD3	2.07	0.54
3:A:974:ASP:OD1	3:A:974:ASP:N	2.40	0.54
4:B:1073:TYR:N	4:B:1073:TYR:CD1	2.74	0.54
3:A:1132:LYS:O	3:A:1135:ARG:CB	2.55	0.54
3:A:1219:THR:HG21	3:A:1271:ILE:HD11	1.90	0.54
3:A:863:VAL:HG23	6:E:170:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:156:LEU:HD21	6:E:197:LYS:HB2	1.88	0.54
6:E:162:ARG:NH2	6:E:166:LYS:HZ2	2.04	0.54
4:B:843:GLN:HB2	4:B:993:THR:HB	1.90	0.54
3:A:273:ASN:N	3:A:296:LEU:CD1	2.70	0.54
4:B:1184:GLY:C	4:B:1186:ASP:N	2.60	0.54
4:B:899:ILE:HD11	4:B:911:ILE:CG2	2.36	0.54
4:B:59:LEU:CD1	4:B:417:PHE:CE2	2.90	0.54
4:B:288:ALA:O	4:B:327:ARG:NH2	2.37	0.54
4:B:356:LEU:O	4:B:357:GLN:HG3	2.07	0.54
7:F:73:ALA:O	7:F:74:ILE:CG1	2.45	0.54
4:B:773:MET:C	4:B:775:LYS:N	2.59	0.54
2:T:5:DT:H2''	2:T:6:DC:C5'	2.29	0.54
4:B:1084:GLN:HB3	5:C:201:TRP:HH2	1.72	0.54
5:C:260:LEU:O	5:C:263:THR:HB	2.08	0.54
8:H:88:SER:O	8:H:89:LEU:HG	2.07	0.54
5:C:92:CYS:SG	5:C:94:LYS:N	2.80	0.54
8:H:77:ARG:O	8:H:78:SER:C	2.46	0.54
6:E:157:SER:O	6:E:159:ASP:N	2.41	0.54
3:A:1236:LEU:C	3:A:1237:ILE:HG13	2.29	0.54
4:B:641:GLU:HB3	4:B:643:ASP:OD2	2.08	0.54
4:B:707:PRO:CD	4:B:708:GLU:H	2.19	0.54
5:C:172:PRO:CD	5:C:173:ALA:H	2.21	0.54
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	1.56	0.54
12:L:29:TYR:C	12:L:30:ILE:HG13	2.27	0.54
4:B:428:ILE:O	4:B:429:PHE:C	2.45	0.54
3:A:530:GLY:O	3:A:653:VAL:CG1	2.56	0.54
3:A:596:THR:O	3:A:597:LEU:C	2.46	0.54
6:E:98:ILE:O	6:E:100:ILE:N	2.40	0.54
9:I:25:LEU:O	9:I:26:LEU:HD23	2.08	0.54
6:E:37:LEU:CG	6:E:37:LEU:O	2.56	0.54
4:B:557:PHE:C	4:B:557:PHE:CD2	2.81	0.54
9:I:56:ALA:O	9:I:57:GLY:C	2.44	0.54
5:C:193:TYR:H	5:C:193:TYR:HD2	1.55	0.54
6:E:173:SER:C	6:E:175:LEU:H	2.11	0.54
6:E:197:LYS:C	6:E:198:ILE:HG13	2.28	0.54
3:A:89:PRO:C	3:A:90:VAL:CG2	2.77	0.54
4:B:469:GLN:CG	4:B:470:LYS:H	2.21	0.54
4:B:1099:VAL:O	4:B:1103:ILE:CD1	2.56	0.54
4:B:1102:LYS:HB2	4:B:1103:ILE:HD13	1.90	0.54
3:A:54:ASN:O	3:A:55:ASP:CB	2.56	0.54
3:A:168:GLY:O	3:A:169:ASN:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.86	0.54
4:B:563:MET:CE	4:B:588:GLY:HA3	2.37	0.54
4:B:378:LEU:O	4:B:382:ILE:HG12	2.08	0.54
3:A:1067:LEU:CD2	3:A:1367:HIS:CE1	2.84	0.54
6:E:115:ASN:O	6:E:116:ILE:HG12	2.08	0.54
5:C:69:LEU:N	5:C:69:LEU:CD1	2.71	0.54
6:E:29:PHE:C	6:E:30:ILE:HG13	2.27	0.54
5:C:80:LEU:HD11	5:C:95:CYS:CA	2.38	0.54
3:A:1220:PHE:O	3:A:1222:ASN:N	2.40	0.54
3:A:537:ARG:CG	3:A:537:ARG:HH11	2.21	0.54
3:A:856:THR:HB	3:A:865:GLN:HB2	1.89	0.54
3:A:863:VAL:HG11	3:A:866:PHE:CE2	2.43	0.54
3:A:306:ASN:N	3:A:306:ASN:ND2	2.55	0.54
4:B:329:THR:C	4:B:332:ASP:HB2	2.27	0.54
3:A:216:VAL:O	3:A:219:PHE:HB2	2.08	0.54
3:A:139:TRP:O	3:A:141:LEU:N	2.40	0.54
3:A:14:VAL:HG23	3:A:1432:GLN:HE22	1.72	0.54
4:B:555:ILE:HD11	4:B:582:VAL:CG1	2.33	0.54
9:I:50:THR:CG2	9:I:52:ILE:CG2	2.83	0.54
3:A:1325:THR:O	6:E:148:GLU:HB2	2.07	0.54
4:B:412:LEU:O	4:B:413:LEU:C	2.46	0.54
3:A:353:ILE:HG21	3:A:487:MET:HB2	1.89	0.54
3:A:370:ILE:HG22	3:A:374:LEU:HD12	1.90	0.54
11:K:65:HIS:CD2	11:K:66:PRO:N	2.76	0.54
3:A:1076:ALA:HA	3:A:1079:MET:CE	2.38	0.54
11:K:71:PHE:C	11:K:71:PHE:CD1	2.82	0.54
11:K:32:VAL:O	11:K:32:VAL:HG12	2.07	0.54
3:A:547:LEU:CD2	11:K:58:PHE:HD1	2.14	0.54
4:B:784:ASN:CG	4:B:788:ARG:HD2	2.27	0.54
4:B:314:LEU:O	4:B:315:LYS:C	2.46	0.54
4:B:1160:VAL:O	4:B:1194:ILE:HD13	2.07	0.54
5:C:99:LEU:CD2	5:C:99:LEU:N	2.70	0.54
4:B:57:TYR:CD1	4:B:57:TYR:N	2.76	0.54
4:B:123:THR:O	4:B:125:SER:N	2.41	0.54
4:B:223:VAL:HG12	4:B:223:VAL:O	2.08	0.54
3:A:77:CYS:SG	3:A:80:HIS:CE1	3.01	0.53
5:C:22:LEU:HD23	5:C:22:LEU:C	2.28	0.53
4:B:426:LYS:O	4:B:430:ARG:CZ	2.56	0.53
4:B:297:ILE:O	4:B:300:HIS:N	2.41	0.53
4:B:590:HIS:CD2	4:B:596:LEU:HD22	2.43	0.53
7:F:76:LYS:O	7:F:79:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:801:LYS:N	10:J:52:THR:CG2	2.71	0.53
6:E:113:GLN:HB3	6:E:137:GLU:CD	2.27	0.53
4:B:233:PRO:HG2	4:B:234:ILE:H	1.73	0.53
3:A:1229:SER:CB	3:A:1233:ASP:OD2	2.56	0.53
3:A:529:CYS:O	3:A:529:CYS:SG	2.66	0.53
3:A:1133:LEU:H	3:A:1133:LEU:HD23	1.71	0.53
4:B:482:VAL:O	4:B:483:LEU:C	2.47	0.53
8:H:84:ALA:HB1	8:H:87:ARG:CB	2.38	0.53
4:B:292:ILE:HD12	4:B:326:ASP:HA	1.90	0.53
5:C:255:VAL:HG12	11:K:91:CYS:HB3	1.90	0.53
4:B:1096:ARG:HG2	4:B:1096:ARG:HH11	1.72	0.53
3:A:401:GLY:CA	3:A:435:HIS:HD2	2.21	0.53
3:A:1203:ASN:O	3:A:1204:ASP:C	2.47	0.53
3:A:16:GLU:HB2	4:B:1217:TYR:HB2	1.91	0.53
3:A:89:PRO:C	3:A:204:THR:CG2	2.77	0.53
3:A:273:ASN:N	3:A:296:LEU:HD11	2.22	0.53
5:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.53
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.32	0.53
3:A:889:SER:CB	3:A:892:ALA:H	2.11	0.53
4:B:361:LEU:HD12	4:B:361:LEU:N	2.22	0.53
5:C:63:ILE:HG22	5:C:67:LEU:HD11	1.91	0.53
5:C:57:VAL:CG2	10:J:57:ILE:HD11	2.37	0.53
3:A:577:ILE:O	3:A:578:LEU:C	2.46	0.53
3:A:805:LEU:HD12	3:A:806:ARG:N	2.22	0.53
3:A:1148:ILE:CD1	3:A:1198:ASP:HB2	2.38	0.53
3:A:1227:ILE:O	3:A:1238:ILE:HA	2.09	0.53
3:A:1326:ARG:O	3:A:1327:ILE:O	2.26	0.53
3:A:857:ARG:NH1	7:F:139:PRO:HG2	2.24	0.53
4:B:638:PHE:HD2	4:B:653:VAL:HG21	1.71	0.53
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.44	0.53
4:B:992:ILE:HD13	11:K:67:PHE:HE2	1.71	0.53
2:T:1:DA:H2''	2:T:2:DC:C5'	2.39	0.53
3:A:896:ARG:HB3	3:A:897:TYR:CD1	2.44	0.53
3:A:913:LEU:HD12	3:A:915:SER:N	2.21	0.53
3:A:107:CYS:O	3:A:111:GLY:HA2	2.09	0.53
3:A:341:MET:HE1	3:A:843:LYS:NZ	2.23	0.53
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	2.23	0.53
4:B:856:PHE:N	4:B:856:PHE:CD1	2.76	0.53
8:H:138:GLU:C	8:H:139:ASN:O	2.46	0.53
11:K:47:ARG:HH11	11:K:47:ARG:HG2	1.73	0.53
6:E:153:HIS:O	6:E:154:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1155:ASP:HB3	3:A:1241:ARG:HH21	1.73	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	1.97	0.53
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.34	0.53
3:A:567:LYS:HG3	3:A:568:PRO:HG2	1.90	0.53
3:A:24:PRO:HG3	3:A:237:THR:HG21	1.89	0.53
3:A:543:LEU:CD1	3:A:547:LEU:HD11	2.39	0.53
3:A:544:ASP:OD1	3:A:545:GLN:N	2.40	0.53
3:A:690:VAL:CG1	3:A:718:VAL:HG13	2.39	0.53
4:B:1147:LEU:O	4:B:1151:LEU:HB2	2.09	0.53
4:B:1158:PHE:CE2	4:B:1160:VAL:HG22	2.43	0.53
4:B:228:LYS:O	4:B:229:ALA:O	2.25	0.53
4:B:877:PRO:O	4:B:878:GLN:CG	2.56	0.53
4:B:487:THR:CG2	4:B:488:TYR:N	2.71	0.53
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.08	0.53
3:A:351:THR:HG21	3:A:466:SER:O	2.08	0.53
12:L:45:ALA:O	12:L:46:VAL:HG23	2.09	0.53
12:L:53:HIS:C	12:L:55:ILE:H	2.11	0.53
3:A:928:LEU:O	3:A:931:GLU:N	2.42	0.53
3:A:1364:ASN:C	3:A:1364:ASN:ND2	2.62	0.53
3:A:947:PHE:HD2	3:A:954:TRP:CZ2	2.27	0.53
5:C:70:ILE:HD11	5:C:144:ILE:HD11	1.86	0.53
4:B:1096:ARG:HG3	4:B:1097:HIS:N	2.23	0.53
3:A:1408:ILE:O	3:A:1412:ALA:HB2	2.07	0.53
3:A:613:ILE:N	3:A:613:ILE:HD13	2.23	0.53
3:A:1105:LEU:HD23	3:A:1384:VAL:HG21	1.89	0.53
3:A:1348:LEU:O	3:A:1352:VAL:HG23	2.09	0.53
4:B:826:ALA:HB2	4:B:1087:PHE:CE1	2.43	0.53
3:A:381:THR:HG23	3:A:382:PRO:CD	2.38	0.53
4:B:321:GLY:O	4:B:324:ILE:N	2.41	0.53
4:B:326:ASP:CG	4:B:329:THR:OG1	2.47	0.53
11:K:49:GLU:C	11:K:51:LEU:H	2.11	0.53
3:A:953:ASN:C	3:A:954:TRP:CD1	2.82	0.53
5:C:60:ASP:CB	12:L:67:PHE:CE1	2.80	0.53
5:C:67:LEU:O	5:C:70:ILE:HB	2.08	0.53
3:A:1444:MET:CB	7:F:133:VAL:HG12	2.38	0.53
7:F:81:THR:CG2	7:F:136:ARG:HH11	2.19	0.53
3:A:582:ILE:HG22	3:A:610:GLY:CA	2.39	0.53
3:A:755:PHE:O	3:A:758:ILE:N	2.42	0.53
4:B:1024:ALA:O	4:B:1025:HIS:C	2.46	0.53
7:F:109:VAL:CG2	7:F:124:GLU:CG	2.87	0.53
3:A:82:GLY:HA3	3:A:241:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:604:ARG:HH21	4:B:614:SER:HA	1.74	0.53
3:A:250:ILE:O	3:A:251:SER:HB3	2.08	0.53
3:A:1134:ILE:O	3:A:1135:ARG:C	2.47	0.53
3:A:1265:ASN:O	3:A:1266:THR:C	2.47	0.53
4:B:712:PRO:O	4:B:712:PRO:CD	2.51	0.53
4:B:466:TRP:HB2	4:B:479:VAL:HG23	1.91	0.53
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.91	0.53
4:B:957:ASN:HD21	4:B:958:GLN:HB2	1.73	0.53
3:A:898:ARG:HD2	3:A:898:ARG:C	2.28	0.53
3:A:382:PRO:HD3	3:A:428:TYR:CE2	2.44	0.53
4:B:274:PRO:HG2	4:B:359:GLU:O	2.09	0.53
8:H:23:VAL:HG12	8:H:24:CYS:N	2.23	0.53
3:A:104:GLU:O	3:A:142:CYS:O	2.26	0.53
3:A:219:PHE:CZ	3:A:230:ARG:HG2	2.44	0.53
5:C:74:SER:HB3	5:C:77:ILE:CG1	2.39	0.53
6:E:113:GLN:C	6:E:114:ASN:HD22	2.11	0.53
3:A:606:LEU:HD22	3:A:614:PHE:CE2	2.43	0.53
7:F:97:ARG:NH2	7:F:108:PHE:CE1	2.77	0.53
4:B:317:CYS:O	4:B:320:ASP:N	2.33	0.53
3:A:116:ASP:O	3:A:118:HIS:N	2.41	0.53
4:B:901:PRO:HA	4:B:949:VAL:HB	1.89	0.53
3:A:1209:MET:O	3:A:1212:VAL:HB	2.09	0.53
4:B:840:ILE:O	4:B:1010:LEU:HD12	2.09	0.53
4:B:844:SER:OG	4:B:996:ARG:N	2.27	0.53
3:A:314:ALA:C	3:A:319:GLY:O	2.47	0.53
4:B:112:LEU:O	4:B:180:TYR:CE1	2.59	0.53
4:B:885:MET:HA	4:B:936:ASP:HB3	1.91	0.53
4:B:1172:ILE:O	4:B:1172:ILE:CG2	2.56	0.53
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.73	0.53
4:B:295:GLY:C	4:B:297:ILE:N	2.55	0.53
4:B:800:GLN:HG3	10:J:52:THR:HB	1.90	0.53
3:A:662:PHE:O	4:B:828:ALA:HA	2.09	0.53
3:A:993:LEU:HB2	3:A:1046:LEU:HD21	1.91	0.53
9:I:111:THR:CG2	9:I:113:ASP:H	2.22	0.53
4:B:942:ARG:HB2	4:B:945:GLU:HB2	1.91	0.53
4:B:805:THR:HA	4:B:809:MET:CE	2.39	0.53
4:B:498:THR:HB	4:B:537:LYS:O	2.08	0.53
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.09	0.53
4:B:635:ARG:CD	4:B:636:PRO:CD	2.78	0.53
4:B:203:PHE:CE1	4:B:212:LEU:HD12	2.44	0.53
4:B:824:ILE:HD11	10:J:45:CYS:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:41:ILE:CG1	5:C:172:PRO:HG3	2.39	0.53
5:C:244:VAL:HG21	11:K:105:PHE:CE1	2.43	0.53
3:A:899:VAL:CG1	3:A:929:LEU:CD1	2.81	0.53
3:A:1299:VAL:CG1	3:A:1300:LYS:H	1.99	0.53
3:A:112:LYS:HG2	3:A:113:LEU:N	2.23	0.53
3:A:550:LEU:HD12	3:A:556:TRP:NE1	2.24	0.53
5:C:181:ASP:OD1	5:C:183:TRP:O	2.26	0.53
5:C:244:VAL:HG21	11:K:105:PHE:CE2	2.45	0.52
3:A:30:ILE:HG13	4:B:1170:THR:CG2	2.38	0.52
3:A:892:ALA:CA	3:A:895:LYS:HB2	2.15	0.52
3:A:254:GLU:HB3	4:B:935:ARG:HH11	1.73	0.52
3:A:567:LYS:O	3:A:569:LYS:N	2.40	0.52
8:H:39:THR:OG1	8:H:124:ARG:HB3	2.08	0.52
3:A:230:ARG:O	3:A:233:TRP:HB2	2.08	0.52
3:A:472:LEU:O	3:A:475:THR:HB	2.09	0.52
5:C:77:ILE:CD1	5:C:129:ILE:HD11	2.38	0.52
8:H:114:VAL:N	8:H:125:LEU:O	2.41	0.52
3:A:660:ASN:ND2	4:B:1082:MET:HB3	2.24	0.52
3:A:667:GLY:O	3:A:669:THR:N	2.42	0.52
3:A:1148:ILE:HG22	3:A:1149:ALA:N	2.24	0.52
4:B:369:GLY:HA2	4:B:371:GLU:OE1	2.09	0.52
5:C:193:TYR:N	5:C:193:TYR:CD2	2.76	0.52
6:E:178:ILE:CG2	6:E:214:CYS:HA	2.39	0.52
3:A:367:PRO:HA	3:A:463:ILE:HD12	1.91	0.52
4:B:847:ASP:HB3	5:C:167:HIS:HD2	1.72	0.52
4:B:843:GLN:HB2	4:B:993:THR:CB	2.39	0.52
4:B:936:ASP:OD2	4:B:938:SER:OG	2.28	0.52
11:K:83:PRO:O	11:K:87:LEU:N	2.37	0.52
3:A:447:GLN:CB	3:A:448:PRO:HA	2.39	0.52
6:E:65:THR:OG1	6:E:67:GLU:CB	2.48	0.52
3:A:184:SER:O	3:A:185:TRP:CB	2.57	0.52
4:B:278:GLN:CG	4:B:279:ASP:H	2.17	0.52
3:A:1146:VAL:HG12	3:A:1201:ALA:HB3	1.91	0.52
3:A:870:GLU:HG2	6:E:208:TYR:CD2	2.44	0.52
4:B:215:GLN:O	4:B:406:LEU:HA	2.09	0.52
4:B:542:MET:HE2	4:B:747:MET:HE2	1.90	0.52
11:K:40:HIS:CE1	11:K:63:VAL:HG13	2.39	0.52
3:A:60:SER:OG	3:A:64:ASN:O	2.25	0.52
3:A:76:GLU:O	3:A:76:GLU:HG3	2.09	0.52
4:B:59:LEU:CD1	4:B:417:PHE:CD2	2.92	0.52
3:A:530:GLY:CA	3:A:532:ARG:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:634:THR:HG1	3:A:642:CYS:HG	1.54	0.52
4:B:800:GLN:HG3	10:J:52:THR:CG2	2.40	0.52
3:A:844:ALA:HB2	3:A:1389:PHE:CD2	2.45	0.52
6:E:35:VAL:C	6:E:37:LEU:H	2.13	0.52
3:A:919:ILE:O	3:A:921:GLY:N	2.42	0.52
3:A:964:ILE:HG22	3:A:965:GLN:N	2.23	0.52
4:B:757:PRO:O	4:B:758:PHE:HB2	2.08	0.52
12:L:34:CYS:SG	12:L:35:SER:N	2.82	0.52
3:A:396:PRO:C	3:A:397:ASN:OD1	2.48	0.52
4:B:708:GLU:C	4:B:710:LEU:N	2.60	0.52
4:B:912:ILE:O	4:B:938:SER:HB2	2.09	0.52
3:A:115:LEU:CG	3:A:142:CYS:HB3	2.40	0.52
4:B:109:THR:HG22	4:B:109:THR:O	2.09	0.52
3:A:453:MET:HE3	3:A:513:SER:HB2	1.91	0.52
5:C:74:SER:CB	5:C:77:ILE:HG13	2.38	0.52
3:A:657:LEU:O	3:A:660:ASN:N	2.41	0.52
3:A:665:GLY:HA2	4:B:1086:PHE:CD1	2.44	0.52
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.10	0.52
5:C:186:LEU:HB3	5:C:188:HIS:CD2	2.44	0.52
4:B:1035:ALA:O	4:B:1036:ALA:C	2.46	0.52
4:B:803:LEU:H	4:B:822:ASN:HD21	1.56	0.52
6:E:15:ALA:O	6:E:19:VAL:HG23	2.09	0.52
3:A:855:THR:HG23	3:A:856:THR:N	2.24	0.52
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.91	0.52
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.74	0.52
4:B:1161:HIS:O	4:B:1162:ILE:HG12	2.09	0.52
3:A:933:TYR:CD2	3:A:933:TYR:O	2.62	0.52
3:A:1207:LEU:HD22	3:A:1208:THR:H	1.74	0.52
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.57	0.52
3:A:777:PHE:CD2	3:A:782:ARG:CA	2.93	0.52
3:A:904:THR:CG2	3:A:905:ASP:H	2.22	0.52
3:A:224:PHE:CD2	3:A:231:PRO:HD3	2.45	0.52
10:J:64:ASN:CB	10:J:65:PRO:CD	2.75	0.52
3:A:15:LYS:HB3	4:B:1220:ARG:HA	1.91	0.52
4:B:778:MET:HE3	4:B:853:SER:HB2	1.90	0.52
3:A:95:PHE:O	3:A:96:ILE:C	2.48	0.52
3:A:1139:GLU:O	3:A:1140:HIS:O	2.28	0.52
4:B:647:GLY:O	4:B:648:HIS:CG	2.63	0.52
4:B:705:MET:H	4:B:710:LEU:CD1	2.22	0.52
3:A:406:ILE:HD12	3:A:431:LYS:O	2.09	0.52
3:A:1076:ALA:C	3:A:1078:GLN:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.90	0.52
6:E:187:TYR:CD2	6:E:188:LEU:HD23	2.32	0.52
3:A:244:PRO:CG	3:A:245:PRO:HD2	2.40	0.52
6:E:90:VAL:N	6:E:120:ALA:HB2	2.24	0.52
3:A:1116:LEU:HD22	3:A:1311:VAL:CG2	2.31	0.52
4:B:858:SER:HA	4:B:966:VAL:O	2.09	0.52
4:B:165:VAL:CG1	4:B:166:PHE:N	2.72	0.52
11:K:91:CYS:O	11:K:95:ILE:HG13	2.10	0.52
4:B:197:PHE:CG	4:B:817:LEU:HD11	2.45	0.52
3:A:447:GLN:HB3	3:A:448:PRO:HA	1.92	0.52
4:B:1065:GLN:NE2	4:B:1067:ARG:N	2.56	0.52
3:A:595:THR:OG1	3:A:603:ASN:HB3	2.10	0.52
4:B:686:ASN:H	4:B:686:ASN:ND2	2.06	0.52
9:I:106:CYS:O	9:I:107:SER:C	2.46	0.52
3:A:1138:ILE:N	3:A:1138:ILE:HD13	2.25	0.52
4:B:25:ILE:HG22	4:B:26:THR:N	2.23	0.52
4:B:955:THR:HG23	12:L:54:ARG:C	2.30	0.52
3:A:898:ARG:CD	3:A:898:ARG:C	2.77	0.52
4:B:448:ILE:HG22	4:B:450:ALA:H	1.75	0.52
3:A:886:ILE:HD11	3:A:944:ARG:N	2.25	0.52
4:B:130:VAL:CG1	4:B:132:VAL:CG2	2.88	0.52
5:C:181:ASP:CG	5:C:186:LEU:HD13	2.29	0.52
3:A:354:SER:HA	3:A:482:PHE:CD2	2.45	0.52
3:A:733:ALA:O	3:A:734:GLU:C	2.45	0.52
4:B:807:ARG:HH11	4:B:807:ARG:HG3	1.74	0.52
4:B:957:ASN:HB3	4:B:961:LEU:CD1	2.35	0.52
3:A:899:VAL:CG2	3:A:1029:ARG:HG2	2.39	0.52
4:B:364:ILE:O	4:B:365:THR:HB	2.10	0.52
8:H:31:THR:O	8:H:32:THR:HB	2.09	0.52
11:K:83:PRO:O	11:K:86:ALA:HB3	2.10	0.52
4:B:280:ILE:CG2	4:B:285:ILE:HG12	2.26	0.52
3:A:741:ASN:HD22	3:A:744:LYS:H	1.58	0.52
3:A:803:SER:C	3:A:805:LEU:N	2.60	0.52
4:B:782:LEU:O	4:B:783:THR:C	2.47	0.52
4:B:554:ILE:O	4:B:555:ILE:C	2.48	0.52
4:B:806:THR:CG2	4:B:808:ALA:H	2.21	0.52
3:A:225:ASN:O	3:A:227:VAL:N	2.43	0.52
6:E:157:SER:C	6:E:159:ASP:N	2.61	0.52
3:A:1068:ALA:O	3:A:1069:ALA:C	2.47	0.52
10:J:28:ASP:OD1	10:J:28:ASP:N	2.43	0.52
3:A:1267:MET:O	3:A:1271:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1339:LEU:HD11	6:E:147:HIS:CD2	2.45	0.51
6:E:195:VAL:CG2	6:E:213:ILE:HD13	2.40	0.51
3:A:780:VAL:HG23	4:B:699:GLU:CD	2.29	0.51
3:A:267:ALA:O	3:A:268:ASP:C	2.48	0.51
4:B:474:SER:HA	4:B:476:ARG:CD	2.40	0.51
5:C:134:ILE:HD12	5:C:141:GLY:HA2	1.90	0.51
3:A:54:ASN:O	3:A:55:ASP:HB3	2.10	0.51
3:A:900:ASP:HA	3:A:926:GLN:NE2	2.25	0.51
3:A:380:VAL:HG21	3:A:430:TRP:HB2	1.91	0.51
4:B:292:ILE:HD11	4:B:327:ARG:N	2.25	0.51
3:A:211:PHE:C	3:A:213:HIS:H	2.13	0.51
3:A:834:THR:HG21	3:A:1077:THR:N	2.23	0.51
3:A:605:MET:HE3	3:A:605:MET:HA	1.91	0.51
4:B:313:MET:HE2	4:B:386:LEU:HD22	1.92	0.51
8:H:11:GLN:HA	8:H:53:ASP:O	2.10	0.51
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.92	0.51
4:B:20:ASP:N	4:B:655:LYS:NZ	2.58	0.51
4:B:1130:PHE:HZ	4:B:1138:MET:HG2	1.75	0.51
3:A:1172:LEU:H	3:A:1172:LEU:HD23	1.75	0.51
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.40	0.51
3:A:464:PRO:HG2	3:A:465:TYR:HD1	1.74	0.51
3:A:1029:ARG:O	3:A:1033:GLN:N	2.32	0.51
6:E:20:LYS:HE2	6:E:60:PHE:CE1	2.45	0.51
8:H:32:THR:HG22	8:H:33:GLN:N	2.24	0.51
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.91	0.51
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.45	0.51
3:A:107:CYS:HB3	3:A:114:LEU:CD2	2.32	0.51
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.10	0.51
4:B:1202:LEU:O	4:B:1203:LEU:C	2.48	0.51
4:B:1084:GLN:HE22	5:C:192:TRP:N	2.05	0.51
3:A:804:TYR:HE1	4:B:1021:MET:HE3	1.75	0.51
11:K:78:THR:HG22	11:K:79:GLU:O	2.10	0.51
9:I:59:VAL:O	9:I:62:ILE:N	2.27	0.51
8:H:102:TYR:HD2	8:H:102:TYR:H	1.55	0.51
3:A:557:ASP:OD2	3:A:559:VAL:CG2	2.58	0.51
6:E:171:LYS:O	6:E:172:GLU:C	2.48	0.51
4:B:701:ILE:CG1	4:B:740:HIS:HE1	2.24	0.51
3:A:322:VAL:O	3:A:323:LYS:CG	2.58	0.51
3:A:909:ASP:CG	3:A:910:PRO:HD3	2.30	0.51
3:A:913:LEU:CD1	3:A:915:SER:H	2.19	0.51
11:K:97:LYS:O	11:K:100:ALA:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:245:GLU:OE1	4:B:551:PRO:HG2	2.09	0.51
4:B:273:LEU:CD2	4:B:360:PHE:HD1	2.24	0.51
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.41	0.51
3:A:209:ASN:O	3:A:210:ILE:C	2.47	0.51
1:R:10:A:C8	1:R:10:A:OP2	2.58	0.51
3:A:1100:ARG:NH2	3:A:1351:GLU:HG2	2.25	0.51
4:B:892:LYS:HE2	4:B:904:ARG:O	2.10	0.51
4:B:1102:LYS:O	4:B:1104:HIS:N	2.40	0.51
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.51
4:B:566:LEU:HD11	4:B:586:TRP:CD2	2.44	0.51
11:K:82:ASP:OD2	11:K:84:LYS:HD2	2.11	0.51
9:I:15:TYR:O	9:I:27:PHE:CD2	2.61	0.51
4:B:816:GLU:C	4:B:818:PRO:HD3	2.30	0.51
3:A:666:ILE:HA	4:B:1026:LEU:CD1	2.41	0.51
3:A:826:ASP:O	3:A:830:LYS:N	2.39	0.51
4:B:686:ASN:C	4:B:688:GLY:H	2.14	0.51
4:B:57:TYR:N	4:B:57:TYR:HD1	2.09	0.51
3:A:359:LEU:HD22	3:A:363:GLN:HB2	1.91	0.51
3:A:1119:TYR:HD2	3:A:1305:VAL:HG22	1.76	0.51
5:C:167:HIS:CD2	5:C:168:ALA:H	2.29	0.51
3:A:324:SER:O	3:A:326:ARG:N	2.36	0.51
3:A:848:ILE:HB	3:A:1065:GLY:CA	2.41	0.51
3:A:737:LEU:H	3:A:737:LEU:HD23	1.75	0.51
10:J:3:VAL:HA	10:J:53:HIS:CD2	2.45	0.51
3:A:694:THR:HA	3:A:714:PHE:HE1	1.75	0.51
5:C:116:LYS:O	5:C:116:LYS:HG2	2.09	0.51
3:A:756:ILE:CG2	3:A:757:ASN:N	2.74	0.51
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	2.09	0.51
4:B:1168:LEU:C	4:B:1170:THR:H	2.13	0.51
3:A:568:PRO:CB	5:C:221:TYR:HE1	2.22	0.51
3:A:552:TRP:NE1	3:A:655:PHE:HD1	2.07	0.51
3:A:552:TRP:CD1	3:A:655:PHE:CD1	2.99	0.51
3:A:743:VAL:CG1	3:A:758:ILE:HD11	2.41	0.51
4:B:981:ALA:HA	4:B:1092:TYR:CD2	2.45	0.51
6:E:143:ASN:OD1	6:E:187:TYR:HE1	1.93	0.51
4:B:1016:ALA:O	4:B:1017:ILE:HD13	2.10	0.51
4:B:516:ASN:H	4:B:516:ASN:HD22	1.58	0.51
4:B:653:VAL:O	4:B:654:ARG:HD3	2.10	0.51
4:B:471:LYS:CG	4:B:472:ALA:H	1.91	0.51
3:A:67:CYS:HB3	3:A:68:GLN:NE2	2.25	0.51
4:B:1159:ARG:HE	4:B:1193:GLN:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:898:ARG:O	3:A:899:VAL:HG23	2.11	0.51
8:H:95:TYR:HE2	8:H:97:MET:SD	2.33	0.51
3:A:24:PRO:HB3	3:A:237:THR:HG21	1.92	0.51
10:J:18:TRP:CZ2	10:J:22:LEU:HD11	2.46	0.51
1:R:8:G:H2'	1:R:9:G:H8	1.76	0.51
8:H:109:LYS:HB3	8:H:110:ASP:OD2	2.10	0.51
3:A:599:SER:C	3:A:601:LYS:N	2.64	0.51
3:A:1105:LEU:O	3:A:1384:VAL:HG23	2.10	0.51
3:A:1389:PHE:HE1	3:A:1390:ASN:OD1	1.93	0.51
9:I:50:THR:HG22	9:I:52:ILE:N	2.24	0.51
4:B:121:ASN:N	4:B:121:ASN:ND2	2.57	0.51
4:B:1215:ARG:O	4:B:1216:LEU:HD23	2.11	0.51
5:C:96:SER:O	5:C:97:VAL:HG23	2.11	0.51
4:B:1187:ASN:OD1	4:B:1190:ASP:O	2.29	0.51
3:A:855:THR:HG23	3:A:857:ARG:CG	2.40	0.51
3:A:818:MET:O	3:A:819:GLY:C	2.49	0.51
4:B:426:LYS:O	4:B:430:ARG:NH1	2.44	0.51
3:A:672:ASP:CG	3:A:674:PRO:HD2	2.31	0.51
9:I:33:SER:O	9:I:34:TYR:C	2.48	0.51
7:F:75:PRO:C	7:F:77:ASP:H	2.14	0.51
10:J:57:ILE:HG23	10:J:58:GLU:N	2.25	0.51
3:A:834:THR:CG2	3:A:1077:THR:HG23	2.40	0.51
5:C:194:GLU:C	5:C:195:GLN:HG3	2.30	0.51
4:B:770:GLN:CG	4:B:983:ARG:O	2.58	0.51
7:F:97:ARG:O	7:F:98:ALA:C	2.49	0.51
3:A:1319:VAL:HB	3:A:1322:ILE:CD1	2.35	0.51
5:C:98:VAL:C	5:C:99:LEU:CD2	2.77	0.51
3:A:697:ALA:HA	3:A:702:LEU:HB2	1.93	0.51
5:C:80:LEU:HD11	5:C:95:CYS:C	2.31	0.51
8:H:49:VAL:O	8:H:50:ALA:HB2	2.10	0.51
3:A:403:LYS:O	3:A:404:TYR:O	2.28	0.51
3:A:970:THR:CG2	3:A:970:THR:O	2.58	0.51
4:B:613:VAL:CG1	4:B:627:PHE:O	2.57	0.51
6:E:85:GLU:OE2	6:E:92:THR:HG21	2.11	0.51
4:B:34:ILE:HD11	4:B:743:ILE:CG2	2.39	0.51
3:A:352:VAL:CG1	3:A:353:ILE:H	2.22	0.51
4:B:933:SER:OG	4:B:934:LYS:N	2.42	0.51
3:A:147:VAL:HB	3:A:149:GLU:H	1.76	0.51
4:B:364:ILE:HD13	4:B:585:VAL:HG22	1.93	0.51
8:H:115:TYR:HA	8:H:123:MET:O	2.11	0.51
3:A:541:ILE:CG2	3:A:546:VAL:HG22	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:655:PHE:CE2	3:A:659:HIS:HD2	2.28	0.51
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.93	0.51
9:I:115:LYS:O	9:I:116:ASN:O	2.29	0.51
4:B:1191:ILE:CG2	4:B:1192:TYR:N	2.74	0.51
3:A:849:MET:HE1	3:A:1061:GLY:CA	2.36	0.51
11:K:28:PRO:O	11:K:29:ASN:C	2.49	0.51
3:A:414:ASP:C	3:A:414:ASP:OD1	2.48	0.51
1:R:4:G:H1	2:T:11:DC:H42	1.59	0.51
12:L:28:LYS:HB2	12:L:39:SER:HA	1.93	0.51
3:A:1118:VAL:HG23	3:A:1306:LEU:HB2	1.92	0.51
3:A:889:SER:HB2	3:A:892:ALA:N	2.12	0.51
4:B:361:LEU:HD23	4:B:377:PHE:CD2	2.45	0.51
7:F:77:ASP:HB3	7:F:78:GLN:HG3	1.92	0.51
4:B:796:LEU:HB3	4:B:799:PRO:CG	2.41	0.51
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.41	0.51
3:A:335:ARG:O	3:A:338:GLY:N	2.43	0.51
5:C:258:ILE:HG22	5:C:259:LEU:N	2.25	0.51
3:A:609:ASP:O	3:A:611:GLN:HB2	2.10	0.51
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.41	0.51
3:A:1101:LEU:HG	3:A:1105:LEU:HD12	1.93	0.51
4:B:781:PHE:HE2	4:B:793:ALA:HB1	1.75	0.51
11:K:27:ALA:CB	11:K:28:PRO:HD3	2.38	0.51
3:A:404:TYR:N	3:A:404:TYR:CD1	2.78	0.51
4:B:694:ASP:O	4:B:695:ALA:C	2.50	0.51
3:A:1127:ASP:CB	3:A:1130:GLN:HB3	2.38	0.50
3:A:1197:LEU:HD12	3:A:1209:MET:SD	2.51	0.50
6:E:147:HIS:HB3	6:E:150:VAL:HG23	1.93	0.50
3:A:91:PHE:N	3:A:297:GLN:NE2	2.58	0.50
4:B:637:LEU:HD23	4:B:742:GLU:OE2	2.11	0.50
4:B:110:HIS:NE2	12:L:53:HIS:HE1	2.09	0.50
3:A:929:LEU:H	3:A:929:LEU:HD23	1.76	0.50
3:A:166:GLY:O	3:A:167:CYS:CB	2.59	0.50
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.93	0.50
3:A:947:PHE:CE2	3:A:954:TRP:CE2	2.99	0.50
4:B:785:TYR:CE2	10:J:60:PHE:HE1	2.29	0.50
3:A:1402:PHE:CD2	3:A:1403:GLU:N	2.76	0.50
4:B:1024:ALA:O	4:B:1027:ILE:N	2.44	0.50
7:F:97:ARG:HG3	7:F:101:ILE:HD11	1.92	0.50
5:C:80:LEU:HD12	5:C:94:LYS:O	2.11	0.50
9:I:119:THR:CG2	9:I:119:THR:O	2.59	0.50
4:B:864:LYS:HG3	4:B:865:LYS:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:40:GLU:OE1	5:C:254:LYS:NZ	2.28	0.50
12:L:25:ALA:O	12:L:26:THR:OG1	2.22	0.50
3:A:511:ILE:HG12	3:A:521:MET:HE2	1.93	0.50
4:B:979:LYS:C	4:B:980:PHE:CD1	2.84	0.50
3:A:1283:VAL:CG1	3:A:1284:MET:N	2.74	0.50
3:A:1327:ILE:HG23	3:A:1327:ILE:O	2.10	0.50
4:B:996:ARG:NH2	5:C:38:ILE:CD1	2.70	0.50
4:B:1170:THR:HG23	4:B:1183:LYS:HZ1	1.75	0.50
3:A:167:CYS:SG	3:A:167:CYS:O	2.70	0.50
7:F:136:ARG:HD2	7:F:146:TRP:CD1	2.46	0.50
4:B:827:ILE:HD12	4:B:1086:PHE:CD2	2.47	0.50
3:A:590:ARG:O	3:A:591:PHE:HB2	2.11	0.50
3:A:691:LEU:O	3:A:694:THR:HB	2.11	0.50
3:A:825:ILE:HD13	4:B:533:CYS:SG	2.52	0.50
8:H:4:THR:CG2	8:H:5:LEU:N	2.73	0.50
9:I:19:ASP:OD2	9:I:24:ARG:NE	2.30	0.50
8:H:7:ASP:O	8:H:8:ASP:CB	2.59	0.50
3:A:680:THR:CG2	3:A:681:GLU:N	2.70	0.50
5:C:249:ASP:O	5:C:253:LYS:HG3	2.11	0.50
3:A:1118:VAL:HG12	3:A:1327:ILE:HG13	1.94	0.50
3:A:1236:LEU:O	3:A:1237:ILE:HG13	2.11	0.50
3:A:491:VAL:CG1	3:A:492:PRO:HD2	2.42	0.50
4:B:844:SER:HG	4:B:996:ARG:H	1.57	0.50
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.46	0.50
3:A:896:ARG:C	3:A:897:TYR:HD1	2.15	0.50
4:B:426:LYS:O	4:B:430:ARG:CD	2.60	0.50
3:A:942:PHE:C	3:A:942:PHE:CD2	2.85	0.50
3:A:1025:ARG:HG2	3:A:1025:ARG:NH1	2.02	0.50
2:T:4:DA:C2'	2:T:5:DT:C6	2.93	0.50
3:A:1412:ALA:HA	3:A:1417:GLU:HG3	1.92	0.50
3:A:1377:THR:C	3:A:1379:GLY:N	2.64	0.50
4:B:901:PRO:O	4:B:949:VAL:O	2.30	0.50
3:A:1127:ASP:C	3:A:1129:GLU:H	2.13	0.50
3:A:1118:VAL:HG12	3:A:1327:ILE:CD1	2.41	0.50
3:A:218:ASP:O	3:A:219:PHE:O	2.30	0.50
3:A:996:ASN:C	3:A:998:LEU:N	2.62	0.50
3:A:858:ASN:ND2	3:A:860:LEU:N	2.59	0.50
4:B:51:PHE:O	4:B:54:PHE:HB3	2.11	0.50
3:A:870:GLU:HB3	6:E:204:THR:HG21	1.94	0.50
6:E:89:GLY:O	6:E:91:LYS:N	2.44	0.50
3:A:1171:GLN:O	3:A:1174:PHE:CZ	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:640:VAL:CG1	4:B:650:GLU:O	2.60	0.50
5:C:173:ALA:O	5:C:233:GLU:O	2.28	0.50
6:E:16:PHE:O	6:E:17:ARG:C	2.49	0.50
3:A:868:TYR:OH	3:A:1366:ARG:HD3	2.12	0.50
5:C:23:SER:O	5:C:25:VAL:HG22	2.11	0.50
3:A:528:LEU:HD12	3:A:528:LEU:C	2.31	0.50
3:A:381:THR:HG23	3:A:382:PRO:HD2	1.94	0.50
3:A:568:PRO:HB3	5:C:221:TYR:CE1	2.46	0.50
8:H:15:VAL:CG2	8:H:26:ILE:HD11	2.42	0.50
3:A:113:LEU:HD12	3:A:218:ASP:OD1	2.11	0.50
4:B:236:HIS:NE2	4:B:389:ALA:HA	2.26	0.50
6:E:97:VAL:HG13	6:E:127:ILE:CG2	2.42	0.50
5:C:46:ILE:HG23	5:C:157:CYS:HB3	1.92	0.50
4:B:1106:ARG:CG	4:B:1107:ALA:N	2.75	0.50
3:A:1045:VAL:O	3:A:1049:ILE:HG13	2.12	0.50
3:A:590:ARG:HH21	3:A:620:LYS:C	2.14	0.50
9:I:55:THR:CG2	9:I:56:ALA:N	2.74	0.50
11:K:47:ARG:NH1	11:K:47:ARG:CB	2.74	0.50
6:E:161:LYS:HD2	6:E:195:VAL:CG2	2.42	0.50
11:K:61:TYR:HD1	11:K:62:LYS:N	2.10	0.50
3:A:296:LEU:O	3:A:300:VAL:HG23	2.12	0.50
4:B:1051:THR:HB	4:B:1054:GLY:H	1.75	0.50
4:B:288:ALA:HB1	4:B:331:LEU:HD13	1.93	0.50
9:I:28:GLU:OE2	9:I:28:GLU:C	2.50	0.50
9:I:32:CYS:SG	9:I:34:TYR:N	2.76	0.50
4:B:1138:MET:HA	4:B:1138:MET:CE	2.40	0.50
7:F:90:ARG:HG3	7:F:94:LEU:HD12	1.94	0.50
10:J:31:ASP:O	10:J:33:GLY:N	2.44	0.50
9:I:51:ASN:O	9:I:54:GLU:HG3	2.12	0.50
6:E:178:ILE:HD13	6:E:185:ALA:HB2	1.94	0.50
4:B:521:LEU:HD23	4:B:635:ARG:CG	2.38	0.50
3:A:491:VAL:H	4:B:1150:ARG:NH2	2.09	0.50
3:A:901:LEU:CG	3:A:926:GLN:HE21	2.04	0.50
4:B:424:LEU:HD12	4:B:448:ILE:HG23	1.93	0.50
4:B:566:LEU:O	4:B:567:GLU:C	2.50	0.50
9:I:7:CYS:SG	9:I:34:TYR:HB3	2.52	0.50
3:A:1400:CYS:O	3:A:1402:PHE:N	2.38	0.50
3:A:335:ARG:HD3	3:A:339:ASN:HD22	1.77	0.50
11:K:32:VAL:HG23	11:K:74:ARG:CB	2.42	0.50
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.75	0.50
4:B:724:ASP:C	4:B:724:ASP:OD1	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:140:ASP:OD1	7:F:141:GLY:N	2.45	0.50
3:A:707:GLY:HA3	3:A:1281:ARG:HD3	1.93	0.50
4:B:465:ASN:O	4:B:467:GLY:N	2.45	0.50
3:A:853:ASP:C	3:A:853:ASP:OD1	2.50	0.50
6:E:147:HIS:O	6:E:148:GLU:C	2.50	0.50
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.11	0.50
3:A:89:PRO:C	3:A:90:VAL:HG23	2.33	0.50
3:A:265:LYS:C	3:A:267:ALA:H	2.15	0.50
5:C:233:GLU:OE2	10:J:43:ARG:NH2	2.45	0.50
10:J:36:LEU:CD1	10:J:47:ARG:HG2	2.39	0.50
3:A:306:ASN:HD21	3:A:324:SER:CB	2.25	0.50
3:A:56:PRO:O	3:A:57:ARG:HG3	2.12	0.50
4:B:885:MET:HA	4:B:936:ASP:CB	2.42	0.50
3:A:908:LEU:HD11	3:A:983:ILE:CD1	2.32	0.50
3:A:937:VAL:O	3:A:938:LYS:C	2.49	0.50
4:B:423:LYS:HA	4:B:426:LYS:NZ	2.27	0.50
4:B:380:TYR:HE1	4:B:579:ARG:HE	1.59	0.50
3:A:332:LYS:O	3:A:334:GLY:N	2.45	0.50
3:A:830:LYS:CE	3:A:1098:VAL:HG21	2.35	0.50
4:B:662:MET:C	4:B:664:THR:N	2.63	0.50
4:B:627:PHE:O	4:B:632:ARG:NH1	2.43	0.50
3:A:88:LYS:HD2	3:A:293:GLU:OE2	2.12	0.50
3:A:321:PRO:C	3:A:322:VAL:HG13	2.32	0.50
4:B:483:LEU:HD22	4:B:491:THR:HG23	1.94	0.50
5:C:41:ILE:O	5:C:41:ILE:HG12	2.11	0.50
3:A:566:ILE:C	3:A:567:LYS:O	2.48	0.50
3:A:144:THR:O	3:A:146:MET:CE	2.59	0.50
7:F:136:ARG:O	7:F:143:PHE:HA	2.12	0.50
3:A:834:THR:HG21	3:A:1077:THR:HA	1.90	0.50
5:C:74:SER:CB	5:C:77:ILE:CG1	2.89	0.50
5:C:27:LEU:O	5:C:30:ALA:N	2.43	0.50
3:A:608:ILE:C	3:A:609:ASP:O	2.48	0.50
3:A:688:LYS:O	3:A:691:LEU:HB3	2.11	0.50
4:B:1177:HIS:O	4:B:1178:ASN:C	2.49	0.50
4:B:979:LYS:O	4:B:980:PHE:CD1	2.65	0.50
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.94	0.49
5:C:141:GLY:O	5:C:142:VAL:O	2.29	0.49
4:B:430:ARG:O	4:B:431:TYR:O	2.30	0.49
4:B:355:ILE:HG22	4:B:356:LEU:HD23	1.94	0.49
4:B:377:PHE:O	4:B:380:TYR:HB3	2.12	0.49
4:B:236:HIS:C	4:B:237:VAL:HG23	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:VAL:C	3:A:95:PHE:H	2.15	0.49
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.94	0.49
3:A:1105:LEU:CD2	3:A:1384:VAL:HG21	2.42	0.49
3:A:1389:PHE:O	3:A:1389:PHE:HD1	1.94	0.49
9:I:103:CYS:SG	9:I:106:CYS:SG	3.09	0.49
3:A:512:VAL:CG1	3:A:512:VAL:O	2.60	0.49
11:K:18:LYS:HE3	11:K:38:GLU:OE2	2.12	0.49
9:I:85:PHE:O	9:I:86:PHE:HB3	2.12	0.49
4:B:374:LYS:O	4:B:375:ALA:C	2.50	0.49
3:A:1225:PHE:C	3:A:1226:VAL:HG23	2.32	0.49
6:E:173:SER:HB2	6:E:177:ARG:NH2	2.27	0.49
3:A:269:ILE:HG13	3:A:299:HIS:HB3	1.93	0.49
3:A:493:GLN:H	4:B:1149:GLU:CD	2.16	0.49
4:B:882:THR:HG23	4:B:882:THR:O	2.12	0.49
3:A:385:ILE:HD11	3:A:428:TYR:CE2	2.48	0.49
3:A:568:PRO:O	5:C:221:TYR:CE1	2.64	0.49
10:J:1:MET:H1	10:J:57:ILE:N	2.10	0.49
3:A:1444:MET:N	7:F:133:VAL:O	2.45	0.49
3:A:1076:ALA:O	3:A:1079:MET:HG3	2.12	0.49
3:A:1410:PHE:O	3:A:1411:GLU:C	2.50	0.49
3:A:92:HIS:CD2	3:A:92:HIS:O	2.65	0.49
3:A:1098:VAL:N	3:A:1099:PRO:HD2	2.27	0.49
4:B:1023:VAL:O	4:B:1027:ILE:HG13	2.11	0.49
3:A:244:PRO:O	3:A:246:VAL:N	2.45	0.49
4:B:525:ALA:O	4:B:527:THR:HG22	2.13	0.49
4:B:614:SER:HB3	4:B:694:ASP:OD1	2.12	0.49
4:B:487:THR:HG22	4:B:489:SER:N	2.27	0.49
5:C:38:ILE:HG12	5:C:176:ILE:HD12	1.94	0.49
3:A:1242:VAL:O	3:A:1243:VAL:HG23	2.12	0.49
3:A:904:THR:CG2	3:A:905:ASP:N	2.75	0.49
3:A:27:VAL:CG1	3:A:238:CYS:SG	3.00	0.49
3:A:1258:HIS:O	3:A:1261:LYS:HB2	2.13	0.49
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.48	0.49
6:E:126:SER:C	6:E:128:PRO:HD3	2.29	0.49
9:I:64:SER:O	9:I:65:ASP:C	2.50	0.49
3:A:399:HIS:CB	3:A:400:PRO:CD	2.90	0.49
9:I:19:ASP:O	9:I:23:ASN:CA	2.58	0.49
6:E:9:ILE:O	6:E:10:SER:C	2.50	0.49
3:A:534:LEU:O	3:A:539:THR:CG2	2.59	0.49
3:A:1169:ILE:O	3:A:1169:ILE:HG22	2.12	0.49
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:34:ILE:O	4:B:35:SER:C	2.50	0.49
4:B:291:ILE:HD12	4:B:291:ILE:H	1.78	0.49
3:A:1156:PRO:HD2	3:A:1157:ASP:H	1.77	0.49
3:A:1191:TRP:HD1	3:A:1256:GLU:CD	2.16	0.49
3:A:1402:PHE:CG	3:A:1403:GLU:N	2.79	0.49
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.27	0.49
3:A:820:GLY:HA2	3:A:823:GLY:H	1.77	0.49
3:A:857:ARG:CZ	7:F:139:PRO:HG2	2.42	0.49
3:A:261:ASP:HB2	3:A:323:LYS:HB3	1.95	0.49
3:A:898:ARG:CD	3:A:899:VAL:N	2.71	0.49
3:A:903:ASN:O	3:A:906:HIS:N	2.46	0.49
3:A:526:ASP:O	3:A:527:THR:C	2.50	0.49
3:A:115:LEU:HD11	3:A:142:CYS:CB	2.43	0.49
4:B:236:HIS:CD2	4:B:389:ALA:HA	2.48	0.49
4:B:785:TYR:CD1	4:B:786:ASN:N	2.81	0.49
3:A:340:LEU:HD22	3:A:1429:ILE:HG23	1.95	0.49
3:A:709:THR:HG22	3:A:711:ARG:N	2.11	0.49
3:A:343:LYS:HE3	4:B:1151:LEU:O	2.13	0.49
4:B:759:PRO:HB2	4:B:767:ASN:HD21	1.76	0.49
4:B:750:GLY:O	4:B:751:VAL:C	2.51	0.49
5:C:193:TYR:N	5:C:193:TYR:HD2	2.11	0.49
3:A:1166:ASP:OD2	3:A:1239:ARG:NE	2.36	0.49
3:A:1160:SER:HA	3:A:1170:ILE:HG21	1.94	0.49
4:B:124:TYR:CB	4:B:204:ILE:HD13	2.42	0.49
3:A:955:PRO:C	3:A:956:LEU:HG	2.31	0.49
3:A:381:THR:HG23	3:A:382:PRO:HG2	1.95	0.49
3:A:1025:ARG:HA	3:A:1030:ARG:HH11	1.75	0.49
3:A:447:GLN:HA	3:A:448:PRO:C	2.33	0.49
3:A:1053:PHE:HD2	3:A:1054:LEU:H	1.59	0.49
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.49
3:A:1007:ILE:O	3:A:1010:ALA:CB	2.60	0.49
3:A:537:ARG:HG2	3:A:537:ARG:HH11	1.77	0.49
4:B:871:THR:O	4:B:872:GLU:O	2.31	0.49
3:A:1370:LEU:O	3:A:1374:VAL:HG23	2.12	0.49
4:B:978:ASP:OD1	4:B:1098:MET:HB3	2.12	0.49
3:A:862:ASN:HA	6:E:174:GLN:HA	1.94	0.49
3:A:818:MET:HG3	4:B:514:LEU:HD23	1.94	0.49
11:K:9:LEU:HD23	11:K:9:LEU:N	2.27	0.49
3:A:35:ILE:HA	3:A:52:GLY:O	2.12	0.49
3:A:896:ARG:HB3	3:A:897:TYR:HD1	1.78	0.49
3:A:927:VAL:HG12	3:A:928:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:PRO:O	5:C:221:TYR:HE1	1.96	0.49
9:I:32:CYS:SG	9:I:33:SER:N	2.82	0.49
5:C:191:TYR:N	5:C:191:TYR:HD1	2.11	0.49
6:E:157:SER:O	6:E:158:SER:C	2.51	0.49
3:A:1116:LEU:CD1	3:A:1329:THR:OG1	2.60	0.49
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.41	0.49
3:A:1308:THR:CG2	3:A:1309:ASP:H	2.24	0.49
3:A:705:LYS:CG	3:A:713:SER:HB3	2.40	0.49
4:B:173:MET:N	4:B:203:PHE:HE2	2.11	0.49
3:A:273:ASN:HA	3:A:296:LEU:CD1	2.43	0.49
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.95	0.49
11:K:53:ASP:OD1	11:K:56:VAL:CG2	2.61	0.49
3:A:106:VAL:CG1	3:A:107:CYS:H	2.24	0.49
3:A:452:LYS:CB	4:B:1141:HIS:HE1	2.13	0.49
3:A:1399:ARG:NH2	3:A:1417:GLU:OE1	2.45	0.49
6:E:114:ASN:O	6:E:115:ASN:CB	2.61	0.49
3:A:543:LEU:HD11	3:A:547:LEU:HD11	1.94	0.49
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.30	0.49
8:H:131:ASN:C	8:H:133:ASN:N	2.66	0.49
6:E:178:ILE:CG1	6:E:179:GLN:H	2.25	0.49
6:E:177:ARG:HD3	6:E:215:MET:SD	2.53	0.49
4:B:515:HIS:CD2	4:B:517:THR:H	2.31	0.49
3:A:351:THR:CG2	3:A:352:VAL:H	2.01	0.49
4:B:826:ALA:HB2	4:B:1087:PHE:CD1	2.48	0.49
4:B:842:ASN:HB3	4:B:845:SER:OG	2.13	0.49
5:C:41:ILE:CD1	5:C:172:PRO:HG3	2.41	0.49
6:E:39:LEU:O	6:E:42:PHE:N	2.38	0.49
6:E:55:ARG:C	6:E:57:MET:N	2.66	0.49
3:A:452:LYS:CB	4:B:1141:HIS:CE1	2.82	0.49
1:R:10:A:O3'	3:A:485:ASP:OD1	2.31	0.49
6:E:64:PRO:HG2	6:E:76:GLY:CA	2.37	0.49
6:E:121:MET:C	6:E:123:LEU:N	2.64	0.49
3:A:1349:TYR:O	3:A:1350:LYS:C	2.49	0.49
3:A:84:ILE:HG22	3:A:241:VAL:HG22	1.92	0.49
3:A:1017:LEU:HD23	3:A:1017:LEU:O	2.13	0.49
4:B:614:SER:OG	4:B:627:PHE:HB2	2.12	0.49
9:I:85:PHE:C	9:I:86:PHE:CD2	2.86	0.49
3:A:1225:PHE:C	3:A:1226:VAL:CG2	2.81	0.49
5:C:100:THR:HB	5:C:119:VAL:HG12	1.93	0.49
3:A:1116:LEU:HB2	3:A:1308:THR:CB	2.43	0.49
3:A:1130:GLN:O	3:A:1134:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1265:ASN:O	3:A:1268:LEU:N	2.46	0.49
4:B:841:MET:O	4:B:993:THR:HA	2.11	0.49
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.95	0.49
4:B:563:MET:O	4:B:563:MET:CG	2.45	0.49
3:A:567:LYS:HB2	8:H:95:TYR:HA	1.95	0.49
7:F:74:ILE:HG23	7:F:75:PRO:HD2	1.93	0.49
5:C:62:PHE:HD2	5:C:62:PHE:O	1.96	0.49
3:A:1076:ALA:HA	3:A:1079:MET:HE3	1.95	0.49
4:B:1084:GLN:NE2	5:C:191:TYR:C	2.66	0.49
3:A:401:GLY:O	3:A:435:HIS:HB2	2.12	0.49
3:A:691:LEU:HD12	3:A:691:LEU:C	2.33	0.49
4:B:317:CYS:O	4:B:319:GLU:N	2.46	0.49
4:B:736:THR:O	4:B:736:THR:CG2	2.51	0.49
3:A:361:LEU:N	3:A:471:ASN:HD22	2.10	0.49
3:A:989:GLY:O	3:A:990:VAL:C	2.51	0.49
3:A:116:ASP:C	3:A:118:HIS:H	2.15	0.49
4:B:224:GLN:O	4:B:238:ALA:HA	2.13	0.49
3:A:294:SER:O	3:A:298:PHE:CB	2.60	0.48
4:B:917:PRO:C	4:B:918:ILE:HD13	2.33	0.48
3:A:531:ILE:CD1	3:A:649:ILE:HG21	2.42	0.48
4:B:291:ILE:HG21	4:B:297:ILE:HD13	1.94	0.48
4:B:352:ALA:O	4:B:354:ASP:N	2.46	0.48
3:A:942:PHE:O	3:A:945:GLU:HB3	2.13	0.48
4:B:1219:ASP:C	4:B:1221:SER:N	2.64	0.48
4:B:780:VAL:CG1	4:B:817:LEU:HD23	2.43	0.48
3:A:1154:TYR:HB2	3:A:1191:TRP:HZ3	1.76	0.48
3:A:1261:LYS:C	3:A:1263:ILE:N	2.63	0.48
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.60	0.48
3:A:139:TRP:C	3:A:141:LEU:N	2.63	0.48
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.53	0.48
4:B:1147:LEU:CD2	4:B:1151:LEU:HD22	2.42	0.48
4:B:51:PHE:O	4:B:54:PHE:N	2.42	0.48
3:A:474:VAL:HG13	3:A:474:VAL:O	2.13	0.48
11:K:47:ARG:NH1	11:K:48:ALA:N	2.61	0.48
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.13	0.48
6:E:66:GLU:HA	6:E:69:ILE:HB	1.94	0.48
3:A:1141:THR:CG2	3:A:1205:LYS:HD2	2.43	0.48
3:A:493:GLN:HA	3:A:493:GLN:NE2	2.28	0.48
4:B:839:MET:CG	4:B:1010:LEU:HD11	2.43	0.48
4:B:843:GLN:O	4:B:843:GLN:HG3	2.12	0.48
5:C:36:VAL:O	5:C:37:MET:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1031:LEU:HD13	4:B:1055:ILE:HD12	1.95	0.48
3:A:107:CYS:N	3:A:114:LEU:CD2	2.75	0.48
3:A:26:GLU:O	3:A:27:VAL:C	2.50	0.48
9:I:15:TYR:O	9:I:27:PHE:HA	2.13	0.48
7:F:136:ARG:O	7:F:143:PHE:HB2	2.12	0.48
3:A:1441:PHE:CZ	7:F:88:TYR:C	2.87	0.48
3:A:335:ARG:HD3	3:A:335:ARG:HA	1.63	0.48
3:A:577:ILE:C	3:A:579:SER:N	2.65	0.48
8:H:109:LYS:C	8:H:111:LEU:H	2.16	0.48
3:A:1098:VAL:O	3:A:1099:PRO:C	2.51	0.48
9:I:113:ASP:OD2	9:I:116:ASN:HB2	2.12	0.48
8:H:5:LEU:CD2	8:H:133:ASN:O	2.58	0.48
4:B:660:LYS:O	4:B:663:ALA:HB3	2.14	0.48
3:A:882:SER:HA	3:A:952:ALA:O	2.13	0.48
3:A:1311:VAL:HG21	3:A:1329:THR:CG2	2.44	0.48
4:B:640:VAL:HG12	4:B:650:GLU:O	2.13	0.48
4:B:654:ARG:C	4:B:656:GLY:N	2.65	0.48
3:A:322:VAL:O	3:A:323:LYS:CB	2.60	0.48
4:B:461:LEU:HD12	4:B:466:TRP:HZ3	1.77	0.48
4:B:847:ASP:OD2	11:K:6:ARG:NH2	2.40	0.48
4:B:976:ILE:HD11	4:B:992:ILE:CD1	2.42	0.48
4:B:861:ASP:OD1	4:B:914:LYS:NZ	2.41	0.48
3:A:897:TYR:HB3	3:A:936:LEU:HD12	1.95	0.48
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.78	0.48
3:A:115:LEU:HB2	3:A:122:MET:HE2	1.95	0.48
10:J:1:MET:H1	10:J:57:ILE:H	1.61	0.48
10:J:59:LYS:O	10:J:62:ARG:CB	2.60	0.48
3:A:1441:PHE:CE1	7:F:89:GLU:HA	2.49	0.48
3:A:472:LEU:HD11	4:B:835:GLN:CD	2.33	0.48
3:A:809:THR:CB	3:A:810:PRO:CD	2.91	0.48
8:H:76:THR:HG23	8:H:77:ARG:NH2	2.27	0.48
3:A:1109:LYS:O	3:A:1111:MET:N	2.43	0.48
3:A:706:HIS:NE2	3:A:1139:GLU:OE2	2.45	0.48
4:B:34:ILE:CD1	4:B:743:ILE:CG2	2.91	0.48
4:B:179:CYS:O	4:B:181:LEU:N	2.47	0.48
4:B:300:HIS:CE1	4:B:376:PHE:CZ	3.01	0.48
6:E:59:SER:CB	6:E:81:GLU:HA	2.43	0.48
10:J:3:VAL:CG2	10:J:18:TRP:CG	2.96	0.48
7:F:109:VAL:HG21	7:F:124:GLU:HG3	1.94	0.48
3:A:241:VAL:HG13	3:A:266:LEU:CD1	2.43	0.48
4:B:195:CYS:SG	4:B:196:PRO:HD2	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:628:THR:CG2	4:B:628:THR:O	2.60	0.48
4:B:1138:MET:HA	4:B:1138:MET:HE3	1.96	0.48
3:A:492:PRO:CB	3:A:497:THR:HG22	2.43	0.48
4:B:1033:LYS:HE3	4:B:1087:PHE:O	2.13	0.48
3:A:68:GLN:NE2	3:A:70:CYS:CB	2.76	0.48
12:L:61:THR:HG22	12:L:62:LYS:H	1.78	0.48
3:A:898:ARG:CA	3:A:933:TYR:CE1	2.97	0.48
6:E:13:TRP:CD2	6:E:39:LEU:HD13	2.48	0.48
3:A:1362:TYR:CE1	3:A:1363:VAL:C	2.87	0.48
8:H:40:LEU:HD13	8:H:123:MET:CE	2.43	0.48
3:A:947:PHE:CD2	3:A:954:TRP:CZ2	3.01	0.48
3:A:484:GLY:O	3:A:485:ASP:C	2.51	0.48
5:C:227:THR:C	5:C:228:PHE:CD1	2.86	0.48
3:A:1041:ALA:O	3:A:1042:PHE:C	2.52	0.48
3:A:590:ARG:HG2	3:A:591:PHE:N	2.29	0.48
4:B:230:ALA:O	4:B:232:SER:N	2.44	0.48
8:H:138:GLU:O	8:H:139:ASN:O	2.31	0.48
11:K:29:ASN:ND2	11:K:78:THR:O	2.46	0.48
3:A:808:LEU:N	3:A:808:LEU:HD12	2.29	0.48
3:A:44:THR:O	3:A:45:GLN:HB2	2.13	0.48
3:A:1313:LEU:O	3:A:1314:SER:C	2.52	0.48
3:A:783:THR:HB	3:A:787:PHE:HD1	1.78	0.48
4:B:653:VAL:O	4:B:654:ARG:HG2	2.13	0.48
4:B:124:TYR:HB3	4:B:204:ILE:HD13	1.95	0.48
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.89	0.48
3:A:935:GLN:C	3:A:937:VAL:N	2.66	0.48
6:E:42:PHE:HZ	6:E:58:MET:HE1	1.78	0.48
3:A:381:THR:CG2	3:A:383:TYR:HB2	2.42	0.48
4:B:796:LEU:CB	4:B:799:PRO:HD3	2.32	0.48
4:B:190:TYR:CZ	10:J:62:ARG:HG2	2.48	0.48
3:A:43:GLU:O	3:A:46:THR:CB	2.60	0.48
4:B:170:LEU:HD13	4:B:457:LEU:HD13	1.96	0.48
4:B:864:LYS:N	4:B:872:GLU:OE1	2.40	0.48
7:F:99:LEU:C	7:F:99:LEU:CD1	2.82	0.48
4:B:652:LYS:O	4:B:653:VAL:O	2.31	0.48
12:L:60:ARG:HG3	12:L:61:THR:O	2.13	0.48
3:A:983:ILE:HD12	3:A:1028:THR:HG21	1.96	0.48
3:A:928:LEU:O	3:A:929:LEU:C	2.52	0.48
6:E:26:ARG:NH2	6:E:109:ILE:HD11	2.28	0.48
3:A:1064:VAL:O	3:A:1065:GLY:C	2.51	0.48
8:H:93:TYR:CD1	8:H:143:LEU:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:114:LEU:HG	3:A:114:LEU:H	1.48	0.48
3:A:549:MET:O	3:A:550:LEU:C	2.50	0.48
3:A:555:ASP:O	3:A:556:TRP:C	2.50	0.48
3:A:137:ALA:O	3:A:138:ILE:O	2.32	0.48
3:A:709:THR:C	3:A:711:ARG:N	2.66	0.48
4:B:234:ILE:HA	4:B:259:TYR:HA	1.95	0.48
4:B:118:ARG:NH2	4:B:194:GLU:OE1	2.47	0.48
3:A:396:PRO:C	3:A:397:ASN:CG	2.73	0.48
3:A:251:SER:OG	3:A:252:PHE:N	2.47	0.48
4:B:463:THR:HG21	4:B:465:ASN:ND2	2.28	0.48
6:E:182:ASP:HA	6:E:183:PRO:HD2	1.57	0.48
3:A:465:TYR:CD2	4:B:976:ILE:HD12	2.49	0.48
5:C:164:ALA:O	5:C:166:GLU:N	2.47	0.48
3:A:50:ILE:C	3:A:52:GLY:H	2.17	0.48
12:L:62:LYS:C	12:L:64:LEU:H	2.17	0.48
3:A:901:LEU:H	3:A:926:GLN:CG	2.27	0.48
3:A:122:MET:O	3:A:123:ARG:C	2.51	0.48
6:E:100:ILE:HD11	6:E:108:GLY:HA2	1.94	0.48
3:A:839:ARG:O	3:A:843:LYS:N	2.41	0.48
4:B:1081:LEU:HA	4:B:1081:LEU:HD23	1.75	0.48
7:F:98:ALA:O	7:F:117:PRO:HB2	2.13	0.48
4:B:1152:MET:O	4:B:1156:ASP:O	2.31	0.48
3:A:1120:LEU:O	3:A:1323:ASP:HB2	2.13	0.48
3:A:419:LYS:HB3	3:A:419:LYS:HZ2	1.79	0.48
3:A:768:GLN:HG3	3:A:816:HIS:HA	1.94	0.48
3:A:18:GLN:HE21	3:A:1418:LEU:HD13	1.78	0.48
3:A:1368:MET:O	3:A:1369:ALA:C	2.52	0.48
6:E:178:ILE:HD11	6:E:185:ALA:HB2	1.95	0.48
4:B:1006:ILE:HG22	4:B:1007:VAL:N	2.28	0.48
4:B:826:ALA:O	4:B:1011:ILE:HG23	2.14	0.48
4:B:1076:HIS:CE1	11:K:40:HIS:CD2	3.02	0.48
11:K:64:GLU:OE1	11:K:72:LYS:HE3	2.14	0.48
3:A:76:GLU:O	3:A:76:GLU:CG	2.61	0.48
3:A:910:PRO:HB3	3:A:916:GLY:CA	2.44	0.48
4:B:431:TYR:CG	4:B:447:ALA:HB1	2.49	0.48
3:A:567:LYS:HD3	8:H:95:TYR:HA	1.96	0.48
5:C:104:PHE:HB2	5:C:152:GLU:HG2	1.96	0.48
6:E:78:LEU:HG	6:E:79:TRP:N	2.28	0.48
7:F:75:PRO:O	7:F:77:ASP:N	2.47	0.48
4:B:780:VAL:HG12	4:B:817:LEU:CD2	2.44	0.48
3:A:399:HIS:O	3:A:401:GLY:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:49:VAL:HG12	5:C:155:LEU:HD22	1.96	0.48
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.95	0.48
7:F:95:GLY:O	7:F:98:ALA:HB3	2.13	0.48
6:E:36:GLU:O	6:E:38:PRO:CD	2.62	0.48
7:F:111:LEU:HD13	7:F:111:LEU:N	2.26	0.48
3:A:1254:ALA:O	3:A:1255:GLU:CB	2.60	0.48
3:A:493:GLN:NE2	3:A:493:GLN:CA	2.77	0.48
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.14	0.48
3:A:70:CYS:C	3:A:71:GLN:CG	2.82	0.48
2:T:1:DA:C2	2:T:2:DC:H5	2.32	0.48
7:F:155:LEU:N	7:F:155:LEU:CD2	2.53	0.48
4:B:129:PHE:CD2	4:B:166:PHE:CB	2.89	0.48
3:A:253:ASN:CG	3:A:254:GLU:H	1.99	0.48
3:A:947:PHE:CE2	3:A:954:TRP:CD2	3.02	0.48
3:A:144:THR:O	3:A:146:MET:HG3	2.14	0.48
3:A:24:PRO:CD	3:A:25:GLU:H	2.27	0.48
3:A:583:PRO:O	3:A:610:GLY:CA	2.54	0.48
5:C:194:GLU:HB2	5:C:200:GLU:OE2	2.14	0.48
3:A:660:ASN:C	3:A:660:ASN:ND2	2.61	0.48
3:A:1041:ALA:O	3:A:1044:TRP:CB	2.60	0.48
3:A:12:ARG:CB	4:B:1218:THR:CG2	2.92	0.48
3:A:1200:ALA:C	3:A:1202:MET:N	2.66	0.48
3:A:416:ARG:HG3	3:A:417:TYR:CD2	2.49	0.48
6:E:157:SER:OG	6:E:160:GLU:HB2	2.14	0.48
3:A:389:THR:OG1	3:A:426:LEU:HD12	2.14	0.48
3:A:89:PRO:O	3:A:90:VAL:HG22	2.14	0.47
3:A:351:THR:HG23	4:B:1103:ILE:HG23	1.94	0.47
4:B:1159:ARG:HH21	4:B:1193:GLN:NE2	2.12	0.47
3:A:914:GLU:C	3:A:916:GLY:N	2.66	0.47
6:E:13:TRP:O	6:E:16:PHE:HB3	2.13	0.47
4:B:63:ILE:HD12	4:B:95:ILE:HD12	1.96	0.47
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.44	0.47
11:K:94:ILE:HD12	11:K:94:ILE:N	2.27	0.47
3:A:209:ASN:HB3	3:A:210:ILE:H	1.43	0.47
10:J:57:ILE:CG2	10:J:58:GLU:N	2.77	0.47
5:C:135:GLN:C	5:C:136:ASP:O	2.48	0.47
7:F:125:LEU:HB2	7:F:130:ILE:CD1	2.41	0.47
3:A:322:VAL:HG11	3:A:323:LYS:HD3	1.85	0.47
5:C:33:LEU:HD12	5:C:37:MET:HE2	1.96	0.47
2:T:1:DA:C2	2:T:2:DC:C5	3.01	0.47
6:E:80:VAL:HA	6:E:109:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:128:LEU:HD12	4:B:128:LEU:HA	1.50	0.47
3:A:213:HIS:C	3:A:214:ILE:O	2.51	0.47
9:I:34:TYR:O	9:I:35:VAL:HG23	2.13	0.47
4:B:186:GLU:O	4:B:189:LEU:HB2	2.14	0.47
3:A:741:ASN:ND2	3:A:743:VAL:HB	2.29	0.47
3:A:591:PHE:HA	3:A:595:THR:HG21	1.96	0.47
3:A:33:ALA:HB3	3:A:83:HIS:N	2.29	0.47
3:A:919:ILE:CG2	3:A:922:ASP:HB2	2.44	0.47
4:B:1077:THR:CG2	4:B:1079:LYS:CB	2.92	0.47
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.39	0.47
8:H:135:LEU:CD2	8:H:136:LYS:HD2	2.43	0.47
4:B:464:GLY:HA2	4:B:479:VAL:O	2.14	0.47
4:B:976:ILE:HA	4:B:990:ILE:CG2	2.45	0.47
4:B:174:LEU:O	4:B:175:ARG:CB	2.62	0.47
3:A:900:ASP:HA	3:A:926:GLN:CD	2.34	0.47
4:B:254:LEU:HD22	4:B:361:LEU:CD1	2.27	0.47
4:B:364:ILE:O	4:B:365:THR:CB	2.62	0.47
3:A:1300:LYS:O	3:A:1302:PRO:HD3	2.14	0.47
3:A:115:LEU:HB2	3:A:122:MET:HE3	1.97	0.47
5:C:191:TYR:CD1	5:C:191:TYR:N	2.80	0.47
6:E:136:ASN:OD1	6:E:137:GLU:N	2.46	0.47
5:C:29:MET:HB2	11:K:45:LEU:CD1	2.44	0.47
11:K:32:VAL:HG23	11:K:74:ARG:HA	1.95	0.47
3:A:244:PRO:CB	3:A:245:PRO:CD	2.92	0.47
1:R:5:A:H2'	1:R:6:G:H8	1.79	0.47
4:B:995:ARG:CZ	4:B:995:ARG:HB2	2.44	0.47
3:A:512:VAL:HA	3:A:519:PRO:HA	1.96	0.47
4:B:803:LEU:N	4:B:822:ASN:HD21	2.13	0.47
3:A:827:THR:C	3:A:829:VAL:H	2.17	0.47
3:A:785:PRO:HB2	4:B:701:ILE:CD1	2.40	0.47
4:B:992:ILE:HD11	11:K:67:PHE:CE2	2.49	0.47
11:K:6:ARG:O	11:K:7:PHE:C	2.51	0.47
4:B:1168:LEU:HB3	4:B:1170:THR:OG1	2.15	0.47
4:B:1183:LYS:O	4:B:1185:CYS:N	2.47	0.47
4:B:1159:ARG:HE	4:B:1193:GLN:CG	2.26	0.47
3:A:900:ASP:CA	3:A:926:GLN:NE2	2.77	0.47
3:A:908:LEU:O	3:A:909:ASP:C	2.53	0.47
3:A:901:LEU:CB	3:A:926:GLN:HG2	2.42	0.47
3:A:902:LEU:CG	3:A:926:GLN:HG3	2.44	0.47
4:B:879:ARG:HB3	4:B:883:LEU:HD22	1.97	0.47
4:B:917:PRO:O	4:B:918:ILE:HD13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:127:ILE:HD11	6:E:132:ILE:HD12	1.95	0.47
3:A:1424:VAL:HG12	3:A:1425:SER:N	2.30	0.47
3:A:1394:THR:HG22	3:A:1395:GLY:H	1.76	0.47
3:A:247:ARG:O	3:A:247:ARG:HG2	2.15	0.47
3:A:982:THR:HB	3:A:985:ASP:H	1.80	0.47
4:B:121:ASN:O	4:B:206:ASN:HA	2.13	0.47
3:A:1152:ILE:CG1	3:A:1260:LEU:HD23	2.44	0.47
3:A:464:PRO:O	3:A:465:TYR:HB2	2.14	0.47
3:A:50:ILE:C	3:A:52:GLY:N	2.67	0.47
3:A:878:ILE:C	3:A:879:GLU:CG	2.82	0.47
4:B:294:ASP:N	9:I:12:ASN:ND2	2.63	0.47
3:A:135:PHE:O	3:A:135:PHE:CD2	2.67	0.47
4:B:816:GLU:OE1	4:B:816:GLU:N	2.48	0.47
4:B:1203:LEU:HD12	4:B:1203:LEU:O	2.14	0.47
6:E:113:GLN:CB	6:E:137:GLU:CD	2.83	0.47
6:E:188:LEU:HB2	6:E:190:LEU:HD21	1.95	0.47
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.14	0.47
3:A:874:ASP:C	3:A:874:ASP:OD1	2.53	0.47
8:H:77:ARG:HB2	8:H:77:ARG:NH1	2.28	0.47
4:B:660:LYS:HE2	4:B:679:TYR:CE2	2.50	0.47
6:E:153:HIS:N	6:E:153:HIS:HD1	2.13	0.47
3:A:51:GLY:HA2	3:A:56:PRO:HG3	1.97	0.47
3:A:935:GLN:HE21	3:A:1023:ARG:NH1	2.13	0.47
3:A:928:LEU:C	3:A:930:ASP:N	2.66	0.47
4:B:298:LEU:H	4:B:298:LEU:HD23	1.78	0.47
3:A:997:LEU:O	3:A:1053:PHE:CE2	2.67	0.47
3:A:1332:PHE:CE1	3:A:1348:LEU:HD13	2.49	0.47
3:A:803:SER:C	3:A:805:LEU:H	2.18	0.47
6:E:204:THR:HG22	6:E:205:SER:H	1.78	0.47
3:A:733:ALA:O	3:A:735:VAL:N	2.47	0.47
5:C:119:VAL:O	5:C:119:VAL:HG12	2.14	0.47
3:A:1279:ILE:O	3:A:1279:ILE:CG2	2.51	0.47
6:E:215:MET:HB3	6:E:215:MET:HE3	1.45	0.47
4:B:653:VAL:O	4:B:654:ARG:CG	2.63	0.47
3:A:352:VAL:HG12	3:A:353:ILE:H	1.76	0.47
4:B:830:TYR:HB3	4:B:831:SER:H	1.46	0.47
5:C:18:VAL:O	5:C:231:ASN:HA	2.15	0.47
3:A:306:ASN:N	3:A:306:ASN:HD22	2.12	0.47
4:B:174:LEU:O	4:B:175:ARG:HB2	2.14	0.47
4:B:202:TYR:N	4:B:202:TYR:CD2	2.82	0.47
4:B:204:ILE:N	4:B:204:ILE:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:925:LEU:O	3:A:926:GLN:C	2.49	0.47
3:A:930:ASP:O	3:A:931:GLU:C	2.52	0.47
4:B:446:LEU:O	4:B:447:ALA:CB	2.60	0.47
4:B:324:ILE:HG22	4:B:324:ILE:O	2.12	0.47
4:B:562:GLY:O	4:B:563:MET:C	2.53	0.47
4:B:291:ILE:CG2	4:B:297:ILE:CD1	2.90	0.47
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.29	0.47
8:H:47:PHE:O	8:H:47:PHE:CG	2.67	0.47
3:A:210:ILE:O	3:A:213:HIS:N	2.44	0.47
6:E:134:THR:C	6:E:135:PHE:HD1	2.17	0.47
5:C:57:VAL:CG1	10:J:60:PHE:CB	2.82	0.47
2:T:4:DA:C5	3:A:831:THR:HG21	2.50	0.47
1:R:9:G:O4'	4:B:1097:HIS:CE1	2.68	0.47
3:A:1445:ILE:H	3:A:1445:ILE:CD1	2.06	0.47
3:A:1436:ILE:HD13	4:B:1139:ILE:HG23	1.97	0.47
3:A:834:THR:HG21	3:A:1077:THR:HG23	1.96	0.47
3:A:100:LYS:NZ	3:A:100:LYS:CB	2.78	0.47
4:B:1029:CYS:O	4:B:1030:LEU:C	2.53	0.47
4:B:1065:GLN:O	4:B:1065:GLN:HG3	2.14	0.47
3:A:714:PHE:CD2	9:I:97:MET:HE1	2.49	0.47
7:F:97:ARG:HE	7:F:124:GLU:CD	2.18	0.47
4:B:794:ASN:ND2	4:B:794:ASN:N	2.54	0.47
3:A:765:VAL:HG21	3:A:800:VAL:CG1	2.40	0.47
8:H:129:TYR:C	8:H:131:ASN:H	2.17	0.47
4:B:45:SER:O	4:B:46:GLN:C	2.52	0.47
5:C:11:ARG:HE	5:C:21:ILE:CD1	2.26	0.47
1:R:5:A:C2	1:R:6:G:C5	3.03	0.47
4:B:384:ARG:HH22	4:B:621:GLU:HG3	1.79	0.47
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.45	0.47
4:B:760:ASP:C	4:B:762:ASN:H	2.16	0.47
3:A:570:PRO:O	3:A:572:TRP:CZ3	2.67	0.47
4:B:890:TYR:CE2	4:B:910:VAL:HG21	2.50	0.47
4:B:34:ILE:CD1	4:B:542:MET:HE1	2.43	0.47
4:B:648:HIS:CD2	4:B:648:HIS:C	2.88	0.47
4:B:474:SER:CA	4:B:476:ARG:CG	2.82	0.47
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.15	0.47
4:B:174:LEU:CD1	4:B:179:CYS:HG	2.27	0.47
6:E:55:ARG:C	6:E:57:MET:H	2.17	0.47
3:A:889:SER:HB3	3:A:891:ALA:HB3	1.97	0.47
4:B:128:LEU:CB	4:B:167:ILE:O	2.61	0.47
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:363:HIS:N	4:B:363:HIS:ND1	2.63	0.47
3:A:210:ILE:HB	3:A:211:PHE:H	1.16	0.47
7:F:135:ARG:O	7:F:135:ARG:CG	2.61	0.47
3:A:476:SER:O	3:A:478:TYR:N	2.48	0.47
5:C:44:LEU:HD22	5:C:129:ILE:HG13	1.97	0.47
11:K:24:ASP:CG	11:K:74:ARG:HH11	2.18	0.47
8:H:112:ILE:HG23	8:H:113:ALA:N	2.30	0.47
3:A:744:LYS:O	3:A:747:VAL:HB	2.15	0.47
3:A:809:THR:CG2	3:A:812:GLU:OE1	2.55	0.47
3:A:635:ARG:HH21	3:A:877:HIS:CA	2.24	0.47
3:A:1017:LEU:CB	6:E:205:SER:HA	2.44	0.47
3:A:518:LYS:CB	3:A:519:PRO:HD2	2.45	0.47
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.46	0.47
9:I:4:PHE:CD2	9:I:4:PHE:N	2.81	0.47
3:A:182:VAL:HG22	3:A:201:VAL:HG13	1.96	0.47
3:A:1192:LEU:CD2	3:A:1239:ARG:NH2	2.76	0.47
6:E:164:LEU:HD13	6:E:211:TYR:HE2	1.74	0.47
4:B:173:MET:N	4:B:203:PHE:CE2	2.82	0.47
4:B:951:GLN:CG	12:L:57:LEU:HD22	2.45	0.47
6:E:12:LEU:HB2	6:E:55:ARG:NH2	2.29	0.47
3:A:1364:ASN:OD1	3:A:1366:ARG:NH1	2.48	0.47
4:B:286:PHE:O	4:B:291:ILE:O	2.33	0.47
8:H:42:ILE:O	8:H:44:VAL:N	2.48	0.47
8:H:44:VAL:O	8:H:44:VAL:CG1	2.62	0.47
3:A:123:ARG:O	3:A:126:LEU:HG	2.14	0.47
6:E:131:THR:CG2	6:E:132:ILE:N	2.65	0.47
2:T:6:DC:C4	2:T:7:DC:C5	3.03	0.47
3:A:65:LEU:CD2	3:A:65:LEU:N	2.67	0.47
3:A:1400:CYS:C	3:A:1402:PHE:H	2.17	0.47
4:B:1165:ILE:CG2	4:B:1166:CYS:H	2.20	0.47
4:B:1106:ARG:NH2	4:B:1109:GLY:CA	2.78	0.47
3:A:1048:ASN:O	3:A:1051:ALA:HB3	2.15	0.47
3:A:1053:PHE:O	3:A:1054:LEU:C	2.53	0.47
3:A:690:VAL:O	3:A:691:LEU:C	2.52	0.47
4:B:530:GLY:O	4:B:533:CYS:HB2	2.15	0.47
10:J:5:VAL:O	10:J:6:ARG:O	2.32	0.47
4:B:1191:ILE:C	4:B:1192:TYR:CD1	2.89	0.47
4:B:393:LYS:NZ	9:I:89:GLN:HB3	2.30	0.47
4:B:216:GLU:OE1	4:B:500:THR:OG1	2.33	0.47
3:A:1151:GLU:O	3:A:1152:ILE:HD12	2.15	0.47
3:A:1189:SER:O	3:A:1241:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1271:ILE:HD13	3:A:1271:ILE:HA	1.62	0.47
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.47
4:B:640:VAL:HG23	4:B:739:THR:C	2.35	0.47
3:A:265:LYS:CE	3:A:323:LYS:CE	2.88	0.47
3:A:265:LYS:HZ1	3:A:322:VAL:CG1	2.28	0.47
4:B:332:ASP:C	4:B:334:ILE:H	2.16	0.47
4:B:236:HIS:O	4:B:237:VAL:CG2	2.64	0.47
3:A:505:CYS:SG	4:B:1141:HIS:CD2	3.06	0.47
4:B:778:MET:HB3	4:B:796:LEU:HD13	1.96	0.47
3:A:1407:GLU:O	3:A:1411:GLU:HG2	2.15	0.47
4:B:1072:MET:HE3	4:B:1085:ILE:CG2	2.39	0.47
3:A:825:ILE:O	3:A:826:ASP:C	2.48	0.47
8:H:89:LEU:HD13	8:H:91:ASP:OD1	2.14	0.47
8:H:11:GLN:HG3	8:H:53:ASP:O	2.14	0.47
5:C:253:LYS:O	5:C:256:ALA:HB3	2.15	0.47
4:B:662:MET:O	4:B:663:ALA:C	2.53	0.47
4:B:666:TYR:C	4:B:668:ASP:H	2.17	0.47
4:B:224:GLN:O	4:B:239:GLU:N	2.47	0.47
3:A:17:VAL:HB	3:A:1419:ASP:HB3	1.96	0.47
3:A:1227:ILE:CG2	3:A:1228:TRP:N	2.77	0.46
3:A:32:VAL:HA	3:A:57:ARG:HH11	1.79	0.46
4:B:956:THR:HA	4:B:963:PHE:HB2	1.96	0.46
3:A:898:ARG:HA	3:A:933:TYR:CE1	2.49	0.46
3:A:382:PRO:HD3	3:A:428:TYR:CD2	2.49	0.46
3:A:1298:TYR:O	3:A:1299:VAL:HG22	2.14	0.46
3:A:93:VAL:HG21	3:A:301:ALA:HA	1.97	0.46
3:A:795:GLU:H	3:A:795:GLU:HG2	1.12	0.46
4:B:827:ILE:O	4:B:828:ALA:CB	2.63	0.46
3:A:618:GLU:CD	3:A:620:LYS:H	2.17	0.46
3:A:1345:ARG:HG3	3:A:1372:VAL:HG12	1.97	0.46
5:C:181:ASP:OD2	5:C:186:LEU:HD13	2.14	0.46
9:I:68:LEU:HD23	9:I:68:LEU:HA	1.67	0.46
4:B:1034:VAL:O	4:B:1037:LEU:HB2	2.15	0.46
5:C:162:GLY:HA3	5:C:170:TRP:CD2	2.51	0.46
3:A:1274:ARG:HG3	3:A:1274:ARG:O	2.14	0.46
4:B:469:GLN:O	4:B:470:LYS:C	2.53	0.46
3:A:68:GLN:HE22	3:A:70:CYS:CB	2.27	0.46
4:B:101:MET:C	4:B:102:VAL:CG2	2.83	0.46
4:B:199:MET:N	4:B:199:MET:SD	2.78	0.46
4:B:202:TYR:CD1	4:B:209:GLU:HB3	2.51	0.46
4:B:911:ILE:HD12	4:B:941:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:928:LEU:HD23	3:A:928:LEU:HA	1.56	0.46
3:A:885:THR:HG22	3:A:940:ARG:HG3	1.97	0.46
11:K:94:ILE:CD1	11:K:94:ILE:N	2.78	0.46
3:A:1422:ARG:NH2	4:B:1220:ARG:HD2	2.28	0.46
4:B:486:TYR:HE2	4:B:778:MET:HG3	1.81	0.46
3:A:92:HIS:C	3:A:92:HIS:CD2	2.88	0.46
4:B:983:ARG:C	4:B:984:HIS:ND1	2.68	0.46
4:B:793:ALA:C	4:B:794:ASN:HD22	2.18	0.46
6:E:143:ASN:OD1	6:E:187:TYR:CE1	2.68	0.46
4:B:38:PHE:CE2	4:B:43:LEU:HD21	2.51	0.46
6:E:170:LEU:HD13	6:E:175:LEU:HD22	1.93	0.46
3:A:254:GLU:HB3	4:B:935:ARG:NH1	2.30	0.46
4:B:300:HIS:CE1	4:B:376:PHE:CE1	3.03	0.46
3:A:106:VAL:HG13	3:A:107:CYS:H	1.81	0.46
3:A:207:ILE:HG13	3:A:207:ILE:H	1.13	0.46
3:A:26:GLU:HA	3:A:29:ALA:CB	2.45	0.46
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	1.97	0.46
5:C:77:ILE:HA	5:C:129:ILE:CD1	2.45	0.46
3:A:1100:ARG:O	3:A:1103:GLU:N	2.48	0.46
6:E:3:GLN:HG3	6:E:4:GLU:N	2.30	0.46
3:A:1009:ASN:ND2	3:A:1012:ARG:HH12	2.12	0.46
3:A:69:THR:HB	4:B:1174:LYS:HE3	1.97	0.46
3:A:1271:ILE:HG22	3:A:1271:ILE:O	2.14	0.46
3:A:779:PHE:CE1	3:A:784:LEU:HA	2.50	0.46
3:A:353:ILE:HD13	3:A:487:MET:HE2	1.95	0.46
4:B:1076:HIS:CG	11:K:40:HIS:CD2	3.02	0.46
3:A:30:ILE:HA	4:B:1183:LYS:NZ	2.30	0.46
6:E:53:PRO:HB2	6:E:55:ARG:NH1	2.31	0.46
4:B:417:PHE:O	4:B:418:LYS:C	2.50	0.46
4:B:282:ILE:HD12	4:B:286:PHE:HD1	1.81	0.46
11:K:49:GLU:HA	11:K:49:GLU:OE1	2.14	0.46
11:K:46:ILE:O	11:K:50:LEU:HB2	2.15	0.46
6:E:100:ILE:HD13	6:E:108:GLY:HA3	1.97	0.46
4:B:486:TYR:CE2	4:B:778:MET:HG3	2.50	0.46
5:C:58:LEU:N	5:C:58:LEU:CD2	2.72	0.46
12:L:48:CYS:HB3	12:L:51:CYS:C	2.35	0.46
5:C:258:ILE:HD12	11:K:42:LEU:HD21	1.95	0.46
4:B:1056:SER:O	4:B:1066:SER:HB2	2.16	0.46
3:A:802:ASN:OD1	4:B:729:ILE:N	2.48	0.46
4:B:40:GLU:OE2	4:B:681:TRP:HB3	2.15	0.46
11:K:28:PRO:C	11:K:30:ALA:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:HG22	9:I:2:THR:O	2.16	0.46
3:A:361:LEU:HA	3:A:471:ASN:ND2	2.30	0.46
12:L:27:LEU:O	12:L:28:LYS:HG2	2.15	0.46
4:B:653:VAL:HG12	4:B:654:ARG:N	2.31	0.46
3:A:269:ILE:C	3:A:271:LYS:N	2.67	0.46
3:A:894:GLU:HG3	3:A:898:ARG:HB2	1.96	0.46
4:B:589:VAL:HG12	4:B:590:HIS:H	1.79	0.46
8:H:32:THR:CG2	8:H:33:GLN:CG	2.88	0.46
3:A:1004:ASN:ND2	6:E:167:ARG:CD	2.52	0.46
5:C:43:THR:CG2	5:C:44:LEU:H	2.28	0.46
7:F:120:ILE:CG2	7:F:121:ALA:N	2.77	0.46
3:A:680:THR:O	3:A:681:GLU:C	2.54	0.46
3:A:8:SER:OG	4:B:1180:PHE:CE1	2.67	0.46
3:A:257:ARG:CG	3:A:258:GLY:H	2.29	0.46
3:A:90:VAL:CG1	3:A:297:GLN:CA	2.78	0.46
3:A:782:ARG:NH1	3:A:785:PRO:HA	2.31	0.46
3:A:783:THR:HB	3:A:787:PHE:CD1	2.50	0.46
3:A:491:VAL:HA	3:A:492:PRO:HD2	1.62	0.46
3:A:899:VAL:HG11	3:A:908:LEU:HD21	1.98	0.46
3:A:908:LEU:C	3:A:909:ASP:O	2.53	0.46
4:B:63:ILE:HG12	4:B:421:PHE:CZ	2.51	0.46
3:A:385:ILE:O	3:A:386:ASP:C	2.53	0.46
1:R:9:G:P	4:B:776:GLN:HE22	2.38	0.46
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.64	0.46
8:H:126:GLU:O	8:H:130:ARG:NH1	2.47	0.46
3:A:714:PHE:CB	9:I:97:MET:HE3	2.45	0.46
4:B:984:HIS:CD2	4:B:1025:HIS:N	2.84	0.46
3:A:809:THR:H	3:A:812:GLU:HB2	1.80	0.46
3:A:182:VAL:CG2	3:A:201:VAL:HG13	2.45	0.46
3:A:1168:GLU:C	3:A:1170:ILE:N	2.68	0.46
3:A:57:ARG:O	3:A:68:GLN:CG	2.64	0.46
3:A:30:ILE:CG1	4:B:1170:THR:HG23	2.46	0.46
3:A:1015:VAL:O	3:A:1018:PHE:N	2.49	0.46
3:A:910:PRO:HA	3:A:916:GLY:HA2	1.96	0.46
3:A:553:VAL:HG22	3:A:652:VAL:HG22	1.97	0.46
3:A:1261:LYS:C	3:A:1263:ILE:H	2.18	0.46
3:A:1441:PHE:HZ	7:F:88:TYR:C	2.19	0.46
3:A:92:HIS:HB2	3:A:236:LEU:HD12	1.95	0.46
3:A:1392:SER:C	3:A:1393:ASN:ND2	2.65	0.46
3:A:590:ARG:NH2	3:A:620:LYS:C	2.68	0.46
4:B:195:CYS:HB2	4:B:784:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:760:ASP:C	4:B:762:ASN:N	2.69	0.46
4:B:854:LEU:HD23	4:B:854:LEU:HA	1.47	0.46
3:A:1152:ILE:HG13	3:A:1260:LEU:HD23	1.97	0.46
3:A:1171:GLN:CB	3:A:1172:LEU:HD23	2.32	0.46
6:E:171:LYS:O	6:E:173:SER:N	2.49	0.46
3:A:777:PHE:CE2	3:A:782:ARG:CA	2.99	0.46
11:K:61:TYR:HA	11:K:72:LYS:O	2.16	0.46
3:A:878:ILE:CG2	3:A:879:GLU:N	2.79	0.46
3:A:215:SER:OG	3:A:216:VAL:N	2.49	0.46
9:I:15:TYR:HD1	9:I:15:TYR:N	2.11	0.46
3:A:336:ILE:HG22	3:A:337:ARG:N	2.30	0.46
3:A:836:TYR:O	3:A:837:ILE:C	2.54	0.46
4:B:1084:GLN:HE22	5:C:191:TYR:CA	2.21	0.46
3:A:666:ILE:HA	4:B:1026:LEU:HD13	1.97	0.46
4:B:737:THR:O	4:B:738:PHE:O	2.33	0.46
3:A:590:ARG:NH2	3:A:621:THR:HA	2.30	0.46
5:C:124:LEU:O	5:C:125:MET:HB2	2.16	0.46
3:A:816:HIS:ND1	3:A:816:HIS:O	2.49	0.46
3:A:823:GLY:O	3:A:824:LEU:C	2.54	0.46
6:E:144:ILE:CG1	6:E:145:THR:N	2.79	0.46
3:A:1211:GLN:O	3:A:1215:ARG:HB2	2.16	0.46
4:B:472:ALA:C	4:B:474:SER:N	2.69	0.46
10:J:8:PHE:H	10:J:49:MET:HE1	1.80	0.46
4:B:113:TYR:O	4:B:114:PRO:C	2.50	0.46
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.98	0.46
3:A:476:SER:HB2	3:A:477:PRO:CD	2.46	0.46
4:B:737:THR:HG21	9:I:66:PRO:C	2.33	0.46
8:H:49:VAL:HG13	8:H:50:ALA:N	2.30	0.46
3:A:414:ASP:O	3:A:416:ARG:N	2.49	0.46
4:B:620:ARG:H	4:B:620:ARG:HG3	1.48	0.46
9:I:92:ARG:HG2	9:I:94:ASP:OD2	2.15	0.46
4:B:1213:THR:HA	4:B:1214:PRO:HD3	1.68	0.46
3:A:1147:THR:HG21	3:A:1268:LEU:HD21	1.98	0.46
3:A:1163:ILE:HA	3:A:1164:PRO:HD2	1.56	0.46
4:B:541:LEU:CD1	4:B:747:MET:HE1	2.43	0.46
5:C:167:HIS:CD2	5:C:168:ALA:N	2.84	0.46
4:B:1161:HIS:CD2	4:B:1173:ALA:HB2	2.51	0.46
6:E:12:LEU:HD21	6:E:58:MET:HE1	1.98	0.46
3:A:841:LEU:HA	3:A:841:LEU:HD23	1.66	0.46
4:B:421:PHE:HA	4:B:453:ILE:HD11	1.97	0.46
4:B:59:LEU:HG	4:B:95:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:361:LEU:CD1	4:B:361:LEU:N	2.78	0.46
8:H:59:ILE:O	8:H:60:ALA:CB	2.61	0.46
4:B:780:VAL:HG12	4:B:817:LEU:HD23	1.96	0.46
3:A:1441:PHE:CZ	7:F:89:GLU:CA	2.92	0.46
9:I:98:VAL:CG1	9:I:99:LEU:N	2.79	0.46
4:B:856:PHE:HA	4:B:968:VAL:O	2.16	0.46
8:H:50:ALA:O	8:H:53:ASP:HB2	2.16	0.46
3:A:726:ARG:CG	3:A:727:ASP:N	2.79	0.46
3:A:181:LEU:HB2	3:A:202:LEU:HB2	1.98	0.46
10:J:23:ASN:O	10:J:27:GLU:HB2	2.15	0.46
3:A:1305:VAL:HG12	3:A:1306:LEU:N	2.30	0.45
3:A:1340:GLY:CA	6:E:183:PRO:HG2	2.46	0.45
3:A:815:PHE:C	3:A:817:ALA:N	2.66	0.45
5:C:41:ILE:HA	5:C:42:PRO:HD3	1.49	0.45
6:E:42:PHE:CZ	6:E:58:MET:HE1	2.51	0.45
3:A:892:ALA:HB2	3:A:895:LYS:HD2	1.98	0.45
1:R:9:G:C5'	4:B:1097:HIS:NE2	2.80	0.45
1:R:8:G:N2	2:T:8:DT:N3	2.64	0.45
7:F:81:THR:CG2	7:F:136:ARG:CD	2.84	0.45
3:A:334:GLY:O	3:A:335:ARG:C	2.55	0.45
3:A:335:ARG:NH1	4:B:1202:LEU:HD12	2.31	0.45
4:B:1064:TYR:N	4:B:1064:TYR:HD1	2.14	0.45
3:A:1349:TYR:CD2	3:A:1350:LYS:N	2.83	0.45
8:H:5:LEU:HB3	8:H:133:ASN:O	2.16	0.45
4:B:435:THR:C	4:B:437:GLU:N	2.70	0.45
4:B:877:PRO:O	4:B:878:GLN:HG2	2.16	0.45
3:A:683:ILE:HD13	3:A:725:ALA:HB1	1.99	0.45
6:E:82:PHE:N	6:E:82:PHE:CD1	2.84	0.45
3:A:1005:GLU:O	3:A:1005:GLU:HG3	2.16	0.45
3:A:785:PRO:CG	4:B:703:ILE:HD12	2.45	0.45
4:B:744:HIS:HA	4:B:745:PRO:HD3	1.50	0.45
3:A:320:ARG:CB	3:A:321:PRO:CB	2.74	0.45
4:B:999:MET:HG2	4:B:1008:PRO:HD2	1.97	0.45
4:B:848:ARG:HH22	4:B:996:ARG:NH1	2.14	0.45
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	2.15	0.45
12:L:30:ILE:HD11	12:L:59:ALA:HA	1.98	0.45
12:L:45:ALA:O	12:L:46:VAL:HG22	2.16	0.45
4:B:550:ASP:HA	4:B:551:PRO:HD3	1.61	0.45
4:B:331:LEU:O	4:B:332:ASP:O	2.34	0.45
4:B:780:VAL:HA	4:B:795:ILE:HG23	1.98	0.45
3:A:1042:PHE:C	3:A:1042:PHE:CD2	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1101:LEU:HD13	3:A:1355:VAL:HG11	1.99	0.45
3:A:151:ASP:C	3:A:152:VAL:CG2	2.85	0.45
3:A:1032:LEU:O	3:A:1036:ARG:HG2	2.17	0.45
4:B:610:ASN:O	4:B:613:VAL:HG23	2.15	0.45
4:B:953:LEU:HD22	4:B:965:LYS:HB2	1.97	0.45
4:B:411:PRO:C	4:B:414:ALA:HB3	2.37	0.45
3:A:376:TYR:CD2	3:A:376:TYR:O	2.69	0.45
3:A:867:ILE:HG22	3:A:872:GLY:N	2.32	0.45
6:E:32:GLN:O	6:E:32:GLN:HG3	2.16	0.45
6:E:173:SER:C	6:E:175:LEU:N	2.69	0.45
3:A:298:PHE:C	3:A:298:PHE:CD2	2.89	0.45
4:B:25:ILE:HD12	4:B:651:LEU:CD1	2.34	0.45
3:A:353:ILE:CG2	3:A:487:MET:HB2	2.46	0.45
5:C:133:ILE:C	5:C:134:ILE:HD13	2.32	0.45
3:A:41:MET:HE2	3:A:61:ILE:CD1	2.46	0.45
3:A:1364:ASN:ND2	3:A:1366:ARG:NH1	2.55	0.45
8:H:58:THR:HG22	8:H:59:ILE:H	1.80	0.45
3:A:406:ILE:CD1	3:A:406:ILE:N	2.58	0.45
6:E:96:PHE:O	6:E:97:VAL:C	2.53	0.45
5:C:62:PHE:CD2	5:C:62:PHE:C	2.90	0.45
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.17	0.45
5:C:118:LEU:HB2	5:C:132:PRO:HG3	1.97	0.45
3:A:139:TRP:O	3:A:140:THR:C	2.55	0.45
4:B:317:CYS:O	4:B:318:VAL:C	2.54	0.45
5:C:120:ILE:HG21	5:C:124:LEU:HD21	1.98	0.45
4:B:501:PRO:O	4:B:502:ILE:CB	2.64	0.45
3:A:682:THR:HA	3:A:685:GLU:OE2	2.16	0.45
9:I:20:LYS:HB2	9:I:21:GLU:H	1.37	0.45
3:A:1159:ARG:HG2	3:A:1159:ARG:H	1.56	0.45
3:A:1189:SER:OG	3:A:1190:PRO:CD	2.62	0.45
5:C:163:ILE:O	5:C:164:ALA:C	2.55	0.45
3:A:903:ASN:O	3:A:904:THR:C	2.53	0.45
4:B:350:GLN:O	4:B:353:LYS:N	2.50	0.45
4:B:562:GLY:HA3	4:B:590:HIS:HE1	1.78	0.45
4:B:589:VAL:CG1	4:B:590:HIS:H	2.28	0.45
8:H:40:LEU:CD1	8:H:123:MET:HE3	2.46	0.45
10:J:57:ILE:C	10:J:59:LYS:N	2.67	0.45
8:H:106:GLU:HG3	8:H:112:ILE:HD11	1.98	0.45
4:B:1072:MET:CE	4:B:1085:ILE:CG2	2.92	0.45
3:A:356:ASP:HA	3:A:357:PRO:HD2	1.79	0.45
3:A:536:LEU:O	3:A:537:ARG:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:14:DT:H2"	3:A:317:LYS:HG2	1.97	0.45
3:A:518:LYS:HG3	3:A:519:PRO:HD2	1.99	0.45
9:I:83:ASN:HA	9:I:102:VAL:O	2.16	0.45
9:I:85:PHE:O	9:I:86:PHE:CB	2.65	0.45
3:A:792:TYR:CD1	3:A:792:TYR:N	2.85	0.45
3:A:1205:LYS:O	3:A:1207:LEU:N	2.50	0.45
4:B:647:GLY:O	4:B:648:HIS:CD2	2.69	0.45
4:B:1099:VAL:O	4:B:1103:ILE:HD11	2.16	0.45
5:C:142:VAL:CG1	5:C:143:LEU:N	2.80	0.45
4:B:848:ARG:NH1	10:J:8:PHE:O	2.49	0.45
3:A:35:ILE:O	3:A:270:LEU:CD1	2.65	0.45
4:B:293:PRO:O	4:B:294:ASP:C	2.55	0.45
5:C:27:LEU:O	5:C:29:MET:N	2.49	0.45
3:A:966:ASN:O	3:A:1044:TRP:CH2	2.70	0.45
3:A:618:GLU:CD	3:A:618:GLU:C	2.75	0.45
3:A:344:ARG:C	3:A:345:VAL:HG13	2.36	0.45
4:B:732:SER:HB3	4:B:734:HIS:CD2	2.51	0.45
3:A:128:ILE:O	3:A:128:ILE:CG2	2.65	0.45
3:A:1151:GLU:C	3:A:1152:ILE:HD12	2.37	0.45
3:A:1210:GLY:O	3:A:1214:GLU:N	2.44	0.45
3:A:91:PHE:CA	3:A:297:GLN:HE22	2.29	0.45
4:B:27:ALA:O	4:B:30:SER:OG	2.34	0.45
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.57	0.45
4:B:476:ARG:O	4:B:477:ALA:C	2.52	0.45
4:B:1173:ALA:C	4:B:1175:LEU:N	2.70	0.45
5:C:3:GLU:CG	5:C:4:GLU:N	2.55	0.45
4:B:428:ILE:HG13	4:B:448:ILE:HD13	1.97	0.45
4:B:569:TYR:CE1	4:B:589:VAL:HG21	2.52	0.45
3:A:1256:GLU:C	3:A:1258:HIS:N	2.63	0.45
7:F:83:PRO:CD	7:F:84:TYR:N	2.79	0.45
3:A:332:LYS:C	3:A:334:GLY:N	2.69	0.45
6:E:136:ASN:O	6:E:137:GLU:C	2.54	0.45
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.19	0.45
9:I:99:LEU:HD23	9:I:99:LEU:HA	1.72	0.45
3:A:535:THR:HG22	3:A:616:VAL:HA	1.96	0.45
11:K:27:ALA:CB	11:K:28:PRO:CD	2.83	0.45
4:B:802:PRO:HB3	4:B:1091:TYR:CG	2.51	0.45
9:I:4:PHE:CE1	9:I:13:MET:CE	3.00	0.45
4:B:487:THR:O	4:B:488:TYR:C	2.55	0.45
4:B:523:CYS:SG	4:B:524:PRO:HD2	2.56	0.45
3:A:49:LYS:HZ2	3:A:60:SER:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:315:LEU:CD1	3:A:319:GLY:HA2	2.27	0.45
4:B:860:MET:CG	4:B:861:ASP:N	2.72	0.45
4:B:899:ILE:HG22	4:B:900:ALA:N	2.32	0.45
3:A:642:CYS:O	3:A:645:LEU:N	2.49	0.45
4:B:274:PRO:O	4:B:275:TYR:C	2.53	0.45
4:B:357:GLN:O	4:B:366:GLN:HA	2.17	0.45
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.82	0.45
3:A:135:PHE:C	3:A:135:PHE:CD2	2.89	0.45
10:J:50:ILE:C	10:J:52:THR:N	2.67	0.45
4:B:1096:ARG:HH11	4:B:1096:ARG:CB	2.30	0.45
3:A:341:MET:HE1	3:A:843:LYS:HZ3	1.80	0.45
4:B:1030:LEU:HD11	4:B:1067:ARG:C	2.37	0.45
4:B:782:LEU:HB3	4:B:784:ASN:OD1	2.17	0.45
4:B:1148:LYS:O	4:B:1152:MET:N	2.50	0.45
3:A:1198:ASP:O	3:A:1202:MET:HG2	2.17	0.45
3:A:870:GLU:C	6:E:204:THR:HG21	2.37	0.45
6:E:82:PHE:N	6:E:82:PHE:HD1	2.15	0.45
3:A:1127:ASP:HB3	3:A:1130:GLN:H	1.82	0.45
3:A:1166:ASP:O	3:A:1170:ILE:CG1	2.62	0.45
3:A:1215:ARG:HA	3:A:1215:ARG:HD2	1.49	0.45
6:E:195:VAL:HG22	6:E:213:ILE:CD1	2.47	0.45
4:B:521:LEU:CD2	4:B:635:ARG:CG	2.84	0.45
4:B:641:GLU:C	4:B:643:ASP:N	2.69	0.45
5:C:41:ILE:HD11	5:C:172:PRO:CG	2.47	0.45
4:B:1051:THR:CG2	4:B:1053:GLU:HB2	2.46	0.45
4:B:282:ILE:CG1	4:B:283:VAL:N	2.79	0.45
4:B:292:ILE:HD11	4:B:327:ARG:H	1.82	0.45
5:C:66:ARG:HH21	10:J:4:PRO:HA	1.82	0.45
10:J:25:LEU:HB2	10:J:26:GLN:H	1.66	0.45
7:F:81:THR:CG2	7:F:136:ARG:NH1	2.64	0.45
6:E:63:ASN:HB3	6:E:64:PRO:CD	2.46	0.45
3:A:738:LYS:HZ1	5:C:194:GLU:HA	1.79	0.45
3:A:694:THR:HA	3:A:714:PHE:CE1	2.51	0.45
3:A:800:VAL:HA	3:A:812:GLU:HG2	1.98	0.45
4:B:270:LYS:HE3	4:B:281:PRO:HG3	1.98	0.45
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.51	0.45
3:A:18:GLN:HE22	3:A:1418:LEU:HB2	1.81	0.45
4:B:574:SER:HB3	4:B:591:ARG:HH21	1.82	0.45
3:A:884:ASP:N	3:A:884:ASP:OD2	2.49	0.45
4:B:105:SER:O	4:B:106:ASP:C	2.54	0.45
3:A:1213:GLY:HA2	3:A:1216:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1313:LEU:O	3:A:1316:VAL:N	2.39	0.45
4:B:744:HIS:CG	4:B:745:PRO:CD	3.00	0.45
3:A:351:THR:O	3:A:486:GLU:HG2	2.16	0.45
4:B:821:GLN:OE1	4:B:851:PHE:N	2.45	0.45
4:B:847:ASP:C	4:B:849:GLY:N	2.71	0.45
3:A:886:ILE:CD1	3:A:944:ARG:HG3	2.47	0.45
4:B:226:PHE:O	4:B:236:HIS:HA	2.16	0.45
4:B:796:LEU:O	4:B:799:PRO:HD2	2.17	0.45
4:B:797:TYR:CE2	5:C:62:PHE:HA	2.52	0.45
4:B:1082:MET:HA	5:C:189:THR:HA	1.98	0.45
5:C:101:LEU:HB3	5:C:155:LEU:HB2	1.98	0.45
4:B:1115:THR:O	4:B:1116:ARG:CB	2.65	0.45
5:C:183:TRP:O	5:C:185:LYS:N	2.49	0.45
3:A:202:LEU:N	3:A:202:LEU:HD12	2.32	0.45
3:A:764:CYS:HB2	3:A:801:GLU:O	2.17	0.45
3:A:1382:THR:HG22	3:A:1388:GLY:CA	2.46	0.45
3:A:1237:ILE:CG2	3:A:1238:ILE:H	2.25	0.45
3:A:1338:VAL:O	6:E:183:PRO:CB	2.64	0.45
3:A:786:HIS:N	3:A:786:HIS:CD2	2.85	0.45
4:B:712:PRO:O	4:B:712:PRO:HD2	2.17	0.45
3:A:67:CYS:C	3:A:68:GLN:NE2	2.70	0.45
3:A:901:LEU:CA	3:A:907:THR:HG23	2.32	0.45
3:A:901:LEU:H	3:A:926:GLN:CD	2.21	0.45
4:B:62:ILE:CG2	4:B:418:LYS:HG2	2.39	0.45
8:H:84:ALA:CB	8:H:87:ARG:CB	2.90	0.45
6:E:23:VAL:CG1	6:E:28:TYR:HB2	2.47	0.45
9:I:65:ASP:HA	9:I:66:PRO:HD3	1.71	0.45
3:A:811:GLN:O	3:A:812:GLU:C	2.54	0.45
3:A:1319:VAL:HG12	3:A:1320:PRO:N	2.32	0.45
4:B:38:PHE:CE2	4:B:43:LEU:CD2	3.01	0.45
3:A:853:ASP:C	3:A:855:THR:H	2.19	0.44
10:J:8:PHE:N	10:J:49:MET:CE	2.80	0.44
3:A:273:ASN:HA	3:A:296:LEU:HD13	1.98	0.44
3:A:32:VAL:HG12	3:A:57:ARG:HD2	1.99	0.44
4:B:859:TYR:OH	4:B:941:LEU:CD2	2.61	0.44
4:B:428:ILE:O	4:B:430:ARG:N	2.50	0.44
4:B:449:ASN:CG	4:B:449:ASN:O	2.56	0.44
4:B:451:LYS:O	4:B:453:ILE:N	2.50	0.44
4:B:360:PHE:CE1	4:B:361:LEU:HD13	2.52	0.44
3:A:1290:LYS:HA	3:A:1299:VAL:O	2.17	0.44
6:E:100:ILE:O	6:E:101:GLN:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:78:LEU:HD23	6:E:78:LEU:C	2.37	0.44
11:K:43:GLY:CA	11:K:71:PHE:CZ	3.01	0.44
3:A:655:PHE:O	3:A:656:TRP:C	2.55	0.44
4:B:170:LEU:CD1	4:B:457:LEU:HD13	2.46	0.44
4:B:573:GLN:HG2	4:B:573:GLN:O	2.16	0.44
3:A:1139:GLU:O	3:A:1140:HIS:C	2.56	0.44
3:A:855:THR:CG2	3:A:857:ARG:CG	2.95	0.44
4:B:461:LEU:HD12	4:B:461:LEU:HA	1.68	0.44
4:B:992:ILE:HG13	4:B:993:THR:H	1.81	0.44
4:B:894:ASP:OD2	12:L:58:LYS:NZ	2.48	0.44
6:E:53:PRO:CB	6:E:55:ARG:NH1	2.81	0.44
4:B:420:LEU:CD2	4:B:468:GLU:OE2	2.65	0.44
4:B:356:LEU:HA	4:B:360:PHE:HB3	1.98	0.44
4:B:191:LYS:C	4:B:193:LYS:H	2.21	0.44
10:J:1:MET:N	10:J:56:LEU:HB2	2.32	0.44
4:B:234:ILE:N	4:B:234:ILE:HD13	2.17	0.44
3:A:1384:VAL:O	3:A:1389:PHE:CE2	2.70	0.44
5:C:80:LEU:HD12	5:C:95:CYS:HA	1.99	0.44
4:B:213:ILE:O	4:B:215:GLN:HG2	2.17	0.44
3:A:1313:LEU:HD23	3:A:1338:VAL:HG21	1.98	0.44
4:B:653:VAL:C	4:B:654:ARG:HG2	2.38	0.44
4:B:542:MET:HG3	4:B:747:MET:HE3	2.00	0.44
3:A:265:LYS:HZ1	3:A:322:VAL:CB	2.30	0.44
4:B:412:LEU:HB3	4:B:466:TRP:CE2	2.52	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.65	0.44
4:B:957:ASN:C	4:B:957:ASN:ND2	2.71	0.44
3:A:167:CYS:O	3:A:169:ASN:ND2	2.51	0.44
3:A:379:VAL:O	3:A:384:ASN:ND2	2.48	0.44
11:K:92:ASN:O	11:K:96:ASN:ND2	2.51	0.44
4:B:801:LYS:O	10:J:52:THR:HG21	2.17	0.44
5:C:144:ILE:HA	5:C:144:ILE:HD13	1.82	0.44
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.99	0.44
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.98	0.44
3:A:551:TYR:CE2	11:K:74:ARG:HB2	2.52	0.44
4:B:1079:LYS:HE3	5:C:188:HIS:ND1	2.32	0.44
3:A:961:ARG:O	3:A:965:GLN:HG3	2.16	0.44
3:A:808:LEU:HD21	3:A:816:HIS:HD2	1.82	0.44
4:B:383:ASN:ND2	4:B:384:ARG:HH11	2.11	0.44
9:I:101:PHE:O	9:I:109:ILE:HA	2.17	0.44
3:A:1387:HIS:O	3:A:1388:GLY:O	2.36	0.44
4:B:745:PRO:HB2	4:B:1047:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:636:PRO:HB2	4:B:637:LEU:H	1.09	0.44
4:B:708:GLU:CG	4:B:709:ASP:N	2.73	0.44
3:A:493:GLN:HE21	3:A:493:GLN:CA	2.30	0.44
3:A:943:LEU:C	3:A:945:GLU:N	2.69	0.44
3:A:209:ASN:O	3:A:212:LYS:HB2	2.18	0.44
4:B:1135:ARG:O	4:B:1136:ASP:C	2.53	0.44
5:C:44:LEU:HD12	5:C:44:LEU:HA	1.73	0.44
4:B:1084:GLN:NE2	5:C:192:TRP:H	2.14	0.44
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.57	0.44
4:B:981:ALA:O	4:B:982:SER:O	2.36	0.44
7:F:121:ALA:HA	7:F:124:GLU:HB2	2.00	0.44
5:C:69:LEU:N	5:C:69:LEU:HD13	2.33	0.44
4:B:42:GLY:C	4:B:43:LEU:HD23	2.38	0.44
3:A:1153:TYR:CD2	3:A:1163:ILE:HD11	2.52	0.44
4:B:1002:THR:HG22	4:B:1006:ILE:O	2.17	0.44
4:B:1033:LYS:HA	4:B:1089:PRO:CG	2.47	0.44
5:C:167:HIS:HD2	5:C:168:ALA:H	1.64	0.44
4:B:996:ARG:CZ	5:C:38:ILE:HD12	2.47	0.44
3:A:273:ASN:CA	3:A:296:LEU:CD1	2.95	0.44
3:A:7:SER:CB	4:B:1193:GLN:HE22	2.12	0.44
3:A:894:GLU:HG3	3:A:898:ARG:CB	2.48	0.44
4:B:1031:LEU:HD13	4:B:1055:ILE:CD1	2.47	0.44
8:H:95:TYR:CE2	8:H:97:MET:SD	3.10	0.44
8:H:98:TYR:N	8:H:118:PHE:HD2	2.16	0.44
3:A:954:TRP:N	3:A:954:TRP:CD1	2.84	0.44
3:A:24:PRO:CG	3:A:237:THR:HG21	2.47	0.44
6:E:98:ILE:C	6:E:100:ILE:N	2.71	0.44
4:B:1202:LEU:HA	4:B:1202:LEU:HD22	1.45	0.44
3:A:1354:ASN:O	3:A:1355:VAL:C	2.55	0.44
4:B:759:PRO:HB2	4:B:767:ASN:ND2	2.32	0.44
8:H:129:TYR:C	8:H:131:ASN:N	2.71	0.44
4:B:766:ARG:HD3	4:B:766:ARG:HA	1.83	0.44
4:B:31:TRP:CD2	4:B:807:ARG:HD2	2.53	0.44
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.18	0.44
3:A:1228:TRP:CA	3:A:1237:ILE:O	2.63	0.44
3:A:901:LEU:HD12	3:A:926:GLN:HG2	1.97	0.44
6:E:12:LEU:HD12	6:E:12:LEU:O	2.18	0.44
4:B:361:LEU:N	4:B:362:PRO:HD3	2.31	0.44
3:A:567:LYS:CD	8:H:96:VAL:H	2.30	0.44
3:A:946:VAL:HG12	3:A:947:PHE:CD1	2.53	0.44
4:B:189:LEU:O	4:B:192:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:197:PHE:CD1	4:B:817:LEU:HD11	2.53	0.44
3:A:834:THR:HG21	3:A:1077:THR:CG2	2.47	0.44
3:A:612:ILE:C	3:A:613:ILE:HD13	2.38	0.44
3:A:658:LEU:HD12	3:A:658:LEU:O	2.18	0.44
7:F:97:ARG:CD	7:F:100:GLN:OE1	2.66	0.44
3:A:504:LEU:CD1	7:F:91:ALA:HB1	2.47	0.44
4:B:1197:PRO:O	4:B:1200:ALA:CB	2.64	0.44
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.38	0.44
4:B:1077:THR:HG23	4:B:1079:LYS:H	1.77	0.44
8:H:7:ASP:OD1	8:H:8:ASP:N	2.50	0.44
4:B:724:ASP:O	4:B:724:ASP:OD1	2.35	0.44
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.82	0.44
3:A:537:ARG:CG	3:A:537:ARG:NH1	2.77	0.44
4:B:1215:ARG:C	4:B:1216:LEU:HD23	2.38	0.44
3:A:699:ALA:C	3:A:701:LEU:H	2.21	0.44
3:A:71:GLN:HB2	3:A:72:GLU:H	1.23	0.44
12:L:61:THR:HG22	12:L:62:LYS:N	2.32	0.44
4:B:321:GLY:C	4:B:323:VAL:N	2.71	0.44
6:E:59:SER:OG	6:E:81:GLU:HG3	2.17	0.44
7:F:86:THR:OG1	7:F:89:GLU:CG	2.60	0.44
3:A:963:ILE:HG21	3:A:1045:VAL:HG13	1.98	0.44
3:A:590:ARG:NH1	3:A:590:ARG:CG	2.78	0.44
4:B:761:HIS:H	4:B:761:HIS:CD2	2.35	0.44
4:B:1144:ALA:O	4:B:1147:LEU:N	2.47	0.44
4:B:626:ILE:HD12	4:B:626:ILE:N	2.33	0.44
3:A:1209:MET:HA	3:A:1212:VAL:CG2	2.48	0.44
3:A:1215:ARG:O	3:A:1219:THR:OG1	2.36	0.44
3:A:1284:MET:HG2	3:A:1306:LEU:HD21	1.99	0.44
4:B:689:LEU:C	4:B:690:VAL:HG23	2.38	0.44
3:A:264:PHE:O	3:A:267:ALA:HB3	2.18	0.44
3:A:51:GLY:CA	3:A:56:PRO:HG2	2.45	0.44
4:B:120:ARG:HD2	4:B:955:THR:CG2	2.16	0.44
4:B:893:LEU:HD23	4:B:897:GLY:C	2.39	0.44
6:E:17:ARG:O	6:E:20:LYS:HB2	2.17	0.44
10:J:1:MET:HB2	10:J:1:MET:HE2	1.88	0.44
2:T:5:DT:C1'	3:A:448:PRO:HB3	2.47	0.44
7:F:134:ILE:HG22	7:F:135:ARG:N	2.32	0.44
3:A:1441:PHE:CZ	7:F:88:TYR:O	2.69	0.44
3:A:129:LYS:O	3:A:130:ASP:OD2	2.36	0.44
3:A:138:ILE:O	3:A:139:TRP:C	2.55	0.44
3:A:657:LEU:HD12	3:A:657:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1096:SER:O	3:A:1099:PRO:CG	2.66	0.44
4:B:751:VAL:HG22	4:B:812:LEU:HD11	1.98	0.44
3:A:1336:MET:HE1	3:A:1381:LEU:HB2	2.00	0.44
4:B:61:ASP:OD1	4:B:61:ASP:N	2.51	0.44
3:A:441:PRO:O	3:A:441:PRO:HG2	2.18	0.44
4:B:518:HIS:O	4:B:519:TRP:C	2.55	0.44
4:B:1159:ARG:HH21	4:B:1193:GLN:HE21	1.66	0.44
12:L:62:LYS:O	12:L:64:LEU:HG	2.18	0.44
4:B:456:GLY:HA3	4:B:468:GLU:OE2	2.18	0.44
3:A:528:LEU:HA	3:A:531:ILE:H	1.82	0.44
4:B:286:PHE:CG	4:B:297:ILE:HD12	2.52	0.44
6:E:61:GLN:HB2	6:E:78:LEU:O	2.17	0.44
3:A:690:VAL:HG22	3:A:718:VAL:HG13	1.98	0.44
3:A:151:ASP:OD1	3:A:163:SER:CB	2.66	0.44
9:I:84:VAL:HG12	9:I:84:VAL:O	2.17	0.44
4:B:868:MET:O	4:B:869:SER:CB	2.66	0.44
3:A:1376:THR:CG2	3:A:1376:THR:O	2.66	0.44
3:A:268:ASP:HB3	3:A:299:HIS:CD2	2.53	0.43
4:B:834:ASN:HB2	4:B:839:MET:HA	2.00	0.43
5:C:237:SER:C	5:C:238:ILE:HG13	2.38	0.43
3:A:54:ASN:OD1	3:A:54:ASN:O	2.36	0.43
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.43
4:B:1183:LYS:CE	4:B:1183:LYS:O	2.66	0.43
3:A:840:ARG:O	3:A:841:LEU:C	2.55	0.43
4:B:427:ASP:HA	4:B:430:ARG:HD2	2.00	0.43
4:B:273:LEU:HD21	4:B:360:PHE:HD1	1.82	0.43
8:H:12:VAL:HA	8:H:28:ALA:HB1	2.00	0.43
3:A:332:LYS:H	3:A:337:ARG:HB2	1.82	0.43
6:E:187:TYR:C	6:E:187:TYR:CD2	2.92	0.43
3:A:919:ILE:HG23	3:A:922:ASP:HB2	1.99	0.43
3:A:1017:LEU:HB2	6:E:206:GLY:N	2.33	0.43
3:A:893:PHE:HD2	3:A:893:PHE:C	2.19	0.43
3:A:1276:VAL:HB	3:A:1279:ILE:HD13	2.00	0.43
3:A:89:PRO:O	3:A:90:VAL:CG2	2.66	0.43
4:B:25:ILE:H	4:B:25:ILE:HG13	1.64	0.43
4:B:483:LEU:HB3	4:B:484:ASN:H	1.60	0.43
4:B:884:ARG:O	4:B:936:ASP:HB3	2.17	0.43
4:B:951:GLN:HG2	12:L:57:LEU:HD22	2.00	0.43
4:B:376:PHE:CZ	4:B:569:TYR:HB3	2.52	0.43
3:A:941:LYS:O	3:A:942:PHE:C	2.56	0.43
9:I:7:CYS:SG	9:I:8:ARG:O	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:80:ALA:O	7:F:81:THR:C	2.57	0.43
4:B:107:GLY:O	4:B:108:VAL:O	2.37	0.43
3:A:1398:MET:O	3:A:1399:ARG:C	2.56	0.43
3:A:445:ASN:ND2	3:A:446:ARG:C	2.72	0.43
3:A:451:HIS:HB3	3:A:453:MET:H	1.82	0.43
3:A:134:ARG:CD	3:A:221:SER:O	2.49	0.43
4:B:1072:MET:HB2	4:B:1085:ILE:CD1	2.49	0.43
3:A:618:GLU:CD	3:A:619:LYS:N	2.70	0.43
3:A:691:LEU:HD11	3:A:695:LYS:HD2	2.00	0.43
7:F:101:ILE:CD1	7:F:120:ILE:HG22	2.48	0.43
9:I:84:VAL:O	9:I:84:VAL:CG1	2.65	0.43
4:B:54:PHE:O	4:B:55:VAL:C	2.56	0.43
8:H:76:THR:O	8:H:76:THR:CG2	2.66	0.43
5:C:204:SER:O	5:C:205:LYS:C	2.55	0.43
3:A:179:LEU:HD11	3:A:298:PHE:HA	1.99	0.43
3:A:88:LYS:HA	3:A:89:PRO:HD2	1.70	0.43
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.53	0.43
4:B:744:HIS:CD2	4:B:745:PRO:HD2	2.53	0.43
4:B:996:ARG:NH2	5:C:174:ALA:O	2.51	0.43
4:B:1001:PHE:CD2	5:C:34:ARG:NH2	2.86	0.43
11:K:4:PRO:O	11:K:5:ASP:C	2.56	0.43
4:B:63:ILE:CG1	4:B:421:PHE:CZ	3.01	0.43
8:H:93:TYR:HD2	8:H:145:ARG:HB3	1.83	0.43
3:A:946:VAL:CG2	6:E:201:LYS:HB3	2.47	0.43
2:T:6:DC:H4'	3:A:447:GLN:OE1	2.18	0.43
5:C:27:LEU:HA	5:C:228:PHE:CZ	2.53	0.43
3:A:583:PRO:HG2	3:A:586:ILE:HG13	2.00	0.43
3:A:547:LEU:CD2	11:K:58:PHE:CD1	2.96	0.43
3:A:1044:TRP:C	3:A:1046:LEU:N	2.69	0.43
3:A:599:SER:O	3:A:602:ASP:N	2.32	0.43
3:A:690:VAL:HG13	3:A:718:VAL:HG22	2.00	0.43
7:F:117:PRO:O	7:F:120:ILE:HB	2.18	0.43
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.48	0.43
3:A:361:LEU:N	3:A:471:ASN:ND2	2.67	0.43
3:A:548:ASN:HD21	11:K:47:ARG:NE	2.15	0.43
4:B:890:TYR:O	4:B:892:LYS:N	2.50	0.43
3:A:1219:THR:HG23	3:A:1271:ILE:HD11	2.00	0.43
3:A:1207:LEU:HD11	3:A:1273:LEU:HD23	2.01	0.43
4:B:705:MET:H	4:B:710:LEU:HD12	1.82	0.43
4:B:173:MET:O	4:B:176:SER:CB	2.66	0.43
4:B:841:MET:SD	4:B:990:ILE:HD11	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:41:ILE:HG12	5:C:172:PRO:HG3	2.00	0.43
10:J:7:CYS:SG	10:J:7:CYS:O	2.74	0.43
10:J:8:PHE:H	10:J:49:MET:HE3	1.81	0.43
3:A:326:ARG:O	3:A:330:LYS:N	2.51	0.43
3:A:7:SER:OG	3:A:9:ALA:HB3	2.17	0.43
4:B:112:LEU:HA	4:B:112:LEU:HD12	1.62	0.43
3:A:1021:LEU:O	3:A:1022:LEU:C	2.56	0.43
3:A:909:ASP:OD1	3:A:911:SER:HB3	2.17	0.43
6:E:39:LEU:C	6:E:41:ASP:N	2.71	0.43
4:B:359:GLU:HA	4:B:362:PRO:HG3	2.01	0.43
11:K:49:GLU:C	11:K:51:LEU:N	2.71	0.43
10:J:1:MET:H1	10:J:56:LEU:HB2	1.84	0.43
3:A:1156:PRO:CD	3:A:1157:ASP:N	2.81	0.43
7:F:81:THR:CB	7:F:144:GLU:OE1	2.67	0.43
2:T:10:DT:OP1	4:B:857:ARG:NH2	2.51	0.43
4:B:1197:PRO:O	4:B:1200:ALA:N	2.50	0.43
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.59	0.43
4:B:55:VAL:O	4:B:56:ASP:C	2.56	0.43
11:K:47:ARG:HD3	11:K:60:ALA:HA	1.99	0.43
4:B:872:GLU:HG3	4:B:916:THR:OG1	2.19	0.43
3:A:867:ILE:HG22	3:A:872:GLY:CA	2.49	0.43
4:B:458:LYS:O	4:B:462:ALA:N	2.52	0.43
3:A:235:ILE:H	3:A:235:ILE:HD12	1.83	0.43
4:B:701:ILE:HG12	4:B:703:ILE:HG13	2.01	0.43
4:B:640:VAL:CG2	4:B:740:HIS:HA	2.39	0.43
4:B:474:SER:O	4:B:476:ARG:N	2.47	0.43
3:A:325:ILE:HG22	4:B:1210:MET:SD	2.59	0.43
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.48	0.43
6:E:20:LYS:O	6:E:21:GLU:C	2.57	0.43
3:A:148:CYS:HB3	3:A:167:CYS:C	2.38	0.43
3:A:427:GLN:O	3:A:428:TYR:O	2.36	0.43
8:H:40:LEU:HD13	8:H:123:MET:HE2	2.00	0.43
7:F:93:ILE:HD11	7:F:134:ILE:HD11	2.00	0.43
4:B:54:PHE:HB3	4:B:55:VAL:H	1.58	0.43
4:B:125:SER:HB2	4:B:171:PRO:N	2.33	0.43
4:B:598:GLU:O	4:B:599:THR:C	2.57	0.43
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.43
5:C:137:LYS:HD3	5:C:138:GLU:HG2	2.00	0.43
4:B:488:TYR:HE2	4:B:813:LYS:HB2	1.83	0.43
3:A:787:PHE:CE1	3:A:796:SER:HA	2.53	0.43
4:B:176:SER:O	4:B:182:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:367:PRO:CB	3:A:466:SER:HA	2.49	0.43
3:A:1362:TYR:CE1	3:A:1363:VAL:O	2.71	0.43
4:B:430:ARG:HB3	4:B:434:ARG:NH1	2.34	0.43
3:A:648:ASN:O	3:A:649:ILE:C	2.56	0.43
3:A:138:ILE:HG22	3:A:139:TRP:N	2.33	0.43
6:E:128:PRO:HA	6:E:129:PRO:HA	1.72	0.43
3:A:1044:TRP:O	3:A:1046:LEU:N	2.52	0.43
3:A:714:PHE:CG	9:I:97:MET:CE	3.01	0.43
12:L:43:THR:HG23	12:L:43:THR:O	2.17	0.43
3:A:986:ILE:HD13	3:A:1032:LEU:HD11	2.01	0.43
3:A:1035:TYR:O	3:A:1037:LEU:HD23	2.19	0.43
3:A:1418:LEU:HD21	4:B:1222:ARG:HG3	2.00	0.43
11:K:17:SER:O	11:K:18:LYS:C	2.55	0.43
4:B:1022:THR:HG23	4:B:1022:THR:O	2.18	0.43
3:A:1430:LEU:N	3:A:1430:LEU:HD23	2.33	0.43
4:B:535:LEU:HA	4:B:535:LEU:HD23	1.71	0.43
4:B:308:TRP:CG	4:B:309:GLN:N	2.86	0.43
3:A:1168:GLU:O	3:A:1171:GLN:N	2.51	0.43
4:B:710:LEU:O	4:B:711:GLU:HB3	2.19	0.43
4:B:211:VAL:CG2	4:B:483:LEU:HG	2.48	0.43
3:A:491:VAL:O	3:A:493:GLN:NE2	2.52	0.43
4:B:842:ASN:O	4:B:846:ILE:HG13	2.18	0.43
4:B:113:TYR:O	4:B:116:GLU:N	2.52	0.43
4:B:423:LYS:CB	4:B:423:LYS:NZ	2.76	0.43
3:A:530:GLY:C	3:A:653:VAL:HG11	2.39	0.43
4:B:254:LEU:HD12	4:B:272:THR:O	2.19	0.43
4:B:365:THR:HG21	4:B:367:LEU:HD12	2.01	0.43
6:E:127:ILE:H	6:E:127:ILE:CD1	2.31	0.43
4:B:1095:LEU:O	4:B:1096:ARG:O	2.35	0.43
2:T:8:DT:OP2	2:T:8:DT:H73	2.18	0.43
3:A:551:TYR:CD1	3:A:551:TYR:C	2.89	0.43
4:B:233:PRO:HG2	4:B:234:ILE:N	2.33	0.43
3:A:12:ARG:HB2	4:B:1218:THR:CG2	2.48	0.43
4:B:170:LEU:HD12	4:B:171:PRO:CD	2.48	0.43
6:E:71:LYS:HD3	6:E:160:GLU:OE2	2.18	0.43
4:B:1058:LEU:HD23	4:B:1058:LEU:HA	1.73	0.43
4:B:991:GLY:O	4:B:992:ILE:HB	2.18	0.43
6:E:46:TYR:CD2	6:E:58:MET:CE	3.02	0.43
5:C:5:GLY:O	5:C:6:PRO:C	2.56	0.43
4:B:169:ARG:HD2	4:B:454:THR:HG21	2.01	0.43
8:H:143:LEU:C	8:H:144:ILE:HG13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG12	8:H:15:VAL:O	2.17	0.43
11:K:82:ASP:HA	11:K:83:PRO:HD2	1.61	0.43
4:B:1132:GLU:O	4:B:1135:ARG:HB3	2.18	0.43
3:A:341:MET:HB3	3:A:341:MET:HE3	1.39	0.43
5:C:260:LEU:O	5:C:264:GLN:CG	2.52	0.43
3:A:793:SER:OG	3:A:795:GLU:HG3	2.18	0.43
3:A:152:VAL:HG13	3:A:153:PRO:HD2	2.00	0.43
4:B:554:ILE:O	4:B:557:PHE:N	2.52	0.43
4:B:368:GLU:HB3	4:B:369:GLY:H	1.71	0.43
3:A:1387:HIS:N	3:A:1387:HIS:ND1	2.67	0.43
3:A:1382:THR:HG22	3:A:1388:GLY:HA3	2.00	0.43
8:H:62:SER:HB2	8:H:63:LEU:H	1.29	0.43
6:E:186:LEU:HA	6:E:186:LEU:HD23	1.91	0.43
3:A:1325:THR:O	6:E:147:HIS:ND1	2.52	0.43
4:B:1007:VAL:HG13	4:B:1008:PRO:N	2.33	0.43
4:B:100:PRO:HG2	4:B:124:TYR:CZ	2.54	0.43
4:B:174:LEU:HD23	4:B:202:TYR:CE1	2.54	0.43
3:A:902:LEU:H	3:A:902:LEU:HG	1.31	0.43
3:A:929:LEU:N	3:A:929:LEU:CD2	2.77	0.43
3:A:407:ARG:HB3	3:A:430:TRP:CZ2	2.54	0.43
4:B:566:LEU:O	4:B:569:TYR:HB2	2.19	0.43
5:C:73:GLN:HE21	5:C:75:MET:HB2	1.83	0.43
4:B:258:LEU:O	4:B:259:TYR:C	2.56	0.43
3:A:1349:TYR:O	3:A:1351:GLU:N	2.52	0.43
3:A:33:ALA:O	3:A:34:LYS:HG3	2.19	0.43
3:A:458:HIS:CE1	3:A:507:VAL:CG2	2.95	0.43
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.27	0.43
3:A:989:GLY:O	3:A:992:ASP:N	2.34	0.43
6:E:117:THR:O	6:E:120:ALA:HB3	2.18	0.43
3:A:778:GLY:HA3	4:B:516:ASN:HB2	2.01	0.43
3:A:707:GLY:O	3:A:1281:ARG:HD3	2.18	0.43
3:A:699:ALA:O	3:A:701:LEU:HG	2.18	0.43
4:B:639:ILE:HD11	4:B:691:GLU:HG3	2.01	0.43
3:A:174:ILE:HG22	3:A:175:ARG:N	2.32	0.43
6:E:95:THR:HG22	6:E:95:THR:O	2.17	0.43
3:A:1331:SER:HG	3:A:1333:ILE:HG22	1.84	0.43
4:B:26:THR:O	4:B:27:ALA:C	2.57	0.43
4:B:638:PHE:O	4:B:740:HIS:HB2	2.18	0.43
5:C:35:ARG:HB2	5:C:36:VAL:H	1.67	0.43
11:K:61:TYR:CD1	11:K:62:LYS:N	2.86	0.43
3:A:76:GLU:O	3:A:76:GLU:OE2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:928:LEU:O	3:A:930:ASP:N	2.51	0.43
4:B:297:ILE:HG22	4:B:298:LEU:N	2.34	0.43
4:B:360:PHE:CD1	4:B:361:LEU:HD13	2.54	0.43
6:E:79:TRP:CE3	6:E:79:TRP:HA	2.53	0.43
3:A:99:ILE:C	3:A:102:VAL:HG23	2.39	0.43
11:K:42:LEU:O	11:K:43:GLY:C	2.58	0.43
3:A:743:VAL:HG11	3:A:758:ILE:HD11	2.01	0.43
4:B:737:THR:O	4:B:738:PHE:C	2.58	0.43
3:A:401:GLY:CA	3:A:435:HIS:CD2	3.01	0.43
7:F:97:ARG:NH2	7:F:124:GLU:OE2	2.52	0.43
4:B:1196:ILE:HD13	4:B:1196:ILE:N	2.33	0.43
3:A:921:GLY:C	3:A:922:ASP:O	2.57	0.43
4:B:554:ILE:HG22	4:B:555:ILE:N	2.33	0.43
3:A:420:ARG:O	3:A:424:ILE:CG1	2.66	0.43
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.43
3:A:473:SER:O	3:A:521:MET:HB3	2.19	0.43
3:A:1127:ASP:O	3:A:1129:GLU:N	2.52	0.42
3:A:1193:LEU:CD1	3:A:1193:LEU:C	2.86	0.42
3:A:463:ILE:CB	3:A:464:PRO:CD	2.97	0.42
3:A:494:SER:HB2	3:A:496:GLU:HG3	2.01	0.42
11:K:44:ASN:HA	11:K:61:TYR:HE2	1.84	0.42
3:A:61:ILE:O	3:A:62:ASP:C	2.50	0.42
4:B:914:LYS:H	4:B:938:SER:HB3	1.83	0.42
4:B:911:ILE:HD11	4:B:941:LEU:HG	2.00	0.42
3:A:924:LYS:HE3	3:A:924:LYS:HB2	1.57	0.42
4:B:294:ASP:H	9:I:12:ASN:HD21	1.67	0.42
8:H:47:PHE:CD2	8:H:95:TYR:CD1	3.04	0.42
9:I:7:CYS:SG	9:I:34:TYR:CB	3.07	0.42
3:A:1000:LEU:HD23	3:A:1000:LEU:HA	1.71	0.42
4:B:1131:GLY:C	4:B:1133:MET:N	2.71	0.42
3:A:185:TRP:HB3	3:A:186:LYS:H	1.69	0.42
3:A:838:GLN:O	3:A:842:VAL:HG23	2.19	0.42
3:A:518:LYS:HG3	3:A:519:PRO:CD	2.49	0.42
3:A:376:TYR:CE2	3:A:377:PRO:O	2.71	0.42
3:A:562:THR:HA	3:A:563:PRO:HD3	1.73	0.42
4:B:653:VAL:HG12	4:B:654:ARG:H	1.84	0.42
4:B:410:GLY:O	4:B:412:LEU:N	2.52	0.42
3:A:320:ARG:NH2	4:B:471:LYS:N	2.67	0.42
3:A:35:ILE:HG22	3:A:270:LEU:CD1	2.44	0.42
4:B:124:TYR:OH	4:B:179:CYS:CA	2.62	0.42
3:A:671:ALA:O	3:A:672:ASP:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:349:ILE:O	4:B:350:GLN:O	2.37	0.42
4:B:376:PHE:CE2	4:B:569:TYR:CD2	3.01	0.42
7:F:77:ASP:HB3	7:F:78:GLN:H	1.60	0.42
3:A:1423:GLY:O	3:A:1424:VAL:C	2.56	0.42
4:B:1084:GLN:CB	5:C:201:TRP:HH2	2.32	0.42
3:A:587:HIS:HE1	3:A:969:GLN:HG2	1.83	0.42
3:A:806:ARG:HH11	3:A:806:ARG:HD2	1.68	0.42
4:B:1116:ARG:HG3	4:B:1198:TYR:CG	2.52	0.42
3:A:754:SER:OG	3:A:757:ASN:ND2	2.51	0.42
4:B:53:GLN:CG	4:B:53:GLN:O	2.67	0.42
9:I:85:PHE:CD1	9:I:86:PHE:N	2.87	0.42
4:B:970:THR:HG22	4:B:971:THR:N	2.34	0.42
3:A:1135:ARG:HB3	3:A:1136:SER:H	1.48	0.42
3:A:1147:THR:HA	3:A:1197:LEU:HD23	2.01	0.42
3:A:1193:LEU:HB2	3:A:1260:LEU:HD21	2.01	0.42
6:E:175:LEU:HB3	6:E:213:ILE:HG22	2.01	0.42
4:B:702:LEU:HA	4:B:702:LEU:HD12	1.46	0.42
4:B:1099:VAL:O	4:B:1101:ASP:N	2.52	0.42
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.82	0.42
4:B:952:VAL:O	12:L:57:LEU:HD23	2.19	0.42
4:B:449:ASN:HD21	4:B:451:LYS:CD	2.33	0.42
3:A:622:VAL:CG2	3:A:622:VAL:O	2.61	0.42
4:B:1084:GLN:CD	4:B:1084:GLN:N	2.68	0.42
3:A:1097:GLY:O	3:A:1098:VAL:C	2.57	0.42
3:A:535:THR:HG21	3:A:616:VAL:HA	2.00	0.42
9:I:106:CYS:SG	9:I:108:HIS:CB	3.08	0.42
10:J:14:VAL:C	10:J:16:ASP:H	2.22	0.42
12:L:34:CYS:O	12:L:35:SER:CB	2.67	0.42
3:A:857:ARG:HB3	3:A:862:ASN:O	2.20	0.42
4:B:745:PRO:O	4:B:748:ILE:HG12	2.20	0.42
3:A:320:ARG:NH2	4:B:470:LYS:C	2.73	0.42
4:B:1099:VAL:HG23	4:B:1099:VAL:H	1.50	0.42
5:C:134:ILE:HD12	5:C:141:GLY:HA3	1.72	0.42
10:J:7:CYS:SG	10:J:10:CYS:N	2.90	0.42
3:A:910:PRO:HB3	3:A:916:GLY:HA3	2.01	0.42
4:B:165:VAL:HG13	4:B:166:PHE:N	2.35	0.42
8:H:40:LEU:HD12	8:H:40:LEU:HA	1.86	0.42
6:E:135:PHE:CB	6:E:140:LEU:HD11	2.27	0.42
3:A:1079:MET:C	3:A:1080:THR:OG1	2.53	0.42
5:C:46:ILE:CD1	5:C:159:ALA:HB2	2.30	0.42
3:A:587:HIS:HA	3:A:607:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1059:LEU:CD1	4:B:1064:TYR:HB2	2.49	0.42
3:A:722:LEU:H	3:A:722:LEU:HD12	1.84	0.42
3:A:1354:ASN:HA	3:A:1357:ALA:HB3	2.01	0.42
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.84	0.42
3:A:343:LYS:HD3	4:B:1155:SER:OG	2.19	0.42
3:A:1139:GLU:CG	3:A:1139:GLU:O	2.67	0.42
4:B:542:MET:CE	4:B:747:MET:HG3	2.49	0.42
6:E:46:TYR:CD2	6:E:57:MET:O	2.72	0.42
4:B:417:PHE:O	4:B:418:LYS:O	2.37	0.42
4:B:297:ILE:O	4:B:299:GLU:N	2.52	0.42
3:A:941:LYS:O	3:A:943:LEU:N	2.52	0.42
4:B:190:TYR:CE1	10:J:62:ARG:HG2	2.54	0.42
5:C:62:PHE:HD2	5:C:62:PHE:C	2.22	0.42
7:F:135:ARG:CG	7:F:137:TYR:HE1	2.26	0.42
11:K:45:LEU:HA	11:K:45:LEU:HD12	1.61	0.42
5:C:261:ALA:HA	5:C:264:GLN:HG3	2.01	0.42
3:A:655:PHE:O	3:A:658:LEU:HB3	2.19	0.42
4:B:1059:LEU:HD23	4:B:1066:SER:HA	2.02	0.42
9:I:111:THR:CG2	9:I:112:SER:N	2.82	0.42
4:B:783:THR:HG22	10:J:63:TYR:CE1	2.45	0.42
5:C:69:LEU:HD12	5:C:169:LYS:HB3	2.01	0.42
3:A:402:ALA:HB1	3:A:433:GLU:O	2.19	0.42
3:A:226:GLU:HB3	3:A:227:VAL:H	1.68	0.42
6:E:85:GLU:HB3	6:E:87:SER:O	2.20	0.42
3:A:723:ASN:O	3:A:724:GLU:C	2.56	0.42
3:A:1227:ILE:C	3:A:1228:TRP:CE3	2.93	0.42
3:A:463:ILE:HB	3:A:464:PRO:CD	2.43	0.42
3:A:314:ALA:O	3:A:319:GLY:O	2.37	0.42
4:B:110:HIS:CD2	4:B:111:ALA:N	2.88	0.42
4:B:957:ASN:HD22	4:B:958:GLN:N	2.16	0.42
4:B:954:VAL:HA	4:B:963:PHE:O	2.20	0.42
4:B:167:ILE:CG2	4:B:424:LEU:CD1	2.76	0.42
4:B:1053:GLU:O	4:B:1055:ILE:N	2.53	0.42
8:H:82:PRO:C	8:H:84:ALA:H	2.10	0.42
8:H:32:THR:CG2	8:H:33:GLN:H	2.26	0.42
8:H:93:TYR:HD2	8:H:145:ARG:HD3	1.82	0.42
3:A:214:ILE:HG22	3:A:215:SER:N	2.35	0.42
4:B:1139:ILE:H	4:B:1139:ILE:HG13	1.61	0.42
7:F:81:THR:HG22	7:F:136:ARG:CZ	2.45	0.42
3:A:332:LYS:C	3:A:334:GLY:H	2.23	0.42
3:A:475:THR:O	3:A:476:SER:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1353:TYR:O	3:A:1354:ASN:C	2.55	0.42
4:B:781:PHE:CE1	4:B:782:LEU:HD12	2.54	0.42
3:A:1319:VAL:HG12	3:A:1320:PRO:CD	2.50	0.42
4:B:759:PRO:CD	4:B:1046:PRO:HG3	2.43	0.42
9:I:75:CYS:CB	9:I:103:CYS:HB2	2.49	0.42
8:H:89:LEU:HB2	8:H:91:ASP:CB	2.49	0.42
3:A:1061:GLY:O	3:A:1062:GLU:C	2.57	0.42
4:B:527:THR:OG1	4:B:528:PRO:CD	2.65	0.42
3:A:1026:LEU:HD23	3:A:1026:LEU:HA	1.71	0.42
4:B:802:PRO:CB	4:B:1091:TYR:CD1	3.03	0.42
4:B:803:LEU:O	4:B:1042:GLY:HA3	2.19	0.42
4:B:606:LYS:HB2	4:B:606:LYS:HE3	1.88	0.42
4:B:478:GLY:C	4:B:479:VAL:O	2.45	0.42
4:B:1032:SER:C	4:B:1089:PRO:HG2	2.40	0.42
4:B:821:GLN:CD	4:B:851:PHE:H	2.22	0.42
5:C:37:MET:SD	5:C:232:VAL:CG2	3.04	0.42
11:K:63:VAL:O	11:K:64:GLU:C	2.57	0.42
3:A:50:ILE:HB	3:A:52:GLY:H	1.85	0.42
4:B:102:VAL:CG2	4:B:112:LEU:CD2	2.88	0.42
4:B:114:PRO:HG3	4:B:181:LEU:HD12	2.01	0.42
4:B:911:ILE:HD11	4:B:941:LEU:CG	2.50	0.42
3:A:939:ASP:HA	3:A:942:PHE:HB3	2.01	0.42
9:I:29:CYS:SG	9:I:31:THR:CG2	3.08	0.42
10:J:54:VAL:O	10:J:56:LEU:N	2.49	0.42
3:A:834:THR:HG21	3:A:1077:THR:OG1	2.18	0.42
3:A:455:MET:C	3:A:456:MET:CG	2.87	0.42
4:B:1023:VAL:O	4:B:1024:ALA:C	2.57	0.42
7:F:120:ILE:HG22	7:F:121:ALA:H	1.81	0.42
3:A:877:HIS:CD2	3:A:1056:SER:HA	2.54	0.42
3:A:151:ASP:OD1	3:A:163:SER:HB3	2.19	0.42
4:B:815:ARG:H	4:B:815:ARG:HG2	1.63	0.42
3:A:423:ASP:HB3	3:A:424:ILE:H	1.49	0.42
4:B:724:ASP:HA	4:B:725:PRO:HD2	1.88	0.42
3:A:290:GLU:HG3	3:A:290:GLU:H	1.44	0.42
3:A:1334:ASP:O	3:A:1335:ILE:C	2.57	0.42
3:A:1167:GLU:O	3:A:1168:GLU:C	2.57	0.42
4:B:1006:ILE:HG23	4:B:1007:VAL:N	2.34	0.42
5:C:31:ASN:O	5:C:34:ARG:N	2.53	0.42
10:J:8:PHE:N	10:J:49:MET:HE3	2.35	0.42
3:A:325:ILE:CG2	4:B:1210:MET:SD	3.08	0.42
4:B:1162:ILE:HD13	4:B:1168:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1362:TYR:CE1	3:A:1364:ASN:HA	2.54	0.42
4:B:276:ILE:CG2	4:B:277:LYS:N	2.81	0.42
4:B:360:PHE:C	4:B:362:PRO:HD3	2.40	0.42
11:K:83:PRO:O	11:K:86:ALA:N	2.52	0.42
3:A:112:LYS:O	3:A:114:LEU:HD23	2.19	0.42
9:I:9:ASP:OD1	9:I:9:ASP:N	2.52	0.42
4:B:796:LEU:O	4:B:799:PRO:CD	2.68	0.42
5:C:61:GLU:O	5:C:64:ALA:HB3	2.20	0.42
5:C:66:ARG:NH1	10:J:2:ILE:HG21	2.35	0.42
4:B:107:GLY:C	4:B:108:VAL:O	2.57	0.42
3:A:923:LEU:HD23	3:A:923:LEU:HA	1.84	0.42
4:B:170:LEU:HA	4:B:171:PRO:HD2	1.50	0.42
3:A:1230:GLU:N	3:A:1233:ASP:OD2	2.52	0.42
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.47	0.42
4:B:906:SER:O	4:B:909:ASP:CG	2.58	0.42
4:B:722:ASP:OD1	4:B:722:ASP:N	2.51	0.42
3:A:1237:ILE:HG23	3:A:1238:ILE:H	1.85	0.42
4:B:638:PHE:HE1	4:B:743:ILE:HA	1.81	0.42
4:B:482:VAL:CG2	4:B:482:VAL:O	2.58	0.42
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.42
12:L:47:ARG:CG	12:L:52:GLY:O	2.68	0.42
11:K:103:THR:O	11:K:106:GLU:HB2	2.19	0.42
3:A:1364:ASN:CG	3:A:1366:ARG:HH11	2.23	0.42
4:B:349:ILE:O	4:B:352:ALA:N	2.49	0.42
4:B:361:LEU:N	4:B:362:PRO:HD2	2.33	0.42
3:A:943:LEU:O	3:A:946:VAL:N	2.53	0.42
6:E:78:LEU:HD23	6:E:78:LEU:O	2.20	0.42
4:B:778:MET:HE3	4:B:853:SER:HB3	1.97	0.42
3:A:453:MET:HB3	3:A:477:PRO:CB	2.50	0.42
3:A:550:LEU:O	3:A:551:TYR:C	2.58	0.42
4:B:1106:ARG:HE	4:B:1109:GLY:N	2.18	0.42
3:A:1100:ARG:NH1	3:A:1104:ILE:HD11	2.34	0.42
4:B:230:ALA:C	4:B:232:SER:H	2.22	0.42
4:B:1192:TYR:CD2	4:B:1218:THR:HG21	2.55	0.42
8:H:104:PHE:CE2	8:H:136:LYS:HA	2.54	0.42
11:K:47:ARG:NH1	11:K:47:ARG:C	2.71	0.42
3:A:1381:LEU:HA	3:A:1381:LEU:HD23	1.48	0.42
5:C:153:LEU:HA	5:C:153:LEU:HD13	1.72	0.42
4:B:581:PHE:CB	4:B:625:LYS:HG2	2.50	0.42
3:A:1119:TYR:CD2	3:A:1305:VAL:HG22	2.54	0.42
3:A:265:LYS:NZ	3:A:322:VAL:HB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:38:ILE:HG12	5:C:176:ILE:CD1	2.50	0.42
3:A:60:SER:HB2	3:A:61:ILE:H	1.44	0.42
3:A:898:ARG:HD3	3:A:933:TYR:CD1	2.55	0.42
6:E:47:CYS:HA	6:E:52:ARG:O	2.19	0.42
3:A:878:ILE:CG2	3:A:956:LEU:N	2.83	0.42
4:B:95:ILE:HA	4:B:129:PHE:O	2.19	0.42
4:B:166:PHE:HE2	4:B:450:ALA:CB	2.33	0.42
3:A:531:ILE:HG12	3:A:622:VAL:CG1	2.27	0.42
4:B:563:MET:CE	4:B:588:GLY:CA	2.98	0.42
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.01	0.42
3:A:211:PHE:CG	3:A:231:PRO:HB2	2.55	0.42
4:B:189:LEU:C	4:B:191:LYS:N	2.69	0.42
3:A:1444:MET:HB3	3:A:1445:ILE:H	1.60	0.42
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.01	0.42
3:A:1408:ILE:O	3:A:1412:ALA:CB	2.68	0.42
5:C:43:THR:HG22	5:C:44:LEU:N	2.34	0.42
5:C:206:ASN:ND2	5:C:229:TYR:CD2	2.88	0.42
7:F:109:VAL:HG12	7:F:110:ASP:N	2.21	0.42
3:A:921:GLY:O	3:A:922:ASP:C	2.58	0.42
3:A:1036:ARG:C	3:A:1037:LEU:O	2.57	0.42
2:T:11:DC:C2'	2:T:12:DG:H8	2.31	0.42
4:B:620:ARG:NH2	9:I:89:GLN:NE2	2.67	0.42
3:A:540:PHE:CE1	8:H:43:ASN:ND2	2.88	0.42
3:A:1227:ILE:CG2	3:A:1228:TRP:H	2.28	0.41
3:A:1340:GLY:HA2	6:E:183:PRO:HG2	2.01	0.41
3:A:787:PHE:CZ	3:A:796:SER:HA	2.54	0.41
4:B:844:SER:O	4:B:847:ASP:HB2	2.20	0.41
4:B:848:ARG:NH2	4:B:996:ARG:NH1	2.68	0.41
5:C:37:MET:HE2	5:C:37:MET:HB2	1.79	0.41
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.55	0.41
3:A:37:PHE:N	3:A:37:PHE:CD1	2.88	0.41
3:A:569:LYS:CD	5:C:221:TYR:O	2.68	0.41
3:A:1291:VAL:HG12	3:A:1292:PRO:HD2	1.97	0.41
10:J:21:TYR:CD2	10:J:22:LEU:HD12	2.54	0.41
5:C:27:LEU:HA	5:C:228:PHE:CE2	2.54	0.41
3:A:588:LEU:HD12	3:A:588:LEU:HA	1.44	0.41
3:A:220:THR:O	3:A:221:SER:C	2.58	0.41
3:A:662:PHE:CE1	3:A:742:ASN:HB3	2.55	0.41
3:A:184:SER:OG	3:A:185:TRP:N	2.52	0.41
9:I:26:LEU:HD23	9:I:26:LEU:HA	1.65	0.41
8:H:128:ASN:CG	8:H:128:ASN:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1057:VAL:HG12	3:A:1058:VAL:O	2.19	0.41
4:B:753:ALA:O	4:B:755:ILE:N	2.53	0.41
3:A:265:LYS:HE3	3:A:323:LYS:HG2	1.97	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
5:C:141:GLY:C	5:C:142:VAL:O	2.56	0.41
11:K:3:ALA:HA	11:K:4:PRO:HD3	1.76	0.41
3:A:324:SER:O	3:A:325:ILE:HB	2.19	0.41
6:E:53:PRO:O	6:E:55:ARG:N	2.52	0.41
4:B:431:TYR:CD1	4:B:447:ALA:HB1	2.54	0.41
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.02	0.41
4:B:291:ILE:CD1	4:B:291:ILE:N	2.80	0.41
3:A:1156:PRO:CG	3:A:1157:ASP:N	2.84	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD3	2.02	0.41
6:E:65:THR:O	6:E:67:GLU:N	2.54	0.41
3:A:582:ILE:HD11	3:A:629:LEU:CD1	2.47	0.41
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.83	0.41
4:B:1106:ARG:HH21	4:B:1109:GLY:CA	2.33	0.41
3:A:997:LEU:O	3:A:1053:PHE:CD2	2.73	0.41
3:A:770:VAL:HG13	3:A:822:GLU:OE1	2.20	0.41
9:I:115:LYS:O	9:I:116:ASN:C	2.59	0.41
11:K:28:PRO:HD2	11:K:28:PRO:O	2.20	0.41
4:B:51:PHE:O	4:B:54:PHE:CB	2.68	0.41
4:B:664:THR:HG22	4:B:664:THR:O	2.20	0.41
4:B:769:TYR:C	4:B:771:SER:N	2.73	0.41
7:F:94:LEU:HA	7:F:94:LEU:HD23	1.69	0.41
3:A:959:ASN:C	3:A:959:ASN:OD1	2.58	0.41
6:E:198:ILE:N	6:E:210:SER:O	2.42	0.41
3:A:783:THR:HG23	3:A:815:PHE:HE2	1.84	0.41
4:B:474:SER:HA	4:B:476:ARG:NE	2.35	0.41
5:C:238:ILE:CG2	5:C:242:GLN:HB2	2.49	0.41
5:C:35:ARG:O	5:C:38:ILE:HB	2.21	0.41
3:A:38:PRO:N	3:A:270:LEU:HD22	2.35	0.41
4:B:179:CYS:C	4:B:181:LEU:N	2.74	0.41
6:E:26:ARG:HH22	6:E:109:ILE:HD11	1.84	0.41
3:A:147:VAL:HB	3:A:149:GLU:N	2.36	0.41
3:A:381:THR:CB	3:A:382:PRO:HD2	2.49	0.41
8:H:58:THR:CG2	8:H:59:ILE:N	2.81	0.41
3:A:1004:ASN:ND2	6:E:167:ARG:CG	2.84	0.41
3:A:208:LEU:HD22	3:A:212:LYS:HG3	2.02	0.41
6:E:78:LEU:CG	6:E:107:THR:HG22	2.51	0.41
7:F:74:ILE:CG2	7:F:75:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:9:G:H5'	4:B:1097:HIS:NE2	2.35	0.41
3:A:95:PHE:O	3:A:99:ILE:HG13	2.20	0.41
3:A:100:LYS:HB3	3:A:100:LYS:HZ1	1.83	0.41
3:A:606:LEU:HA	3:A:606:LEU:HD12	1.68	0.41
3:A:1348:LEU:HA	3:A:1348:LEU:HD12	1.73	0.41
4:B:982:SER:HB2	4:B:983:ARG:H	1.56	0.41
3:A:1212:VAL:O	3:A:1215:ARG:CB	2.69	0.41
4:B:746:SER:O	4:B:749:LEU:HB2	2.20	0.41
10:J:43:ARG:HD2	10:J:45:CYS:SG	2.60	0.41
12:L:46:VAL:HG12	12:L:47:ARG:N	2.35	0.41
3:A:903:ASN:HD22	3:A:906:HIS:HB2	1.85	0.41
4:B:427:ASP:CA	4:B:430:ARG:HD2	2.50	0.41
4:B:431:TYR:CG	4:B:447:ALA:CB	3.03	0.41
8:H:25:ARG:HB2	8:H:25:ARG:HE	1.29	0.41
3:A:1289:ARG:HG2	3:A:1291:VAL:HG23	2.01	0.41
3:A:947:PHE:HE2	3:A:954:TRP:CE3	2.39	0.41
4:B:225:VAL:HG11	4:B:385:LEU:HA	2.02	0.41
7:F:81:THR:O	7:F:82:THR:O	2.38	0.41
3:A:453:MET:HE3	3:A:513:SER:CB	2.51	0.41
3:A:588:LEU:HB3	3:A:607:ILE:HB	2.02	0.41
3:A:608:ILE:HG12	3:A:613:ILE:CG1	2.50	0.41
4:B:1106:ARG:HG3	4:B:1107:ALA:N	2.35	0.41
3:A:399:HIS:CG	3:A:400:PRO:N	2.88	0.41
4:B:1027:ILE:H	4:B:1027:ILE:HG13	1.54	0.41
3:A:548:ASN:OD1	11:K:60:ALA:HB1	2.20	0.41
4:B:1035:ALA:O	4:B:1039:GLY:N	2.44	0.41
6:E:149:LEU:O	6:E:151:PRO:HD3	2.21	0.41
12:L:27:LEU:H	12:L:27:LEU:HD23	1.86	0.41
3:A:1286:LYS:HB2	3:A:1304:TRP:CH2	2.55	0.41
3:A:1282:VAL:HG13	3:A:1283:VAL:N	2.34	0.41
4:B:685:LEU:HD13	4:B:690:VAL:HG12	2.03	0.41
3:A:491:VAL:HG13	3:A:492:PRO:HD2	2.02	0.41
3:A:751:SER:O	3:A:752:LYS:HG2	2.21	0.41
5:C:231:ASN:C	5:C:231:ASN:ND2	2.74	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
4:B:879:ARG:HB2	4:B:880:THR:H	1.02	0.41
4:B:575:PRO:C	4:B:577:ALA:N	2.71	0.41
9:I:14:LEU:HB3	9:I:28:GLU:C	2.41	0.41
10:J:1:MET:N	10:J:56:LEU:H	2.18	0.41
3:A:1000:LEU:HD23	3:A:1001:ARG:H	1.86	0.41
3:A:837:ILE:C	3:A:839:ARG:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:821:ARG:O	3:A:822:GLU:C	2.58	0.41
5:C:51:VAL:HG13	5:C:155:LEU:HD23	2.03	0.41
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.38	0.41
6:E:35:VAL:HG12	6:E:36:GLU:N	2.36	0.41
6:E:168:TYR:HA	6:E:168:TYR:HD2	1.67	0.41
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.21	0.41
4:B:393:LYS:HE3	9:I:89:GLN:O	2.20	0.41
10:J:14:VAL:O	10:J:16:ASP:N	2.54	0.41
3:A:824:LEU:HD23	3:A:824:LEU:HA	1.73	0.41
3:A:368:LYS:HA	3:A:462:VAL:CG1	2.51	0.41
8:H:18:GLY:O	8:H:19:ARG:O	2.39	0.41
3:A:1274:ARG:HB2	3:A:1274:ARG:HE	1.44	0.41
3:A:818:MET:HA	4:B:514:LEU:HB3	2.01	0.41
4:B:685:LEU:CD1	4:B:690:VAL:HG12	2.50	0.41
3:A:302:THR:CB	3:A:313:GLN:NE2	2.83	0.41
6:E:39:LEU:HD12	6:E:39:LEU:HA	1.80	0.41
4:B:428:ILE:O	4:B:432:MET:HE2	2.20	0.41
4:B:563:MET:O	4:B:564:GLU:C	2.57	0.41
8:H:100:THR:HG22	8:H:101:ALA:N	2.35	0.41
4:B:236:HIS:CD2	4:B:389:ALA:CA	3.04	0.41
5:C:104:PHE:HA	5:C:151:GLN:O	2.20	0.41
6:E:124:VAL:HG12	6:E:125:PRO:N	2.35	0.41
3:A:1154:TYR:H	9:I:41:PRO:HB2	1.85	0.41
4:B:1135:ARG:O	4:B:1139:ILE:HG13	2.20	0.41
3:A:336:ILE:HA	3:A:340:LEU:HB2	2.01	0.41
3:A:573:SER:O	3:A:574:GLY:C	2.59	0.41
5:C:260:LEU:HD11	5:C:264:GLN:HE21	1.86	0.41
3:A:709:THR:O	3:A:712:GLU:N	2.54	0.41
8:H:36:CYS:HB2	8:H:130:ARG:HH22	1.86	0.41
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.20	0.41
3:A:1345:ARG:CG	3:A:1372:VAL:CG1	2.99	0.41
4:B:322:PHE:CZ	9:I:30:ARG:CD	2.92	0.41
4:B:1196:ILE:CB	4:B:1197:PRO:CD	2.96	0.41
7:F:128:LYS:HD3	7:F:148:VAL:O	2.21	0.41
5:C:181:ASP:CB	5:C:186:LEU:HD13	2.50	0.41
3:A:985:ASP:O	3:A:986:ILE:C	2.58	0.41
3:A:518:LYS:HG3	3:A:519:PRO:N	2.35	0.41
11:K:34:THR:CG2	11:K:35:PHE:N	2.83	0.41
3:A:1210:GLY:O	3:A:1211:GLN:C	2.57	0.41
3:A:1239:ARG:HH12	3:A:1241:ARG:HH12	1.68	0.41
3:A:91:PHE:C	3:A:297:GLN:HE22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:473:MET:O	4:B:475:SER:N	2.51	0.41
5:C:244:VAL:HG23	5:C:245:VAL:N	2.35	0.41
12:L:46:VAL:O	12:L:47:ARG:CB	2.63	0.41
3:A:904:THR:O	3:A:906:HIS:N	2.54	0.41
4:B:272:THR:O	4:B:273:LEU:HG	2.19	0.41
4:B:294:ASP:N	9:I:12:ASN:HD21	2.18	0.41
3:A:567:LYS:HD3	8:H:96:VAL:H	1.86	0.41
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.51	0.41
3:A:211:PHE:O	3:A:212:LYS:C	2.59	0.41
6:E:24:LYS:HG2	6:E:25:ASP:N	2.34	0.41
3:A:335:ARG:CD	3:A:339:ASN:HD22	2.33	0.41
3:A:99:ILE:CG1	3:A:234:MET:SD	3.09	0.41
4:B:737:THR:CG2	9:I:66:PRO:CA	2.98	0.41
4:B:781:PHE:CD1	4:B:782:LEU:HD12	2.55	0.41
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.36	0.41
6:E:103:LYS:O	6:E:104:ASN:C	2.59	0.41
6:E:153:HIS:C	6:E:154:ILE:HG12	2.41	0.41
8:H:19:ARG:O	8:H:20:TYR:CG	2.74	0.41
4:B:311:LEU:HA	4:B:311:LEU:HD23	1.78	0.41
3:A:1172:LEU:N	3:A:1172:LEU:CD2	2.78	0.41
6:E:164:LEU:CD2	6:E:211:TYR:CD2	3.04	0.41
5:C:245:VAL:C	5:C:247:GLY:N	2.73	0.41
4:B:1184:GLY:O	4:B:1186:ASP:CG	2.59	0.41
4:B:179:CYS:C	4:B:181:LEU:H	2.24	0.41
4:B:898:LEU:O	4:B:899:ILE:C	2.59	0.41
3:A:878:ILE:C	3:A:879:GLU:HG3	2.41	0.41
3:A:147:VAL:C	3:A:149:GLU:H	2.23	0.41
3:A:381:THR:HG23	3:A:382:PRO:CG	2.51	0.41
3:A:596:THR:C	3:A:598:LEU:N	2.73	0.41
3:A:947:PHE:CD1	3:A:947:PHE:N	2.89	0.41
3:A:946:VAL:HG12	3:A:947:PHE:N	2.35	0.41
3:A:23:SER:O	3:A:27:VAL:HG23	2.20	0.41
6:E:78:LEU:HG	6:E:107:THR:HG22	2.03	0.41
7:F:77:ASP:O	7:F:78:GLN:C	2.59	0.41
5:C:129:ILE:O	5:C:131:HIS:HD2	2.03	0.41
4:B:1084:GLN:CG	5:C:201:TRP:CH2	3.02	0.41
6:E:118:PRO:O	6:E:122:LYS:CD	2.68	0.41
3:A:660:ASN:O	4:B:1081:LEU:HD22	2.20	0.41
3:A:606:LEU:HB2	3:A:614:PHE:CE1	2.56	0.41
7:F:101:ILE:HG21	7:F:120:ILE:HG21	2.02	0.41
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:117:ASP:N	5:C:117:ASP:OD1	2.53	0.41
4:B:44:VAL:HG11	4:B:495:LEU:HD13	2.02	0.41
6:E:202:SER:C	6:E:204:THR:H	2.24	0.41
4:B:1060:ARG:O	4:B:1061:GLU:C	2.59	0.41
9:I:62:ILE:HG22	9:I:63:GLY:N	2.34	0.41
6:E:151:PRO:O	6:E:153:HIS:ND1	2.53	0.41
4:B:487:THR:HG22	4:B:489:SER:H	1.84	0.41
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.41	0.41
3:A:1279:ILE:N	3:A:1279:ILE:HD12	2.35	0.41
4:B:545:ILE:C	4:B:634:TYR:HE2	2.25	0.41
4:B:36:ALA:HB2	4:B:661:LEU:HD22	2.03	0.41
4:B:701:ILE:CG1	4:B:703:ILE:HG13	2.51	0.41
4:B:705:MET:H	4:B:710:LEU:HD11	1.86	0.41
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.74	0.41
4:B:474:SER:HA	4:B:476:ARG:HE	1.86	0.41
4:B:476:ARG:C	4:B:478:GLY:N	2.73	0.41
5:C:31:ASN:C	5:C:33:LEU:N	2.74	0.41
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.41	0.41
5:C:245:VAL:O	5:C:247:GLY:N	2.53	0.41
3:A:62:ASP:O	3:A:64:ASN:N	2.54	0.41
3:A:50:ILE:O	3:A:52:GLY:N	2.54	0.41
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.54	0.41
4:B:957:ASN:C	4:B:957:ASN:HD22	2.24	0.41
4:B:893:LEU:HD23	4:B:897:GLY:O	2.21	0.41
6:E:43:LYS:HA	6:E:47:CYS:SG	2.61	0.41
5:C:6:PRO:O	5:C:7:GLN:HG2	2.20	0.41
3:A:1362:TYR:HE1	3:A:1363:VAL:O	2.04	0.41
3:A:528:LEU:CD1	3:A:531:ILE:CG2	2.99	0.41
3:A:639:PRO:HG2	3:A:640:GLN:N	2.34	0.41
4:B:563:MET:HE1	4:B:588:GLY:CA	2.51	0.41
11:K:86:ALA:O	11:K:90:ALA:HB2	2.21	0.41
11:K:50:LEU:CD2	11:K:75:ILE:HD13	2.44	0.41
6:E:124:VAL:H	6:E:125:PRO:CD	2.29	0.41
3:A:1191:TRP:CZ2	3:A:1257:ASP:OD1	2.74	0.41
9:I:42:LEU:C	9:I:43:VAL:HG23	2.41	0.41
3:A:1399:ARG:O	3:A:1400:CYS:C	2.59	0.41
3:A:453:MET:HB3	3:A:477:PRO:HB2	2.03	0.41
3:A:92:HIS:CG	3:A:236:LEU:HD11	2.55	0.41
4:B:1067:ARG:HB2	4:B:1069:PHE:CD1	2.56	0.41
4:B:737:THR:HG21	9:I:66:PRO:CA	2.51	0.41
3:A:997:LEU:HA	3:A:997:LEU:HD22	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:591:PHE:CD2	3:A:595:THR:CG2	3.04	0.41
3:A:603:ASN:O	3:A:604:GLY:O	2.39	0.41
3:A:601:LYS:HB3	3:A:603:ASN:CG	2.41	0.41
4:B:1027:ILE:O	4:B:1028:GLU:C	2.59	0.41
4:B:792:MET:O	4:B:793:ALA:HB2	2.21	0.41
4:B:281:PRO:HG2	4:B:320:ASP:OD2	2.21	0.41
3:A:990:VAL:HG12	3:A:991:LYS:N	2.36	0.41
4:B:485:ARG:NH1	4:B:485:ARG:CG	2.76	0.41
4:B:953:LEU:O	4:B:964:VAL:HA	2.21	0.41
4:B:43:LEU:HA	4:B:43:LEU:HD23	1.64	0.41
4:B:1217:TYR:N	4:B:1217:TYR:CD1	2.89	0.41
3:A:359:LEU:HD22	3:A:363:GLN:CB	2.51	0.41
5:C:119:VAL:O	5:C:119:VAL:CG1	2.69	0.41
6:E:32:GLN:CG	6:E:32:GLN:O	2.69	0.41
3:A:1334:ASP:HA	3:A:1337:GLU:OE1	2.21	0.41
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.21	0.41
3:A:789:LYS:CE	9:I:67:THR:OG1	2.69	0.41
3:A:856:THR:O	3:A:864:ILE:HB	2.21	0.41
6:E:147:HIS:O	6:E:150:VAL:N	2.38	0.41
4:B:541:LEU:HB2	4:B:747:MET:HE3	2.03	0.41
4:B:472:ALA:O	4:B:473:MET:C	2.59	0.41
3:A:746:MET:HB3	3:A:751:SER:OG	2.21	0.41
4:B:992:ILE:HG13	4:B:993:THR:N	2.35	0.41
4:B:1168:LEU:C	4:B:1170:THR:N	2.74	0.41
3:A:379:VAL:HG13	3:A:380:VAL:HG23	2.03	0.41
11:K:83:PRO:HA	11:K:86:ALA:CB	2.50	0.41
3:A:144:THR:O	3:A:146:MET:HE2	2.21	0.41
5:C:63:ILE:O	5:C:66:ARG:N	2.46	0.41
10:J:50:ILE:C	10:J:52:THR:H	2.25	0.41
4:B:1096:ARG:CG	4:B:1097:HIS:N	2.84	0.41
7:F:133:VAL:HG22	7:F:146:TRP:C	2.42	0.41
3:A:1437:GLY:CA	7:F:88:TYR:CD2	2.99	0.41
3:A:1410:PHE:C	3:A:1412:ALA:N	2.71	0.41
11:K:31:VAL:HG13	11:K:32:VAL:N	2.35	0.41
3:A:141:LEU:HD23	3:A:141:LEU:HA	1.79	0.41
3:A:660:ASN:ND2	4:B:1082:MET:CB	2.84	0.41
3:A:391:LEU:O	3:A:394:ASN:HB2	2.21	0.41
3:A:695:LYS:O	3:A:696:GLU:C	2.58	0.41
7:F:109:VAL:HG11	7:F:123:LYS:HG2	2.03	0.41
4:B:554:ILE:HA	4:B:554:ILE:HD13	1.86	0.41
4:B:457:LEU:HD23	4:B:457:LEU:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:986:ILE:CD1	3:A:1032:LEU:HD11	2.51	0.41
3:A:537:ARG:C	3:A:539:THR:H	2.23	0.41
3:A:808:LEU:CD2	3:A:816:HIS:HD2	2.34	0.41
3:A:980:ASP:C	3:A:980:ASP:OD2	2.58	0.41
4:B:802:PRO:HA	4:B:1091:TYR:CD1	2.55	0.41
3:A:715:GLU:O	3:A:716:ASP:C	2.57	0.41
4:B:953:LEU:C	4:B:953:LEU:HD23	2.42	0.41
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.56	0.41
9:I:20:LYS:O	9:I:21:GLU:O	2.38	0.41
11:K:111:LEU:N	11:K:111:LEU:HD23	2.36	0.41
3:A:265:LYS:HZ2	3:A:322:VAL:HB	1.84	0.40
4:B:461:LEU:HD11	4:B:466:TRP:CH2	2.52	0.40
3:A:58:LEU:O	3:A:59:GLY:C	2.55	0.40
4:B:1170:THR:HG23	4:B:1183:LYS:NZ	2.35	0.40
4:B:113:TYR:HA	4:B:114:PRO:HD2	1.98	0.40
4:B:956:THR:HA	4:B:961:LEU:O	2.22	0.40
3:A:875:ALA:HA	3:A:878:ILE:CD1	2.48	0.40
4:B:430:ARG:C	4:B:431:TYR:O	2.55	0.40
3:A:642:CYS:O	3:A:643:ALA:C	2.58	0.40
3:A:382:PRO:HG2	3:A:383:TYR:H	1.85	0.40
4:B:297:ILE:HD13	4:B:297:ILE:HA	1.70	0.40
4:B:225:VAL:O	4:B:226:PHE:CD2	2.74	0.40
10:J:3:VAL:N	10:J:53:HIS:CE1	2.89	0.40
10:J:57:ILE:O	10:J:59:LYS:N	2.54	0.40
7:F:83:PRO:HD2	7:F:84:TYR:H	1.84	0.40
11:K:24:ASP:CG	11:K:74:ARG:NH1	2.74	0.40
8:H:107:VAL:C	8:H:108:SER:O	2.57	0.40
3:A:804:TYR:O	4:B:761:HIS:HB3	2.21	0.40
4:B:230:ALA:O	4:B:261:ARG:HD2	2.21	0.40
4:B:582:VAL:HG22	4:B:626:ILE:HB	2.03	0.40
9:I:58:VAL:C	9:I:59:VAL:HG23	2.41	0.40
3:A:515:GLN:HG2	3:A:516:SER:OG	2.21	0.40
5:C:16:ASP:O	5:C:233:GLU:HA	2.21	0.40
10:J:43:ARG:O	10:J:47:ARG:N	2.54	0.40
4:B:110:HIS:CG	4:B:111:ALA:H	2.39	0.40
3:A:598:LEU:O	3:A:600:PRO:N	2.54	0.40
4:B:800:GLN:HG3	10:J:52:THR:CB	2.52	0.40
2:T:4:DA:H3'	2:T:4:DA:P	2.60	0.40
3:A:1437:GLY:C	7:F:88:TYR:HB3	2.42	0.40
4:B:1131:GLY:O	4:B:1134:GLU:N	2.53	0.40
6:E:63:ASN:CB	6:E:64:PRO:CD	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1077:THR:O	3:A:1078:GLN:NE2	2.54	0.40
9:I:111:THR:HG22	9:I:113:ASP:HB3	2.04	0.40
4:B:791:THR:O	4:B:792:MET:O	2.38	0.40
5:C:186:LEU:N	5:C:186:LEU:HD12	2.36	0.40
4:B:493:SER:HB2	4:B:751:VAL:HG11	2.02	0.40
3:A:1057:VAL:CG1	3:A:1058:VAL:H	2.32	0.40
6:E:117:THR:O	6:E:119:SER:N	2.55	0.40
4:B:694:ASP:O	4:B:697:GLU:N	2.54	0.40
3:A:557:ASP:OD2	3:A:559:VAL:HG23	2.21	0.40
4:B:499:ASN:OD1	4:B:500:THR:N	2.54	0.40
3:A:369:SER:CB	11:K:2:ASN:OD1	2.69	0.40
3:A:1119:TYR:CD2	3:A:1326:ARG:NH2	2.90	0.40
3:A:90:VAL:O	3:A:235:ILE:HG22	2.22	0.40
3:A:815:PHE:O	3:A:818:MET:N	2.54	0.40
4:B:461:LEU:HD12	4:B:466:TRP:CH2	2.54	0.40
4:B:847:ASP:O	5:C:65:HIS:HE1	2.04	0.40
12:L:53:HIS:C	12:L:55:ILE:N	2.73	0.40
4:B:429:PHE:C	4:B:433:GLN:OE1	2.60	0.40
8:H:25:ARG:HB2	8:H:41:ASP:OD1	2.20	0.40
3:A:567:LYS:HD3	8:H:95:TYR:CA	2.51	0.40
3:A:567:LYS:CB	8:H:95:TYR:HA	2.52	0.40
3:A:886:ILE:HA	3:A:886:ILE:HD13	1.85	0.40
6:E:79:TRP:HE3	6:E:79:TRP:HA	1.85	0.40
11:K:58:PHE:CE2	11:K:74:ARG:NE	2.61	0.40
5:C:196:ASP:C	5:C:198:ALA:N	2.74	0.40
3:A:794:PRO:CG	3:A:795:GLU:H	2.26	0.40
3:A:690:VAL:HG13	3:A:718:VAL:HG13	2.03	0.40
4:B:512:ARG:HB3	4:B:533:CYS:O	2.21	0.40
4:B:369:GLY:C	4:B:370:PHE:HD1	2.24	0.40
11:K:107:THR:O	11:K:111:LEU:HD23	2.22	0.40
8:H:16:ASP:HA	8:H:17:PRO:HD2	1.75	0.40
3:A:1329:THR:C	3:A:1331:SER:N	2.75	0.40
3:A:857:ARG:HD3	3:A:861:GLY:O	2.21	0.40
4:B:514:LEU:HD12	4:B:518:HIS:HD2	1.86	0.40
3:A:269:ILE:C	3:A:271:LYS:H	2.24	0.40
4:B:212:LEU:HD23	4:B:212:LEU:HA	1.70	0.40
4:B:831:SER:CB	4:B:994:TYR:OH	2.70	0.40
4:B:847:ASP:C	4:B:849:GLY:H	2.25	0.40
3:A:312:PRO:C	3:A:313:GLN:HG3	2.30	0.40
12:L:57:LEU:HD23	12:L:57:LEU:HA	1.89	0.40
11:K:103:THR:HG22	11:K:104:ASN:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:422:LYS:O	4:B:425:THR:HG22	2.21	0.40
8:H:82:PRO:O	8:H:83:GLN:CB	2.51	0.40
8:H:15:VAL:O	8:H:15:VAL:HG13	2.19	0.40
11:K:21:ILE:O	11:K:21:ILE:HG22	2.21	0.40
9:I:32:CYS:SG	9:I:34:TYR:CB	3.09	0.40
3:A:744:LYS:HE2	3:A:748:MET:HE2	2.04	0.40
4:B:792:MET:H	4:B:857:ARG:HA	1.86	0.40
7:F:132:LEU:HD23	7:F:132:LEU:HA	1.82	0.40
3:A:1017:LEU:HA	3:A:1017:LEU:HD23	1.76	0.40
11:K:47:ARG:CD	11:K:60:ALA:HA	2.51	0.40
6:E:77:SER:HB3	6:E:105:PHE:CD2	2.50	0.40
4:B:583:ASN:OD1	4:B:628:THR:HB	2.21	0.40
3:A:376:TYR:HA	3:A:377:PRO:HD2	1.85	0.40
3:A:789:LYS:HD2	9:I:67:THR:OG1	2.22	0.40
4:B:529:GLU:H	4:B:529:GLU:HG3	1.64	0.40
3:A:1284:MET:HA	3:A:1306:LEU:CD2	2.44	0.40
4:B:515:HIS:H	4:B:518:HIS:CD2	2.40	0.40
4:B:469:GLN:C	4:B:471:LYS:H	2.25	0.40
5:C:248:ILE:H	5:C:248:ILE:HG13	1.51	0.40
3:A:62:ASP:O	3:A:63:ARG:C	2.60	0.40
4:B:101:MET:C	4:B:102:VAL:HG23	2.42	0.40
3:A:899:VAL:CG2	3:A:1029:ARG:NH1	2.85	0.40
11:K:101:LEU:O	11:K:102:LYS:C	2.60	0.40
11:K:99:GLY:O	11:K:100:ALA:C	2.60	0.40
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.84	0.40
4:B:300:HIS:HE1	4:B:376:PHE:CZ	2.38	0.40
6:E:79:TRP:CD1	6:E:100:ILE:HG13	2.55	0.40
6:E:25:ASP:C	6:E:27:GLY:N	2.74	0.40
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.40
3:A:543:LEU:O	3:A:544:ASP:C	2.58	0.40
3:A:993:LEU:HB2	3:A:1046:LEU:CD2	2.51	0.40
3:A:605:MET:CE	3:A:614:PHE:O	2.69	0.40
3:A:266:LEU:HD22	3:A:266:LEU:HA	1.63	0.40
3:A:343:LYS:HZ1	4:B:1197:PRO:CB	2.27	0.40
8:H:135:LEU:HD22	8:H:136:LYS:CD	2.52	0.40
3:A:404:TYR:HB2	3:A:433:GLU:HG3	2.04	0.40
3:A:1036:ARG:HG3	3:A:1036:ARG:NH1	2.32	0.40
4:B:802:PRO:HB3	4:B:1091:TYR:CE1	2.55	0.40
10:J:16:ASP:C	10:J:16:ASP:OD1	2.60	0.40
4:B:755:ILE:HA	4:B:755:ILE:HD13	1.85	0.40
4:B:755:ILE:O	4:B:755:ILE:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1383/1733 (80%)	851 (62%)	315 (23%)	217 (16%)	0	4
4	B	1088/1224 (89%)	730 (67%)	214 (20%)	144 (13%)	0	6
5	C	264/318 (83%)	187 (71%)	49 (19%)	28 (11%)	0	10
6	E	212/215 (99%)	142 (67%)	41 (19%)	29 (14%)	0	6
7	F	82/155 (53%)	49 (60%)	26 (32%)	7 (8%)	1	14
8	H	129/146 (88%)	87 (67%)	16 (12%)	26 (20%)	0	2
9	I	117/122 (96%)	74 (63%)	24 (20%)	19 (16%)	0	4
10	J	63/70 (90%)	42 (67%)	11 (18%)	10 (16%)	0	4
11	K	112/120 (93%)	81 (72%)	20 (18%)	11 (10%)	1	12
12	L	44/70 (63%)	20 (46%)	10 (23%)	14 (32%)	0	0
All	All	3494/4173 (84%)	2263 (65%)	726 (21%)	505 (14%)	0	5

All (505) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	44	THR
3	A	50	ILE
3	A	55	ASP
3	A	56	PRO
3	A	57	ARG
3	A	59	GLY
3	A	62	ASP
3	A	63	ARG
3	A	69	THR
3	A	72	GLU
3	A	74	MET
3	A	76	GLU

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Mol	Chain	Res	Type
3	A	89	PRO
3	A	93	VAL
3	A	99	ILE
3	A	124	GLN
3	A	130	ASP
3	A	131	SER
3	A	132	LYS
3	A	138	ILE
3	A	149	GLU
3	A	167	CYS
3	A	169	ASN
3	A	185	TRP
3	A	209	ASN
3	A	214	ILE
3	A	219	PHE
3	A	223	GLY
3	A	244	PRO
3	A	248	PRO
3	A	250	ILE
3	A	253	ASN
3	A	254	GLU
3	A	283	GLY
3	A	285	PRO
3	A	286	HIS
3	A	290	GLU
3	A	312	PRO
3	A	313	GLN
3	A	314	ALA
3	A	317	LYS
3	A	318	SER
3	A	320	ARG
3	A	321	PRO
3	A	322	VAL
3	A	323	LYS
3	A	331	GLY
3	A	335	ARG
3	A	336	ILE
3	A	385	ILE
3	A	399	HIS
3	A	404	TYR
3	A	415	LEU
3	A	476	SER

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Mol	Chain	Res	Type
3	A	567	LYS
3	A	568	PRO
3	A	593	GLU
3	A	597	LEU
3	A	610	GLY
3	A	668	ASP
3	A	888	GLY
3	A	889	SER
3	A	895	LYS
3	A	903	ASN
3	A	904	THR
3	A	909	ASP
3	A	922	ASP
3	A	972	HIS
3	A	986	ILE
3	A	998	LEU
3	A	1036	ARG
3	A	1053	PHE
3	A	1054	LEU
3	A	1080	THR
3	A	1110	ASN
3	A	1139	GLU
3	A	1140	HIS
3	A	1169	ILE
3	A	1200	ALA
3	A	1201	ALA
3	A	1223	ASP
3	A	1255	GLU
3	A	1257	ASP
3	A	1274	ARG
3	A	1280	GLU
3	A	1314	SER
3	A	1327	ILE
3	A	1389	PHE
3	A	1392	SER
3	A	1394	THR
3	A	1401	SER
3	A	1425	SER
4	B	21	GLU
4	B	23	ALA
4	B	29	ASP
4	B	38	PHE

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Mol	Chain	Res	Type
4	B	55	VAL
4	B	65	GLU
4	B	108	VAL
4	B	168	GLY
4	B	229	ALA
4	B	231	PRO
4	B	248	SER
4	B	249	ARG
4	B	274	PRO
4	B	275	TYR
4	B	294	ASP
4	B	327	ARG
4	B	332	ASP
4	B	333	PHE
4	B	346	GLU
4	B	351	TYR
4	B	367	LEU
4	B	419	THR
4	B	432	MET
4	B	450	ALA
4	B	466	TRP
4	B	468	GLU
4	B	469	GLN
4	B	470	LYS
4	B	473	MET
4	B	476	ARG
4	B	531	GLN
4	B	635	ARG
4	B	636	PRO
4	B	637	LEU
4	B	642	ASP
4	B	643	ASP
4	B	645	SER
4	B	646	LEU
4	B	653	VAL
4	B	708	GLU
4	B	709	ASP
4	B	723	VAL
4	B	734	HIS
4	B	738	PHE
4	B	869	SER
4	B	878	GLN

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Mol	Chain	Res	Type
4	B	958	GLN
4	B	982	SER
4	B	1046	PRO
4	B	1061	GLU
4	B	1097	HIS
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1178	ASN
4	B	1181	GLU
4	B	1183	LYS
4	B	1214	PRO
5	C	107	SER
5	C	142	VAL
5	C	174	ALA
5	C	213	PRO
5	C	215	GLU
5	C	240	VAL
6	E	3	GLN
6	E	36	GLU
6	E	37	LEU
6	E	38	PRO
6	E	59	SER
6	E	77	SER
6	E	90	VAL
6	E	97	VAL
6	E	103	LYS
6	E	111	VAL
6	E	115	ASN
6	E	162	ARG
6	E	174	GLN
7	F	73	ALA
7	F	74	ILE
7	F	112	GLU
7	F	128	LYS
8	H	3	ASN
8	H	32	THR
8	H	34	ASP
8	H	43	ASN
8	H	77	ARG
8	H	80	ARG
8	H	81	PRO

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Mol	Chain	Res	Type
8	H	86	ASP
8	H	91	ASP
8	H	109	LYS
8	H	135	LEU
8	H	140	ALA
9	I	15	TYR
9	I	16	PRO
9	I	21	GLU
9	I	33	SER
9	I	34	TYR
9	I	79	HIS
9	I	116	ASN
10	J	2	ILE
10	J	6	ARG
10	J	55	ASP
10	J	64	ASN
11	K	7	PHE
11	K	27	ALA
11	K	28	PRO
12	L	26	THR
12	L	35	SER
12	L	43	THR
12	L	45	ALA
12	L	47	ARG
12	L	54	ARG
12	L	55	ILE
12	L	59	ALA
12	L	64	LEU
3	A	54	ASN
3	A	61	ILE
3	A	68	GLN
3	A	117	GLU
3	A	129	LYS
3	A	139	TRP
3	A	178	GLY
3	A	210	ILE
3	A	212	LYS
3	A	255	SER
3	A	257	ARG
3	A	315	LEU
3	A	409	SER
3	A	428	TYR

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Mol	Chain	Res	Type
3	A	473	SER
3	A	538	ASP
3	A	609	ASP
3	A	672	ASP
3	A	776	ALA
3	A	819	GLY
3	A	846	GLU
3	A	852	TYR
3	A	854	ASN
3	A	916	GLY
3	A	958	VAL
3	A	979	SER
3	A	980	ASP
3	A	985	ASP
3	A	1002	GLY
3	A	1028	THR
3	A	1135	ARG
3	A	1221	LYS
3	A	1231	ASP
3	A	1386	ARG
3	A	1388	GLY
3	A	1424	VAL
3	A	1437	GLY
4	B	27	ALA
4	B	37	PHE
4	B	94	LYS
4	B	124	TYR
4	B	132	VAL
4	B	200	GLY
4	B	266	ALA
4	B	318	VAL
4	B	350	GLN
4	B	365	THR
4	B	452	THR
4	B	472	ALA
4	B	485	ARG
4	B	641	GLU
4	B	695	ALA
4	B	712	PRO
4	B	731	VAL
4	B	751	VAL
4	B	761	HIS

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Mol	Chain	Res	Type
4	B	774	GLY
4	B	792	MET
4	B	793	ALA
4	B	872	GLU
4	B	891	ASP
4	B	942	ARG
4	B	959	ASP
4	B	1017	ILE
4	B	1021	MET
4	B	1185	CYS
4	B	1202	LEU
5	C	5	GLY
5	C	28	ALA
5	C	46	ILE
5	C	110	THR
5	C	245	VAL
6	E	31	THR
6	E	40	GLU
6	E	45	LYS
6	E	148	GLU
6	E	168	TYR
6	E	183	PRO
8	H	8	ASP
8	H	20	TYR
8	H	52	GLN
8	H	82	PRO
8	H	90	ALA
8	H	139	ASN
9	I	3	THR
9	I	10	CYS
9	I	11	ASN
9	I	23	ASN
9	I	60	GLN
10	J	8	PHE
10	J	32	GLU
11	K	5	ASP
11	K	13	GLY
11	K	78	THR
11	K	90	ALA
12	L	53	HIS
3	A	5	GLN
3	A	48	ALA

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Mol	Chain	Res	Type
3	A	66	LYS
3	A	109	HIS
3	A	220	THR
3	A	251	SER
3	A	259	GLU
3	A	268	ASP
3	A	306	ASN
3	A	333	GLU
3	A	517	ASN
3	A	529	CYS
3	A	556	TRP
3	A	600	PRO
3	A	604	GLY
3	A	737	LEU
3	A	838	GLN
3	A	902	LEU
3	A	905	ASP
3	A	923	LEU
3	A	942	PHE
3	A	1037	LEU
3	A	1046	LEU
3	A	1098	VAL
3	A	1115	SER
3	A	1133	LEU
3	A	1353	TYR
3	A	1403	GLU
4	B	45	SER
4	B	180	TYR
4	B	230	ALA
4	B	264	SER
4	B	265	SER
4	B	398	ARG
4	B	410	GLY
4	B	411	PRO
4	B	451	LYS
4	B	471	LYS
4	B	477	ALA
4	B	707	PRO
4	B	713	ALA
4	B	725	PRO
4	B	754	SER
4	B	937	ALA

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Mol	Chain	Res	Type
4	B	1144	ALA
4	B	1220	ARG
5	C	4	GLU
5	C	6	PRO
5	C	48	SER
5	C	184	ASN
5	C	206	ASN
5	C	212	PRO
6	E	203	GLU
7	F	81	THR
7	F	141	GLY
8	H	19	ARG
9	I	47	GLU
9	I	54	GLU
9	I	86	PHE
10	J	51	LEU
10	J	53	HIS
11	K	8	GLU
11	K	83	PRO
3	A	108	MET
3	A	140	THR
3	A	184	SER
3	A	245	PRO
3	A	400	PRO
3	A	543	LEU
3	A	583	PRO
3	A	963	ILE
3	A	1051	ALA
3	A	1077	THR
3	A	1168	GLU
3	A	1174	PHE
3	A	1204	ASP
3	A	1206	ASP
3	A	1242	VAL
3	A	1261	LYS
3	A	1287	TYR
3	A	1367	HIS
3	A	1383	SER
3	A	1398	MET
4	B	46	GLN
4	B	58	THR
4	B	179	CYS

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Mol	Chain	Res	Type
4	B	298	LEU
4	B	394	ASP
4	B	464	GLY
4	B	598	GLU
4	B	711	GLU
4	B	828	ALA
4	B	865	LYS
4	B	879	ARG
4	B	1066	SER
5	C	165	LYS
5	C	202	PRO
5	C	214	ASN
6	E	16	PHE
6	E	124	VAL
6	E	137	GLU
6	E	161	LYS
7	F	96	THR
8	H	33	GLN
8	H	44	VAL
8	H	48	PRO
8	H	78	SER
8	H	83	GLN
8	H	89	LEU
9	I	20	LYS
9	I	115	LYS
12	L	30	ILE
3	A	10	PRO
3	A	96	ILE
3	A	104	GLU
3	A	153	PRO
3	A	271	LYS
3	A	284	ALA
3	A	288	ALA
3	A	418	SER
3	A	424	ILE
3	A	526	ASP
3	A	599	SER
3	A	691	LEU
3	A	1050	GLU
3	A	1127	ASP
3	A	1233	ASP
3	A	1270	ASN

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Mol	Chain	Res	Type
3	A	1366	ARG
3	A	1421	CYS
4	B	114	PRO
4	B	323	VAL
4	B	353	LYS
4	B	368	GLU
4	B	744	HIS
4	B	818	PRO
4	B	842	ASN
4	B	899	ILE
4	B	1108	ARG
4	B	1157	ALA
5	C	32	SER
5	C	64	ALA
5	C	195	GLN
5	C	264	GLN
8	H	51	ALA
9	I	84	VAL
9	I	97	MET
11	K	4	PRO
11	K	88	LYS
12	L	56	LEU
3	A	51	GLY
3	A	316	GLN
3	A	625	SER
3	A	706	HIS
3	A	926	GLN
3	A	1049	ILE
3	A	1136	SER
4	B	28	GLU
4	B	324	ILE
4	B	418	LYS
4	B	724	ASP
5	C	136	ASP
5	C	185	LYS
6	E	8	ASN
6	E	172	GLU
12	L	48	CYS
3	A	477	PRO
3	A	756	ILE
3	A	1148	ILE
4	B	974	PRO

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Mol	Chain	Res	Type
4	B	992	ILE
5	C	172	PRO
6	E	118	PRO
3	A	27	VAL
3	A	325	ILE
3	A	382	PRO
3	A	530	GLY
3	A	825	ILE
3	A	837	ILE
4	B	201	GLY
4	B	284	ILE
4	B	285	ILE
4	B	555	ILE
10	J	15	GLY
12	L	46	VAL
3	A	162	VAL
3	A	289	ILE
4	B	171	PRO
5	C	243	VAL
10	J	14	VAL
3	A	531	ILE
3	A	1045	VAL
3	A	1335	ILE
4	B	247	GLY
4	B	292	ILE
4	B	870	ILE
4	B	877	PRO
6	E	127	ILE
3	A	639	PRO
4	B	467	GLY
6	E	76	GLY

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1218/1520 (80%)	859 (70%)	359 (30%)	0	3
4	B	960/1061 (90%)	718 (75%)	242 (25%)	1	6
5	C	234/274 (85%)	175 (75%)	59 (25%)	1	6
6	E	196/197 (100%)	141 (72%)	55 (28%)	0	4
7	F	74/137 (54%)	57 (77%)	17 (23%)	1	8
8	H	117/128 (91%)	80 (68%)	37 (32%)	0	3
9	I	113/116 (97%)	84 (74%)	29 (26%)	0	5
10	J	60/65 (92%)	42 (70%)	18 (30%)	0	3
11	K	99/102 (97%)	81 (82%)	18 (18%)	2	14
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
All	All	3111/3657 (85%)	2264 (73%)	847 (27%)	0	4

All (847) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	TYR
3	A	18	GLN
3	A	22	PHE
3	A	25	GLU
3	A	28	ARG
3	A	31	SER
3	A	32	VAL
3	A	38	PRO
3	A	41	MET
3	A	47	ARG
3	A	49	LYS
3	A	50	ILE
3	A	53	LEU
3	A	56	PRO
3	A	60	SER
3	A	62	ASP
3	A	64	ASN
3	A	65	LEU
3	A	67	CYS
3	A	68	GLN
3	A	69	THR
3	A	71	GLN

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Mol	Chain	Res	Type
3	A	72	GLU
3	A	74	MET
3	A	80	HIS
3	A	83	HIS
3	A	84	ILE
3	A	93	VAL
3	A	96	ILE
3	A	100	LYS
3	A	102	VAL
3	A	105	CYS
3	A	107	CYS
3	A	113	LEU
3	A	114	LEU
3	A	115	LEU
3	A	116	ASP
3	A	121	LEU
3	A	123	ARG
3	A	132	LYS
3	A	140	THR
3	A	142	CYS
3	A	143	LYS
3	A	147	VAL
3	A	150	THR
3	A	151	ASP
3	A	162	VAL
3	A	167	CYS
3	A	169	ASN
3	A	170	THR
3	A	180	LYS
3	A	184	SER
3	A	185	TRP
3	A	186	LYS
3	A	207	ILE
3	A	208	LEU
3	A	215	SER
3	A	219	PHE
3	A	222	LEU
3	A	225	ASN
3	A	227	VAL
3	A	229	SER
3	A	235	ILE
3	A	237	THR

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Mol	Chain	Res	Type
3	A	238	CYS
3	A	239	LEU
3	A	240	PRO
3	A	247	ARG
3	A	248	PRO
3	A	249	SER
3	A	250	ILE
3	A	254	GLU
3	A	256	GLN
3	A	257	ARG
3	A	263	THR
3	A	265	LYS
3	A	266	LEU
3	A	270	LEU
3	A	271	LYS
3	A	275	SER
3	A	279	LEU
3	A	282	ASN
3	A	287	HIS
3	A	291	GLU
3	A	295	LEU
3	A	296	LEU
3	A	297	GLN
3	A	302	THR
3	A	304	MET
3	A	306	ASN
3	A	307	ASP
3	A	308	ILE
3	A	315	LEU
3	A	318	SER
3	A	320	ARG
3	A	321	PRO
3	A	323	LYS
3	A	324	SER
3	A	325	ILE
3	A	335	ARG
3	A	337	ARG
3	A	344	ARG
3	A	348	SER
3	A	350	ARG
3	A	356	ASP
3	A	359	LEU

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Mol	Chain	Res	Type
3	A	364	VAL
3	A	380	VAL
3	A	381	THR
3	A	387	ARG
3	A	388	LEU
3	A	391	LEU
3	A	397	ASN
3	A	398	GLU
3	A	403	LYS
3	A	404	TYR
3	A	406	ILE
3	A	407	ARG
3	A	412	ARG
3	A	419	LYS
3	A	423	ASP
3	A	424	ILE
3	A	433	GLU
3	A	434	ARG
3	A	437	MET
3	A	438	ASP
3	A	441	PRO
3	A	443	LEU
3	A	445	ASN
3	A	449	SER
3	A	450	LEU
3	A	452	LYS
3	A	453	MET
3	A	455	MET
3	A	456	MET
3	A	462	VAL
3	A	466	SER
3	A	475	THR
3	A	476	SER
3	A	481	ASP
3	A	489	LEU
3	A	493	GLN
3	A	495	GLU
3	A	496	GLU
3	A	500	GLU
3	A	501	LEU
3	A	512	VAL
3	A	513	SER

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Mol	Chain	Res	Type
3	A	514	PRO
3	A	521	MET
3	A	524	VAL
3	A	525	GLN
3	A	531	ILE
3	A	533	LYS
3	A	552	TRP
3	A	567	LYS
3	A	573	SER
3	A	576	GLN
3	A	577	ILE
3	A	589	GLN
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	601	LYS
3	A	608	ILE
3	A	612	ILE
3	A	614	PHE
3	A	618	GLU
3	A	621	THR
3	A	625	SER
3	A	629	LEU
3	A	630	ILE
3	A	648	ASN
3	A	652	VAL
3	A	653	VAL
3	A	658	LEU
3	A	660	ASN
3	A	666	ILE
3	A	674	PRO
3	A	680	THR
3	A	682	THR
3	A	685	GLU
3	A	687	LYS
3	A	691	LEU
3	A	695	LYS
3	A	702	LEU
3	A	710	LEU
3	A	711	ARG
3	A	713	SER

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Mol	Chain	Res	Type
3	A	720	ARG
3	A	722	LEU
3	A	732	LEU
3	A	735	VAL
3	A	737	LEU
3	A	738	LYS
3	A	740	LEU
3	A	752	LYS
3	A	754	SER
3	A	756	ILE
3	A	764	CYS
3	A	765	VAL
3	A	768	GLN
3	A	771	GLU
3	A	774	ARG
3	A	788	SER
3	A	795	GLU
3	A	803	SER
3	A	805	LEU
3	A	816	HIS
3	A	821	ARG
3	A	826	ASP
3	A	829	VAL
3	A	830	LYS
3	A	831	THR
3	A	839	ARG
3	A	853	ASP
3	A	854	ASN
3	A	855	THR
3	A	857	ARG
3	A	858	ASN
3	A	879	GLU
3	A	882	SER
3	A	884	ASP
3	A	886	ILE
3	A	889	SER
3	A	890	ASP
3	A	893	PHE
3	A	896	ARG
3	A	897	TYR
3	A	898	ARG
3	A	902	LEU

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Mol	Chain	Res	Type
3	A	904	THR
3	A	905	ASP
3	A	907	THR
3	A	911	SER
3	A	913	LEU
3	A	918	GLU
3	A	923	LEU
3	A	924	LYS
3	A	925	LEU
3	A	927	VAL
3	A	929	LEU
3	A	932	GLU
3	A	934	LYS
3	A	940	ARG
3	A	941	LYS
3	A	964	ILE
3	A	968	GLN
3	A	969	GLN
3	A	973	ILE
3	A	978	PRO
3	A	980	ASP
3	A	988	LEU
3	A	990	VAL
3	A	993	LEU
3	A	995	GLU
3	A	996	ASN
3	A	997	LEU
3	A	998	LEU
3	A	1001	ARG
3	A	1004	ASN
3	A	1006	ILE
3	A	1009	ASN
3	A	1017	LEU
3	A	1019	CYS
3	A	1022	LEU
3	A	1024	SER
3	A	1025	ARG
3	A	1029	ARG
3	A	1032	LEU
3	A	1037	LEU
3	A	1046	LEU
3	A	1060	PRO

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Mol	Chain	Res	Type
3	A	1070	GLN
3	A	1077	THR
3	A	1079	MET
3	A	1092	LYS
3	A	1095	THR
3	A	1103	GLU
3	A	1107	VAL
3	A	1116	LEU
3	A	1120	LEU
3	A	1122	PRO
3	A	1128	GLN
3	A	1132	LYS
3	A	1133	LEU
3	A	1134	ILE
3	A	1138	ILE
3	A	1146	VAL
3	A	1150	SER
3	A	1156	PRO
3	A	1162	VAL
3	A	1163	ILE
3	A	1171	GLN
3	A	1172	LEU
3	A	1173	HIS
3	A	1187	GLN
3	A	1190	PRO
3	A	1193	LEU
3	A	1199	ARG
3	A	1207	LEU
3	A	1208	THR
3	A	1215	ARG
3	A	1223	ASP
3	A	1227	ILE
3	A	1231	ASP
3	A	1234	GLU
3	A	1235	LYS
3	A	1243	VAL
3	A	1262	LYS
3	A	1264	GLU
3	A	1265	ASN
3	A	1267	MET
3	A	1272	THR
3	A	1273	LEU

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Mol	Chain	Res	Type
3	A	1274	ARG
3	A	1277	GLU
3	A	1280	GLU
3	A	1281	ARG
3	A	1285	MET
3	A	1290	LYS
3	A	1292	PRO
3	A	1295	THR
3	A	1299	VAL
3	A	1300	LYS
3	A	1309	ASP
3	A	1315	GLU
3	A	1318	THR
3	A	1322	ILE
3	A	1325	THR
3	A	1326	ARG
3	A	1333	ILE
3	A	1336	MET
3	A	1349	TYR
3	A	1355	VAL
3	A	1359	ASP
3	A	1362	TYR
3	A	1364	ASN
3	A	1376	THR
3	A	1384	VAL
3	A	1385	THR
3	A	1387	HIS
3	A	1389	PHE
3	A	1390	ASN
3	A	1391	ARG
3	A	1393	ASN
3	A	1398	MET
3	A	1400	CYS
3	A	1405	THR
3	A	1407	GLU
3	A	1411	GLU
3	A	1420	ASP
3	A	1422	ARG
3	A	1425	SER
3	A	1433	MET
3	A	1435	PRO
3	A	1441	PHE

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Mol	Chain	Res	Type
3	A	1445	ILE
4	B	20	ASP
4	B	24	PRO
4	B	28	GLU
4	B	34	ILE
4	B	49	ASP
4	B	61	ASP
4	B	63	ILE
4	B	65	GLU
4	B	66	ASP
4	B	68	THR
4	B	94	LYS
4	B	97	VAL
4	B	98	THR
4	B	104	GLU
4	B	109	THR
4	B	119	LEU
4	B	120	ARG
4	B	128	LEU
4	B	130	VAL
4	B	131	ASP
4	B	134	LYS
4	B	166	PHE
4	B	174	LEU
4	B	175	ARG
4	B	177	LYS
4	B	185	THR
4	B	188	ASP
4	B	194	GLU
4	B	206	ASN
4	B	217	ARG
4	B	218	SER
4	B	222	ILE
4	B	223	VAL
4	B	225	VAL
4	B	231	PRO
4	B	234	ILE
4	B	246	LYS
4	B	249	ARG
4	B	251	ILE
4	B	252	SER
4	B	253	THR

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Mol	Chain	Res	Type
4	B	257	LYS
4	B	261	ARG
4	B	268	THR
4	B	274	PRO
4	B	275	TYR
4	B	276	ILE
4	B	283	VAL
4	B	298	LEU
4	B	304	ASP
4	B	305	VAL
4	B	315	LYS
4	B	316	PRO
4	B	319	GLU
4	B	322	PHE
4	B	329	THR
4	B	331	LEU
4	B	333	PHE
4	B	346	GLU
4	B	347	LYS
4	B	359	GLU
4	B	362	PRO
4	B	365	THR
4	B	367	LEU
4	B	372	SER
4	B	373	ARG
4	B	385	LEU
4	B	387	LEU
4	B	393	LYS
4	B	401	PHE
4	B	404	LYS
4	B	408	LEU
4	B	411	PRO
4	B	416	LEU
4	B	419	THR
4	B	423	LYS
4	B	424	LEU
4	B	425	THR
4	B	426	LYS
4	B	429	PHE
4	B	431	TYR
4	B	433	GLN
4	B	436	VAL

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Mol	Chain	Res	Type
4	B	451	LYS
4	B	458	LYS
4	B	461	LEU
4	B	469	GLN
4	B	471	LYS
4	B	474	SER
4	B	482	VAL
4	B	485	ARG
4	B	499	ASN
4	B	511	PRO
4	B	513	GLN
4	B	519	TRP
4	B	521	LEU
4	B	531	GLN
4	B	537	LYS
4	B	539	LEU
4	B	540	SER
4	B	547	VAL
4	B	552	MET
4	B	554	ILE
4	B	556	THR
4	B	563	MET
4	B	570	VAL
4	B	572	HIS
4	B	573	GLN
4	B	574	SER
4	B	592	ASN
4	B	598	GLU
4	B	613	VAL
4	B	617	ARG
4	B	623	GLU
4	B	624	LEU
4	B	635	ARG
4	B	638	PHE
4	B	640	VAL
4	B	641	GLU
4	B	642	ASP
4	B	644	GLU
4	B	646	LEU
4	B	648	HIS
4	B	658	ILE
4	B	667	GLN

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Mol	Chain	Res	Type
4	B	679	TYR
4	B	682	SER
4	B	686	ASN
4	B	701	ILE
4	B	709	ASP
4	B	710	LEU
4	B	714	GLU
4	B	723	VAL
4	B	724	ASP
4	B	728	ARG
4	B	730	ARG
4	B	732	SER
4	B	740	HIS
4	B	741	CYS
4	B	748	ILE
4	B	751	VAL
4	B	760	ASP
4	B	762	ASN
4	B	764	SER
4	B	766	ARG
4	B	778	MET
4	B	789	MET
4	B	790	ASP
4	B	791	THR
4	B	794	ASN
4	B	795	ILE
4	B	807	ARG
4	B	810	GLU
4	B	812	LEU
4	B	815	ARG
4	B	817	LEU
4	B	822	ASN
4	B	837	ASP
4	B	838	SER
4	B	856	PHE
4	B	858	SER
4	B	861	ASP
4	B	865	LYS
4	B	866	TYR
4	B	871	THR
4	B	878	GLN
4	B	879	ARG

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Mol	Chain	Res	Type
4	B	882	THR
4	B	883	LEU
4	B	886	LYS
4	B	889	THR
4	B	893	LEU
4	B	895	ASP
4	B	896	ASP
4	B	901	PRO
4	B	914	LYS
4	B	916	THR
4	B	933	SER
4	B	938	SER
4	B	941	LEU
4	B	944	THR
4	B	953	LEU
4	B	956	THR
4	B	957	ASN
4	B	958	GLN
4	B	962	LYS
4	B	968	VAL
4	B	976	ILE
4	B	983	ARG
4	B	984	HIS
4	B	986	GLN
4	B	989	THR
4	B	993	THR
4	B	995	ARG
4	B	996	ARG
4	B	999	MET
4	B	1007	VAL
4	B	1019	SER
4	B	1020	ARG
4	B	1021	MET
4	B	1034	VAL
4	B	1048	THR
4	B	1049	ASP
4	B	1064	TYR
4	B	1065	GLN
4	B	1073	TYR
4	B	1074	ASN
4	B	1077	THR
4	B	1082	MET

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Mol	Chain	Res	Type
4	B	1096	ARG
4	B	1103	ILE
4	B	1108	ARG
4	B	1113	VAL
4	B	1116	ARG
4	B	1119	VAL
4	B	1120	GLU
4	B	1123	SER
4	B	1124	ARG
4	B	1138	MET
4	B	1141	HIS
4	B	1145	SER
4	B	1147	LEU
4	B	1152	MET
4	B	1162	ILE
4	B	1171	VAL
4	B	1172	ILE
4	B	1181	GLU
4	B	1183	LYS
4	B	1185	CYS
4	B	1189	ILE
4	B	1190	ASP
4	B	1191	ILE
4	B	1194	ILE
4	B	1195	HIS
4	B	1196	ILE
4	B	1202	LEU
4	B	1203	LEU
4	B	1206	GLU
4	B	1210	MET
4	B	1218	THR
4	B	1219	ASP
4	B	1222	ARG
5	C	11	ARG
5	C	23	SER
5	C	25	VAL
5	C	26	ASP
5	C	27	LEU
5	C	33	LEU
5	C	34	ARG
5	C	41	ILE
5	C	46	ILE

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Mol	Chain	Res	Type
5	C	50	GLU
5	C	53	THR
5	C	55	THR
5	C	56	THR
5	C	58	LEU
5	C	62	PHE
5	C	67	LEU
5	C	69	LEU
5	C	70	ILE
5	C	77	ILE
5	C	89	GLU
5	C	91	HIS
5	C	99	LEU
5	C	110	THR
5	C	111	THR
5	C	117	ASP
5	C	119	VAL
5	C	122	SER
5	C	135	GLN
5	C	137	LYS
5	C	138	GLU
5	C	140	ASN
5	C	143	LEU
5	C	145	CYS
5	C	151	GLN
5	C	153	LEU
5	C	154	LYS
5	C	163	ILE
5	C	166	GLU
5	C	172	PRO
5	C	178	PHE
5	C	189	THR
5	C	193	TYR
5	C	197	SER
5	C	199	LYS
5	C	209	TYR
5	C	215	GLU
5	C	229	TYR
5	C	231	ASN
5	C	233	GLU
5	C	234	SER
5	C	240	VAL

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Mol	Chain	Res	Type
5	C	249	ASP
5	C	250	THR
5	C	258	ILE
5	C	260	LEU
5	C	264	GLN
5	C	265	MET
5	C	267	GLN
5	C	268	ASP
6	E	3	GLN
6	E	4	GLU
6	E	6	GLU
6	E	9	ILE
6	E	31	THR
6	E	35	VAL
6	E	37	LEU
6	E	38	PRO
6	E	40	GLU
6	E	58	MET
6	E	60	PHE
6	E	61	GLN
6	E	68	SER
6	E	73	PRO
6	E	77	SER
6	E	78	LEU
6	E	87	SER
6	E	92	THR
6	E	94	LYS
6	E	100	ILE
6	E	101	GLN
6	E	105	PHE
6	E	107	THR
6	E	109	ILE
6	E	110	PHE
6	E	117	THR
6	E	121	MET
6	E	122	LYS
6	E	123	LEU
6	E	124	VAL
6	E	127	ILE
6	E	129	PRO
6	E	131	THR
6	E	134	THR

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Mol	Chain	Res	Type
6	E	144	ILE
6	E	145	THR
6	E	146	HIS
6	E	153	HIS
6	E	155	ARG
6	E	156	LEU
6	E	158	SER
6	E	165	LEU
6	E	168	TYR
6	E	169	ARG
6	E	172	GLU
6	E	175	LEU
6	E	180	ARG
6	E	187	TYR
6	E	188	LEU
6	E	190	LEU
6	E	196	VAL
6	E	204	THR
6	E	211	TYR
6	E	212	ARG
6	E	215	MET
7	F	79	ARG
7	F	82	THR
7	F	87	LYS
7	F	90	ARG
7	F	92	ARG
7	F	99	LEU
7	F	104	ASN
7	F	110	ASP
7	F	111	LEU
7	F	115	THR
7	F	119	ARG
7	F	120	ILE
7	F	125	LEU
7	F	133	VAL
7	F	148	VAL
7	F	151	LEU
7	F	155	LEU
8	H	2	SER
8	H	8	ASP
8	H	14	GLU
8	H	15	VAL

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Mol	Chain	Res	Type
8	H	21	ASN
8	H	25	ARG
8	H	27	GLU
8	H	30	SER
8	H	31	THR
8	H	33	GLN
8	H	36	CYS
8	H	37	LYS
8	H	38	LEU
8	H	39	THR
8	H	48	PRO
8	H	49	VAL
8	H	61	SER
8	H	63	LEU
8	H	76	THR
8	H	77	ARG
8	H	82	PRO
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	97	MET
8	H	102	TYR
8	H	103	LYS
8	H	105	GLU
8	H	110	ASP
8	H	112	ILE
8	H	124	ARG
8	H	129	TYR
8	H	130	ARG
8	H	136	LYS
8	H	138	GLU
8	H	142	LEU
8	H	143	LEU
9	I	10	CYS
9	I	12	ASN
9	I	13	MET
9	I	14	LEU
9	I	15	TYR
9	I	16	PRO
9	I	19	ASP
9	I	22	ASN
9	I	24	ARG

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Mol	Chain	Res	Type
9	I	26	LEU
9	I	28	GLU
9	I	29	CYS
9	I	30	ARG
9	I	31	THR
9	I	34	TYR
9	I	42	LEU
9	I	45	ARG
9	I	46	HIS
9	I	55	THR
9	I	83	ASN
9	I	84	VAL
9	I	91	ARG
9	I	101	PHE
9	I	104	LEU
9	I	107	SER
9	I	117	LYS
9	I	118	ARG
9	I	119	THR
9	I	120	GLN
10	J	1	MET
10	J	7	CYS
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	19	GLU
10	J	27	GLU
10	J	28	ASP
10	J	31	ASP
10	J	32	GLU
10	J	36	LEU
10	J	43	ARG
10	J	48	ARG
10	J	51	LEU
10	J	54	VAL
10	J	55	ASP
10	J	60	PHE
10	J	62	ARG
11	K	1	MET
11	K	9	LEU
11	K	17	SER
11	K	34	THR

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Mol	Chain	Res	Type
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	53	ASP
11	K	56	VAL
11	K	61	TYR
11	K	71	PHE
11	K	76	GLN
11	K	81	TYR
11	K	101	LEU
11	K	108	GLU
11	K	111	LEU
11	K	113	THR
11	K	114	LEU
12	L	27	LEU
12	L	28	LYS
12	L	31	CYS
12	L	38	LEU
12	L	40	LEU
12	L	41	SER
12	L	42	ARG
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	4	GLN
3	A	18	GLN
3	A	68	GLN
3	A	71	GLN
3	A	83	HIS
3	A	92	HIS
3	A	169	ASN
3	A	171	GLN
3	A	297	GLN
3	A	306	ASN
3	A	313	GLN

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Mol	Chain	Res	Type
3	A	339	ASN
3	A	358	ASN
3	A	435	HIS
3	A	445	ASN
3	A	471	ASN
3	A	493	GLN
3	A	587	HIS
3	A	631	HIS
3	A	650	GLN
3	A	659	HIS
3	A	660	ASN
3	A	741	ASN
3	A	742	ASN
3	A	745	GLN
3	A	757	ASN
3	A	786	HIS
3	A	858	ASN
3	A	903	ASN
3	A	906	HIS
3	A	926	GLN
3	A	935	GLN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1009	ASN
3	A	1078	GLN
3	A	1110	ASN
3	A	1171	GLN
3	A	1173	HIS
3	A	1278	ASN
3	A	1364	ASN
3	A	1367	HIS
3	A	1390	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	115	GLN
4	B	121	ASN
4	B	206	ASN
4	B	300	HIS
4	B	325	GLN
4	B	366	GLN
4	B	383	ASN

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Mol	Chain	Res	Type
4	B	400	HIS
4	B	415	GLN
4	B	465	ASN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	572	HIS
4	B	657	HIS
4	B	686	ASN
4	B	734	HIS
4	B	740	HIS
4	B	744	HIS
4	B	786	ASN
4	B	794	ASN
4	B	822	ASN
4	B	842	ASN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1065	GLN
4	B	1117	GLN
4	B	1141	HIS
4	B	1161	HIS
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN
5	C	112	ASN
5	C	123	ASN
5	C	131	HIS
5	C	167	HIS
5	C	206	ASN
5	C	242	GLN
5	C	264	GLN
6	E	5	ASN
6	E	99	HIS
6	E	104	ASN
6	E	114	ASN
6	E	147	HIS
8	H	33	GLN
8	H	137	GLN
9	I	12	ASN
9	I	83	ASN

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Mol	Chain	Res	Type
9	I	89	GLN
9	I	116	ASN
11	K	40	HIS
11	K	65	HIS
11	K	96	ASN
12	L	53	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	5	A
1	R	10	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	R	10/10 (100%)	1.37	2 (20%) 1 1	30, 82, 200, 200	0
2	T	14/14 (100%)	1.08	4 (28%) 1 1	30, 107, 200, 200	0
3	A	1395/1733 (80%)	-0.12	25 (1%) 71 57	30, 32, 134, 200	0
4	B	1106/1224 (90%)	-0.20	11 (0%) 84 73	30, 30, 118, 198	0
5	C	266/318 (83%)	-0.31	0 100 100	30, 30, 84, 140	0
6	E	214/215 (99%)	0.31	16 (7%) 17 12	30, 67, 153, 200	0
7	F	84/155 (54%)	-0.05	0 100 100	30, 31, 93, 141	0
8	H	133/146 (91%)	-0.05	3 (2%) 64 49	30, 47, 138, 190	0
9	I	119/122 (97%)	-0.06	0 100 100	30, 32, 114, 163	0
10	J	65/70 (92%)	-0.37	0 100 100	30, 30, 96, 141	0
11	K	114/120 (95%)	-0.33	0 100 100	30, 30, 73, 107	0
12	L	46/70 (65%)	-0.21	1 (2%) 65 50	30, 45, 132, 158	0
All	All	3566/4197 (84%)	-0.13	62 (1%) 73 59	30, 31, 130, 200	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	866	TYR	5.8
3	A	316	GLN	4.9
2	T	1	DA	4.9
3	A	1175	SER	4.6
3	A	149	GLU	4.5
6	E	83	CYS	4.5
3	A	44	THR	4.4
3	A	161	LEU	4.3
4	B	715	ALA	4.1
3	A	1176	LEU	4.0
3	A	183	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
3	A	253	ASN	3.5
3	A	199	LEU	3.3
3	A	256	GLN	3.2
3	A	173	THR	3.2
8	H	86	ASP	3.2
2	T	2	DC	3.2
4	B	869	SER	3.1
8	H	85	GLY	3.0
4	B	433	GLN	3.0
4	B	1189	ILE	3.0
1	R	3	C	2.9
3	A	152	VAL	2.9
1	R	1	A	2.8
4	B	868	MET	2.8
3	A	311	GLN	2.8
6	E	87	SER	2.7
6	E	100	ILE	2.7
3	A	186	LYS	2.7
2	T	3	DG	2.7
3	A	69	THR	2.7
6	E	48	ASP	2.6
3	A	200	ARG	2.6
3	A	1255	GLU	2.6
3	A	56	PRO	2.6
2	T	14	DT	2.5
3	A	121	LEU	2.5
3	A	255	SER	2.5
6	E	127	ILE	2.5
6	E	84	ASP	2.5
4	B	647	GLY	2.5
8	H	83	GLN	2.4
6	E	125	PRO	2.4
3	A	153	PRO	2.4
6	E	122	LYS	2.4
6	E	110	PHE	2.3
3	A	66	LYS	2.3
4	B	865	LYS	2.3
4	B	882	THR	2.3
6	E	93	MET	2.3
3	A	171	GLN	2.2
3	A	254	GLU	2.2
6	E	121	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	250	ILE	2.2
12	L	50	ASP	2.1
6	E	66	GLU	2.1
4	B	134	LYS	2.1
6	E	117	THR	2.1
6	E	49	SER	2.1
6	E	119	SER	2.1
4	B	429	PHE	2.1
6	E	96	PHE	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(Å ²)	Q<0.9
13	ZN	A	1734	1/1	0.84	0.29	-0.48	22,22,22,22	0
13	ZN	I	204	1/1	0.96	0.17	-0.68	22,22,22,22	0
13	ZN	I	203	1/1	0.93	0.21	-0.72	22,22,22,22	0
13	ZN	B	1307	1/1	0.91	0.11	-1.61	22,22,22,22	0
13	ZN	L	105	1/1	0.98	0.06	-1.93	22,22,22,22	0
13	ZN	A	1735	1/1	0.87	0.10	-2.07	22,22,22,22	0
13	ZN	C	319	1/1	0.98	0.06	-2.66	22,22,22,22	0
13	ZN	J	101	1/1	0.94	0.11	-4.98	22,22,22,22	0
14	MG	A	2000	1/1	0.70	0.19	-	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.