



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:17 am BST

PDB ID : 4YFK
Title : Escherichia coli RNA polymerase in complex with squaramide compound 8.
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.;
McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

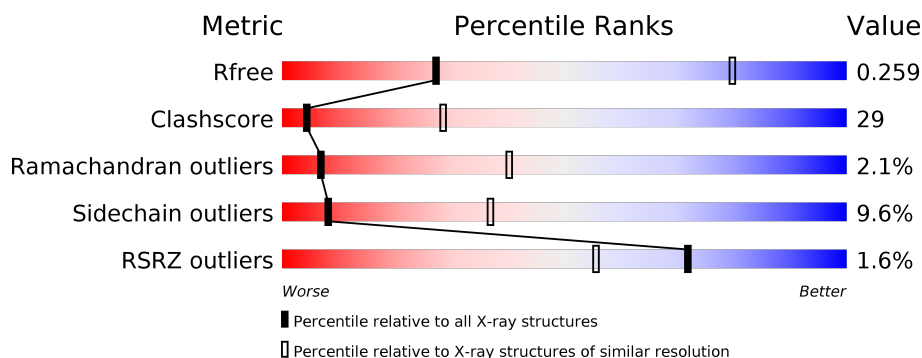
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>2%</div> <div> <div>37%</div> <div>45%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	329	<div> <div>0%</div> <div> <div>30%</div> <div>33%</div> <div>•</div> <div>34%</div> </div> </div>
1	G	329	<div> <div>33%</div> <div>30%</div> <div>6%</div> <div>31%</div> </div>
1	H	329	<div> <div>2%</div> <div> <div>28%</div> <div>34%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>0%</div> <div> <div>48%</div> <div>46%</div> <div>6%</div> </div> </div>
2	I	1342	<div> <div>3%</div> <div> <div>49%</div> <div>45%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>37%40%6%17%</div></div>
3	J	1407	<div><div>%</div><div>39%37%5%18%</div></div>
4	E	91	<div><div></div><div>60%35%. .</div></div>
4	K	91	<div><div>10%</div><div>40%43%.13%</div></div>
5	F	613	<div><div>2%</div><div>38%33%5%24%</div></div>
5	L	613	<div><div>2%</div><div>33%39%5%23%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9050	5690	1620	1694	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8990	5654	1608	1682	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

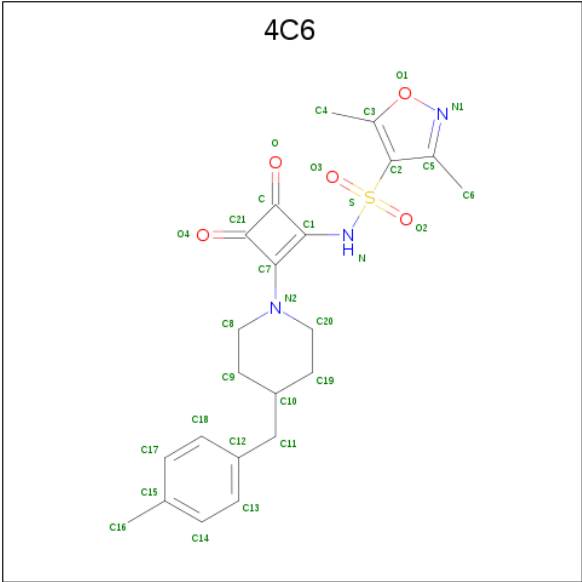
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

- Molecule 8 is 3,5-dimethyl-N-{2-[4-(4-methylbenzyl)piperidin-1-yl]-3,4-dioxocyclobut-1-en-1-yl}-1,2-oxazole-4-sulfonamide (three-letter code: 4C6) (formula: C₂₂H₂₅N₃O₅S).

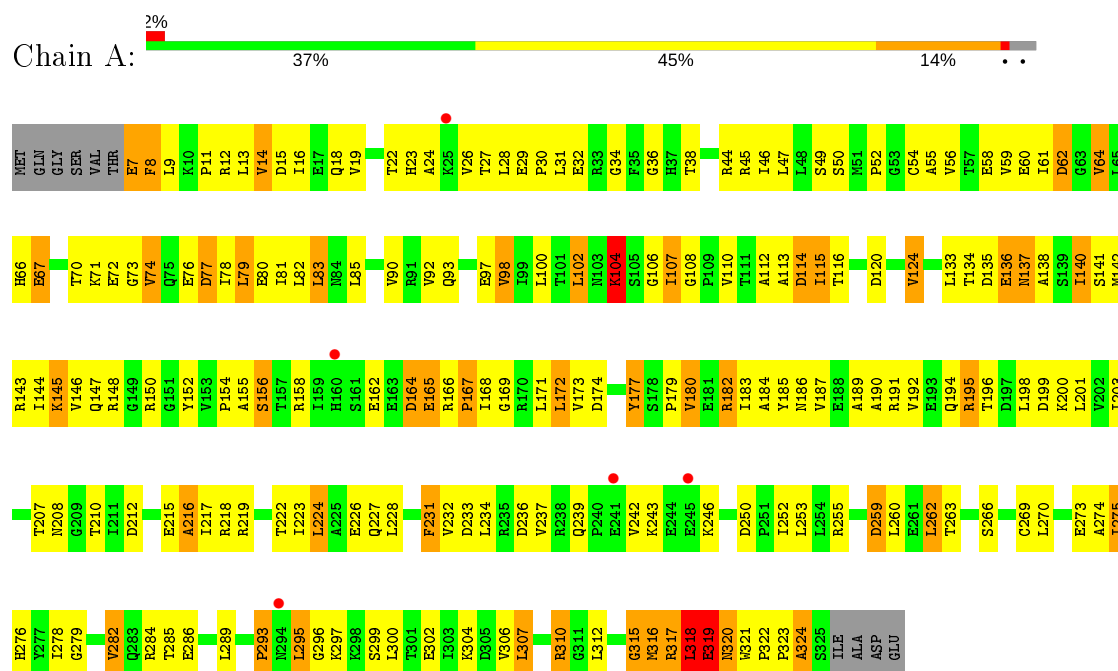


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			31	22	3	5	1		
8	J	1	Total	C	N	O	S	0	0
			31	22	3	5	1		

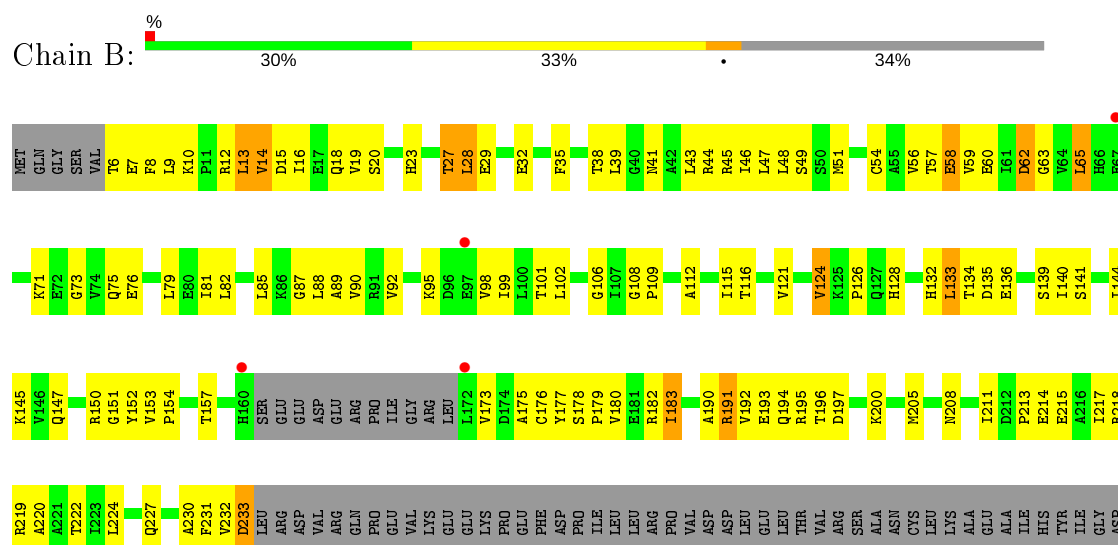
3 Residue-property plots [i](#)

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



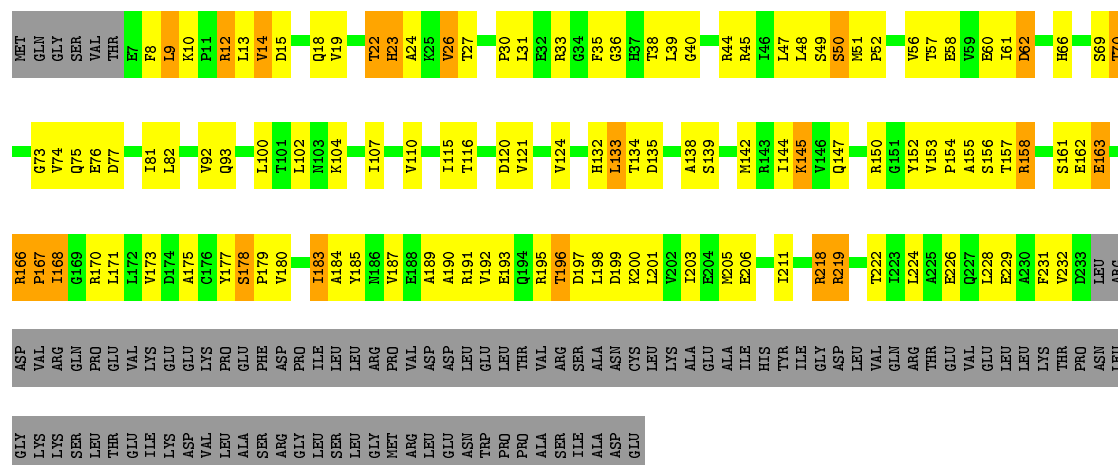
• Molecule 1: DNA-directed RNA polymerase subunit alpha



LEU VAL GLN GLY ARG THR VAL VAL GLU LEU LEU LYS THR PRO ASN LEU GLY LYS LYS SER LEU THR LEU LEU ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU LEU ASN TRP PRO PRO ALA SER ILE ALA ASP GLU

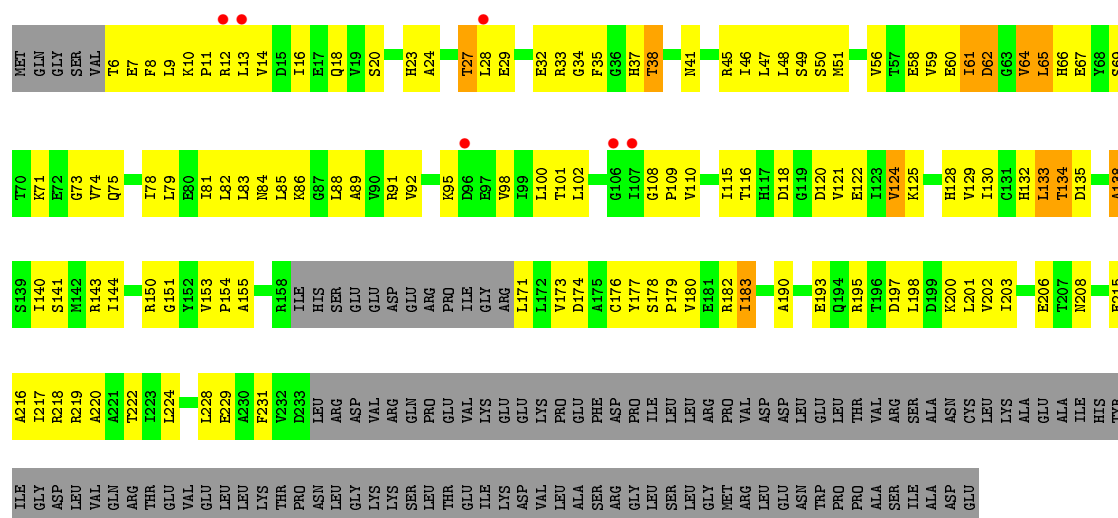
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G: 33% 30% 6% 31%



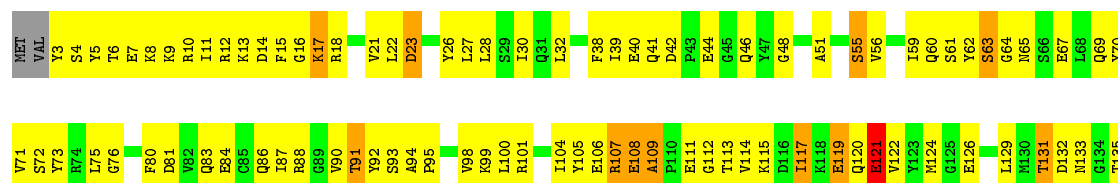
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H: 2% 28% 34% 34%



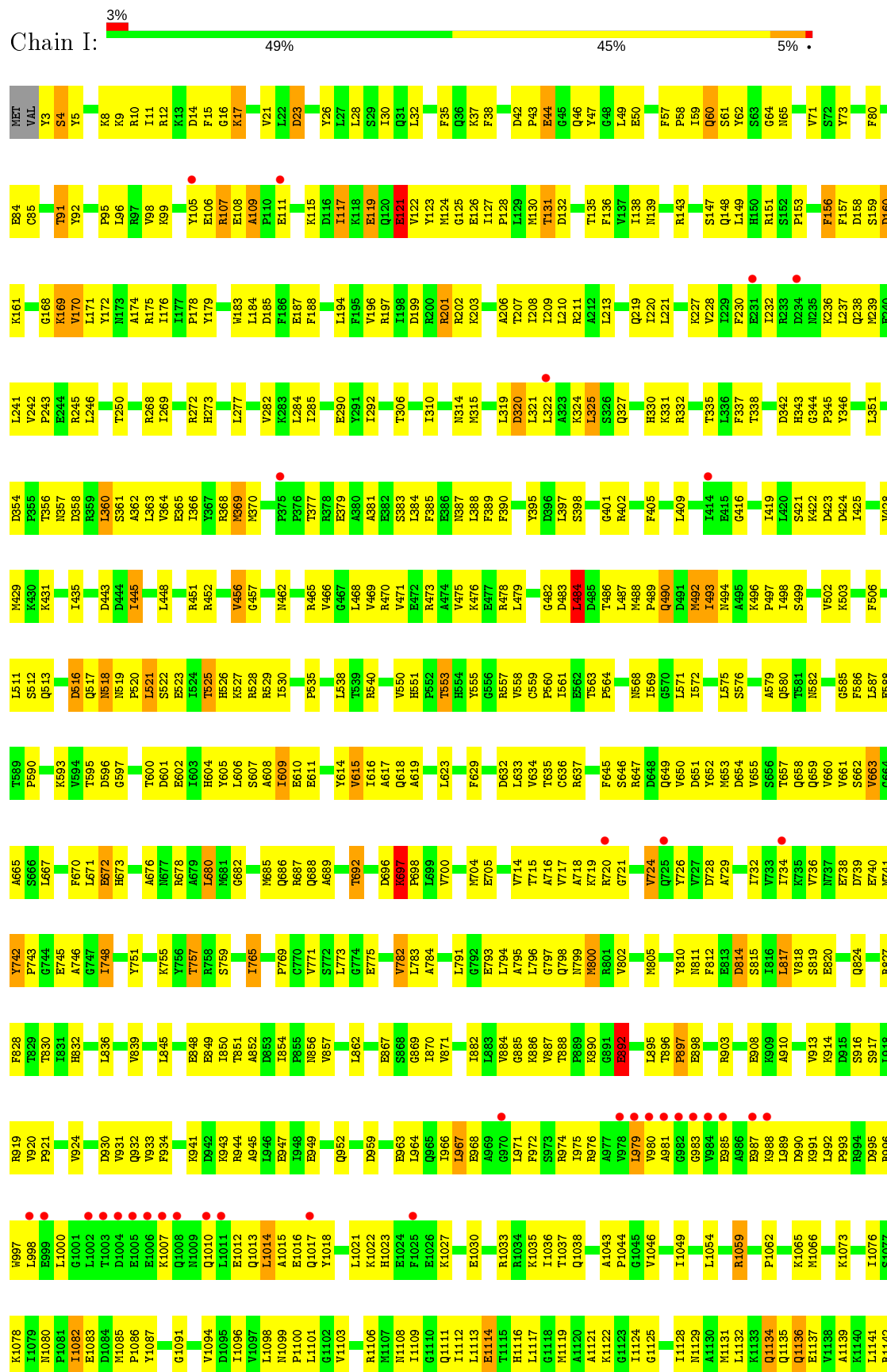
• Molecule 2: DNA-directed RNA polymerase subunit beta

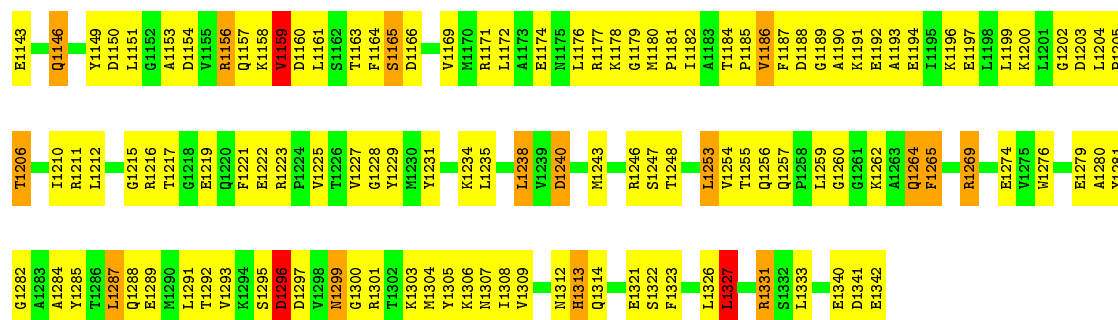
Chain C: 48% 46% 6%



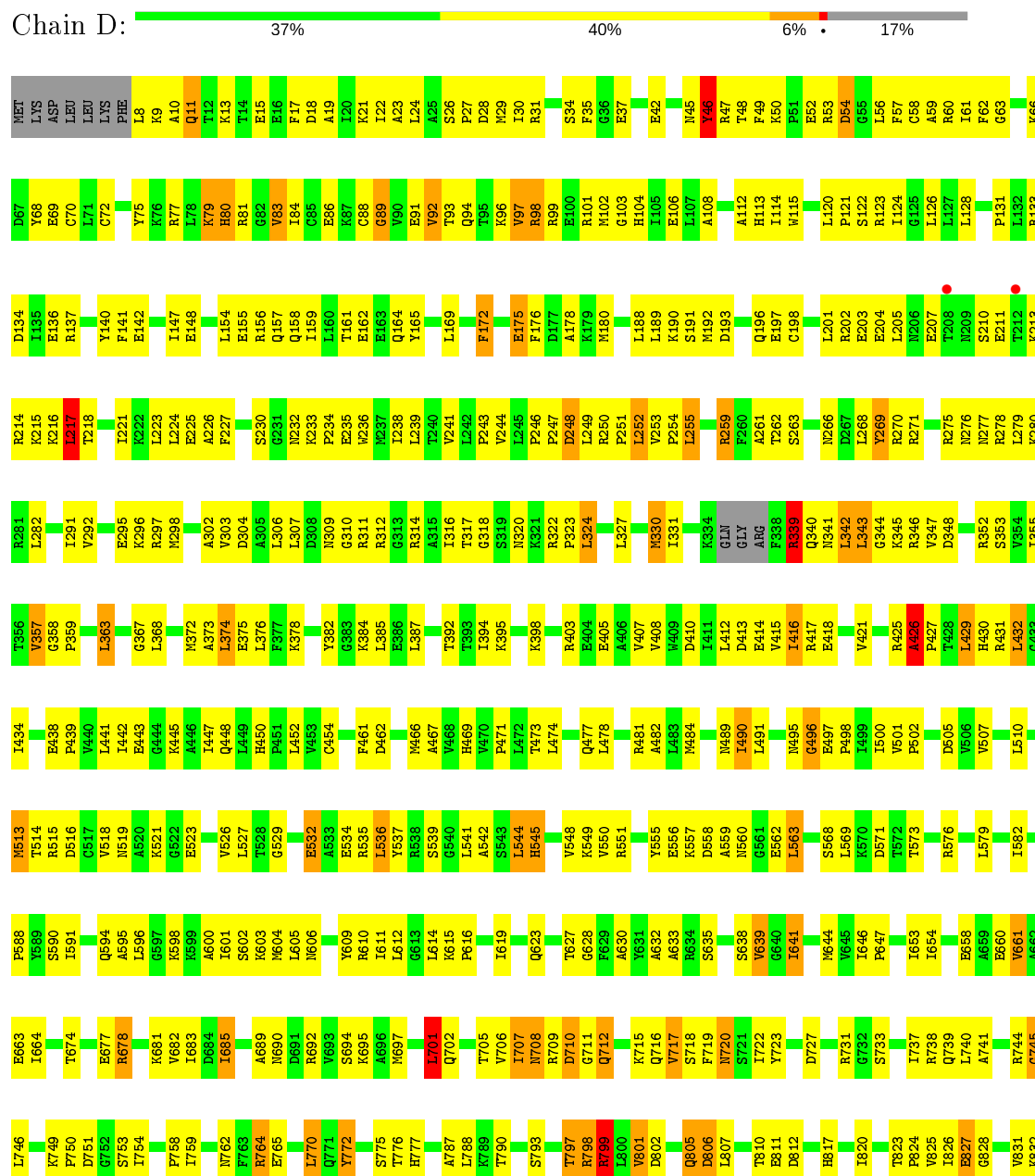
Q1288	L1212	R1142	G1071	E985	Q884	N811	D728	V650	G570	M488	A380	T306	E218	F136
E1289	R1216	Q1146	M1072	A986	L985	D814	A729	D651	L571	P489	A381	T309	Q219	V137
M1290	T1217	Q987	K1073	K988	T986	S730	S730	M652	I572	Q490	E382	L310	I138	I138
L1291	G1218	Y1149	I1076	D989	E988	L817	I732	M653	L575	I493	L384	C311	L221	N139
T1292	E1219	D1150	S1077	K991	E989	V818	V736	V655	N582	M494	Y395	N314	F224	G140
K1294	G1222	L1151	K1078	K991	K900	S819	T737	S656	F586	P497	K404	F316	F225	R143
S1295	R1223	A1152	I1079	L992	L901	Q824	E738	Q658	L587	I498	S403	S318	I229	V146
D1296	G1228	V1155	P1081	R993	L902	D826	E740	Q659	F590	F506	L419	D320	E231	S147
D1297	V1229	R1156	I1082	R994	R903	F828	V742	V660	V591	I591	L420	L322	E231	Q148
G1298	Y1229	Q1157	E1083	Q997	F906	T829	V742	V663	H592	Q510	L420	L322	K236	L149
N1299	M1230	K1158	D1084	L998	A910	H832	A746	V663	H592	Q510	L420	L322	K236	H150
G1300	Y1231	T1159	M1085	L998	A910	H832	A746	V663	H592	Q510	L420	L322	K236	R151
R1301	M1232	V1160	P1086	L1002	V913	H832	A746	V663	H592	Q510	L420	L322	K236	F157
K1303	K1234	L1161	M1090	L1002	V913	H832	A746	V663	H592	Q510	L420	L322	K236	D158
N1307	L1235	S1162	M1090	L1002	V913	H832	A746	V663	H592	Q510	L420	L322	K236	S159
I1308	M1236	T1163	M1090	L1002	V913	H832	A746	V663	H592	Q510	L420	L322	K236	D160
G1311	H1237	F1164	V1094	E1006	S916	A837	G747	V670	V699	Q517	V428	H330	L246	K161
N1312	L1238	S1165	D1095	K1007	S917	C838	E775	E671	T600	N518	V428	H330	L246	H165
H1313	D1240	D1166	I1096	Q1010	L918	V839	E775	E671	T600	N518	V428	H330	L246	G168
Q1314	M1243	V1169	L1098	L1014	P921	S840	E775	E671	T600	N518	V428	H330	L246	K169
P1317	R1246	M1170	M1099	Q1017	V924	I850	E775	E671	T600	N518	V428	H330	L246	V170
G1318	S1247	R1171	P1100	L1021	D930	A852	E775	E671	T600	N518	V428	H330	L246	L171
M1319	T1248	N1175	L1101	L1021	V931	I854	E775	E671	T600	N518	V428	H330	L246	G175
E1320	G1249	G1179	P1104	K1028	D942	I854	E775	E671	T600	N518	V428	H330	L246	I176
S1322	S1250	M1180	S1105	K1031	K943	V857	E775	E671	T600	N518	V428	H330	L246	I177
L1326	I1251	P1181	M1107	K1032	R944	G858	E775	E671	T600	N518	V428	H330	L246	P178
L1327	S1252	I1182	M1108	K1033	A945	A861	E775	E671	T600	N518	V428	H330	L246	S182
R1331	V1254	A1183	I1109	R1034	L946	L862	E775	E671	T600	N518	V428	H330	L246	D185
S1332	T1255	V1186	Q1111	I1036	E949	L865	E775	E671	T600	N518	V428	H330	L246	F188
L1333	Q1256	F1187	I1112	T1037	E950	D866	E775	E671	T600	N518	V428	H330	L246	D189
P1258	L1257	D1188	L1113	Q1038	N951	E867	E775	E671	T600	N518	V428	H330	L246	P190
G1260	G1260	G1189	E1114	Q1038	Q952	G869	E775	E671	T600	N518	V428	H330	L246	N193
Q1264	F1265	K1191	H1116	P1044	L960	I870	E775	E671	T600	N518	V428	H330	L246	L194
G1266	G1267	A1193	G1118	V1046	L960	V871	E775	E671	T600	N518	V428	H330	L246	F195
Q1268	Q1268	E1196	L1117	L1047	E963	G874	E775	E671	T600	N518	V428	H330	L246	V196
R1269	W1276	L1199	A1120	K1048	E963	G874	E775	E671	T600	N518	V428	H330	L246	R197
G1279	E1279	D1202	I1128	R1058	R974	V884	E775	E671	T600	N518	V428	H330	L246	I198
Y1281	Y1281	L1204	M1131	R1059	R975	G885	E775	E671	T600	N518	V428	H330	L246	R201
G1282	G1282	P1205	Q1061	I1060	R976	K886	E775	E671	T600	N518	V428	H330	L246	R202
A1283	S1207	T1206	Q1135	P1062	L979	V888	E775	E671	T600	N518	V428	H330	L246	A206
A1284	G1286	G1286	Q1136	G1063	V980	T888	E775	E671	T600	N518	V428	H330	L246	T207
Y1285	Y1285	Y1285	E1137	D1064	A981	K890	E775	E671	T600	N518	V428	H330	L246	I208
L1287	L1287	L1287	L1141	K1065	G982	E892	E775	E671	T600	N518	V428	H330	L246	I209
				H1070	V984	T993	E775	E671	T600	N518	V428	H330	L246	L210
														R211
														Y215

● Molecule 2: DNA-directed RNA polymerase subunit beta

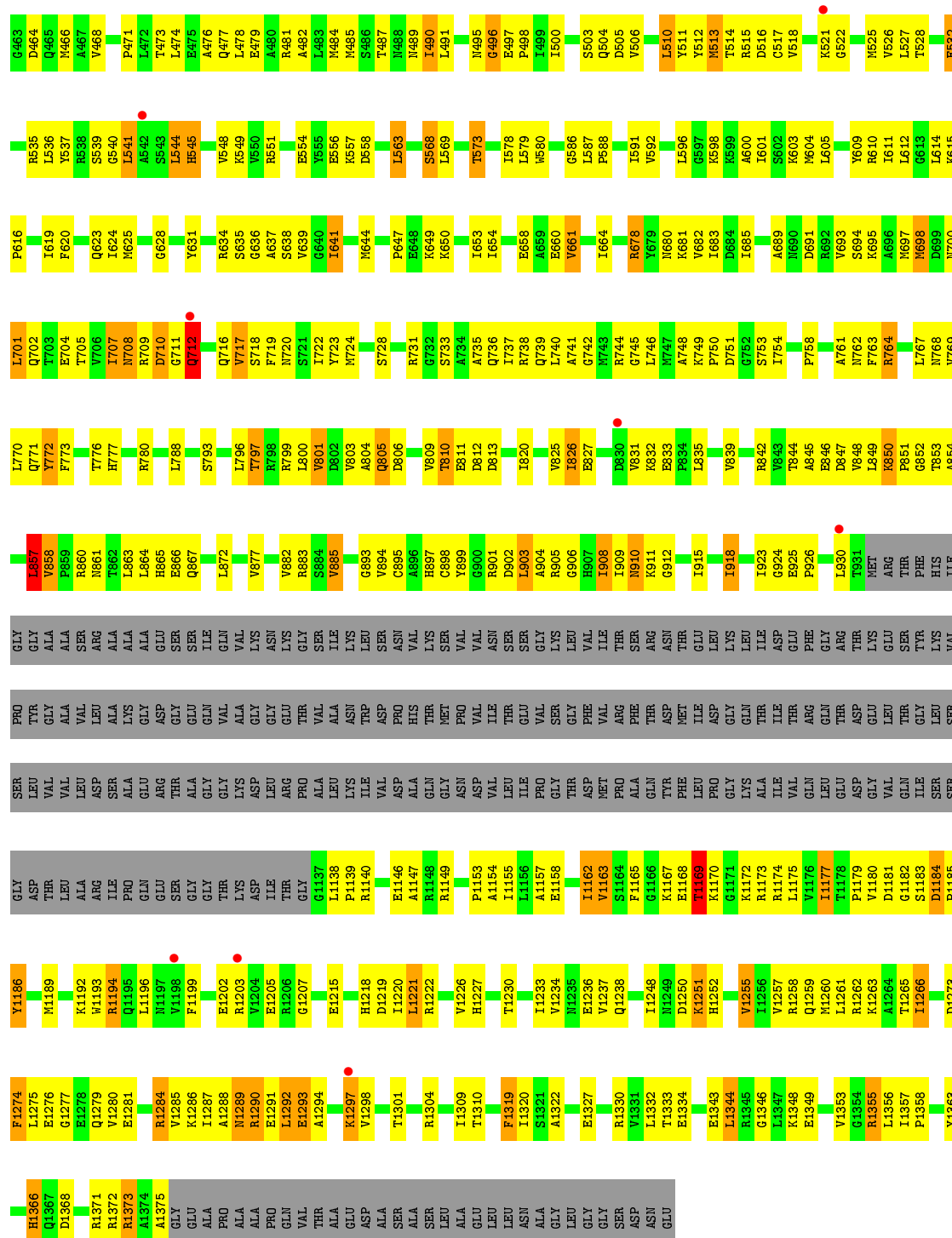




- Molecule 3: DNA-directed RNA polymerase subunit beta'

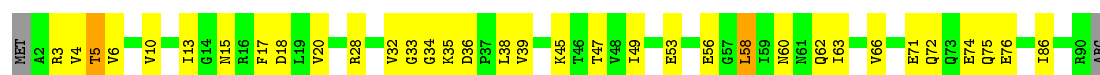




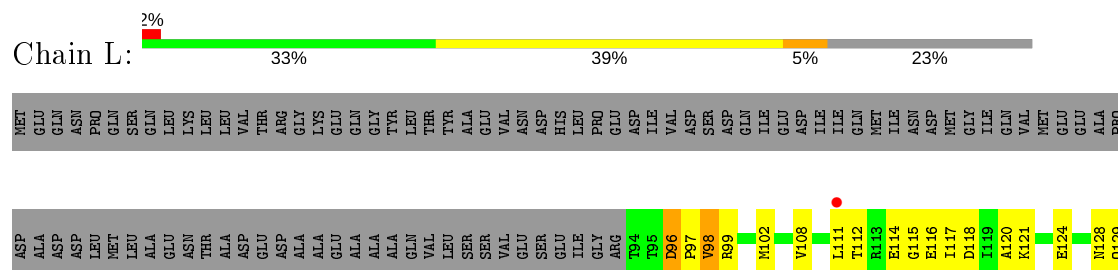
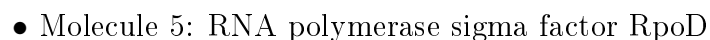
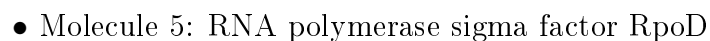


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



- Molecule 4: DNA-directed RNA polymerase subunit omega





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.10Å 206.44Å 307.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.57 31.02 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.96-3.57) 92.3 (31.02-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.252 0.227 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55782	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4C6, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	0/2524	0.91	2/3421 (0.1%)
1	B	0.86	3/1697 (0.2%)	0.97	4/2300 (0.2%)
1	G	0.80	0/1777	0.92	1/2408 (0.0%)
1	H	0.83	1/1681 (0.1%)	0.94	1/2278 (0.0%)
2	C	0.84	1/10739 (0.0%)	0.89	9/14489 (0.1%)
2	I	0.79	2/10735 (0.0%)	0.87	10/14484 (0.1%)
3	D	0.90	6/9188 (0.1%)	0.95	18/12404 (0.1%)
3	J	0.78	2/9128 (0.0%)	0.89	10/12322 (0.1%)
4	E	0.73	0/693	0.75	0/935
4	K	1.03	0/629	0.89	0/847
5	F	0.83	1/3864 (0.0%)	0.87	3/5194 (0.1%)
5	L	0.83	1/3872 (0.0%)	0.83	2/5205 (0.0%)
All	All	0.83	17/56527 (0.0%)	0.90	60/76287 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	4
3	D	0	2
3	J	0	1
5	F	0	1
All	All	0	11

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	799	ARG	CB-CG	-10.16	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	339	ARG	CZ-NH2	8.46	1.44	1.33
3	D	799	ARG	CG-CD	8.42	1.73	1.51
2	I	1296	ASP	CG-OD2	8.26	1.44	1.25
3	D	339	ARG	CB-CG	-8.08	1.30	1.52
3	J	345	LYS	CE-NZ	-6.64	1.32	1.49
3	D	339	ARG	CG-CD	-6.43	1.35	1.51
1	B	233	ASP	CA-CB	6.32	1.67	1.53
1	B	232	VAL	CB-CG1	-6.17	1.39	1.52
1	B	233	ASP	CB-CG	-5.75	1.39	1.51
2	I	1269	ARG	NE-CZ	-5.72	1.25	1.33
1	H	14	VAL	CA-CB	5.28	1.65	1.54
5	L	326	TRP	CB-CG	5.27	1.59	1.50
3	D	827	GLU	CG-CD	5.21	1.59	1.51
5	F	315	TRP	CB-CG	5.16	1.59	1.50
3	J	831	VAL	CA-CB	5.09	1.65	1.54
2	C	1112	ILE	CA-CB	-5.01	1.43	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1269	ARG	NE-CZ-NH1	15.48	128.04	120.30
2	I	1269	ARG	NE-CZ-NH2	-11.03	114.79	120.30
2	I	484	LEU	CA-CB-CG	9.30	136.69	115.30
2	I	1269	ARG	CD-NE-CZ	9.27	136.57	123.60
2	C	1161	LEU	CA-CB-CG	-9.26	94.01	115.30
3	D	799	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	233	ASP	CB-CG-OD2	-9.13	110.08	118.30
3	D	798	ARG	NE-CZ-NH1	8.43	124.51	120.30
3	D	426	ALA	C-N-CD	7.94	145.07	128.40
3	J	1344	LEU	CA-CB-CG	-7.84	97.25	115.30
3	D	799	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	C	1151	LEU	CA-CB-CG	-7.57	97.88	115.30
5	L	530	LEU	CA-CB-CG	7.37	132.24	115.30
2	I	817	LEU	CA-CB-CG	6.71	130.74	115.30
3	D	339	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	28	LEU	CB-CG-CD2	-6.56	99.84	111.00
1	B	65	LEU	CA-CB-CG	6.54	130.34	115.30
3	J	217	LEU	CA-CB-CG	6.28	129.74	115.30
3	D	799	ARG	CB-CG-CD	6.21	127.74	111.60
3	D	860	ARG	NE-CZ-NH1	6.18	123.39	120.30
5	F	486	ARG	NE-CZ-NH1	6.05	123.33	120.30
3	D	701	LEU	CA-CB-CG	6.01	129.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	857	LEU	CA-CB-CG	6.00	129.11	115.30
3	D	432	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	D	799	ARG	CA-CB-CG	5.97	126.54	113.40
2	I	1296	ASP	CB-CG-OD2	5.94	123.64	118.30
3	J	426	ALA	C-N-CD	5.82	140.62	128.40
3	D	217	LEU	CA-CB-CG	5.77	128.58	115.30
3	D	605	LEU	CA-CB-CG	-5.73	102.12	115.30
2	C	1326	LEU	CB-CG-CD2	-5.67	101.37	111.00
2	I	1327	LEU	CB-CG-CD1	-5.63	101.43	111.00
3	D	1347	LEU	CA-CB-CG	5.60	128.18	115.30
3	D	342	LEU	CA-CB-CG	5.55	128.06	115.30
3	D	339	ARG	CB-CA-C	-5.54	99.33	110.40
3	D	911	LYS	CD-CE-NZ	5.53	124.41	111.70
2	C	149	LEU	CB-CG-CD2	-5.52	101.61	111.00
3	J	343	LEU	CB-CG-CD2	5.47	120.30	111.00
3	J	701	LEU	CA-CB-CG	5.47	127.88	115.30
1	H	29	GLU	C-N-CD	-5.47	108.58	120.60
5	F	573	LEU	CA-CB-CG	-5.41	102.86	115.30
5	L	488	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	318	LEU	CA-CB-CG	5.36	127.62	115.30
2	I	1014	LEU	CA-CB-CG	-5.24	103.26	115.30
2	C	484	LEU	CA-CB-CG	5.23	127.33	115.30
2	C	1287	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	224	LEU	CA-CB-CG	-5.19	103.36	115.30
2	C	667	LEU	CB-CG-CD1	-5.17	102.20	111.00
5	F	519	LEU	CB-CG-CD1	-5.17	102.20	111.00
3	J	857	LEU	CA-CB-CG	5.17	127.20	115.30
3	J	1275	LEU	CA-CB-CG	5.16	127.18	115.30
3	D	903	LEU	CA-CB-CG	5.14	127.13	115.30
3	J	541	LEU	CA-CB-CG	5.12	127.08	115.30
3	J	1373	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	C	544	GLY	N-CA-C	-5.09	100.38	113.10
2	I	1295	SER	N-CA-C	5.06	124.66	111.00
3	J	343	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	G	177	TYR	CA-CB-CG	5.04	122.98	113.40
1	B	233	ASP	CB-CG-OD1	5.04	122.84	118.30
2	I	325	LEU	CA-CB-CG	5.01	126.83	115.30
2	C	448	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1264	GLN	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	1264	GLN	Peptide
2	I	1296	ASP	Mainchain
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2542	204	0
1	B	1677	0	1703	105	0
1	G	1755	0	1773	122	0
1	H	1662	0	1687	131	0
2	C	10570	0	10582	606	0
2	I	10566	0	10576	626	0
3	D	9050	0	9218	641	0
3	J	8990	0	9173	595	0
4	E	691	0	695	24	0
4	K	627	0	634	47	0
5	F	3813	0	3880	203	0
5	L	3821	0	3884	244	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	0	25	1	0
8	J	31	0	25	2	0
All	All	55782	0	56397	3255	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 29.

All (3255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.29	1.14
1:A:45:ARG:HG2	1:B:38:THR:HB	1.31	1.12
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.30	1.08
2:I:1269:ARG:HD3	3:J:343:LEU:HD21	1.35	1.08
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.17	1.07
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.33	1.06
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.19	1.05
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.39	1.04
1:G:12:ARG:H	1:G:30:PRO:HD2	1.24	1.02
2:I:17:LYS:HZ1	2:I:1154:ASP:HB3	1.24	1.02
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.40	1.00
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.23	0.99
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.45	0.99
1:A:156:SER:HB3	2:C:1059:ARG:HH22	1.30	0.96
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.47	0.96
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.48	0.95
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.46	0.94
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.49	0.94
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.13	0.94
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.48	0.94
2:C:324:LYS:O	2:C:327:GLN:NE2	1.99	0.93
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.50	0.93
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.49	0.93
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.05	0.92
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.52	0.92
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.47	0.92
1:G:45:ARG:HG2	1:H:38:THR:HB	1.51	0.92
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.49	0.92
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.53	0.91
1:G:187:VAL:HG12	1:G:201:LEU:HD13	1.52	0.90
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.53	0.90
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.07	0.90
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.37	0.90
2:I:148:GLN:NE2	2:I:535:PRO:O	2.04	0.89
3:D:156:ARG:NH2	3:D:191:SER:OG	2.05	0.89
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.55	0.88
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.87	0.88
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.54	0.87
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.08	0.87
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.56	0.87
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.38	0.87
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.55	0.87
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.55	0.86
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.56	0.86
2:I:1269:ARG:CD	3:J:343:LEU:HD21	2.05	0.86
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.58	0.86
2:C:810:TYR:HE1	2:C:1078:LYS:HZ3	1.23	0.86
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.41	0.86
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.41	0.86
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.38	0.86
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.41	0.86
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.57	0.86
1:H:9:LEU:HD12	1:H:195:ARG:HH21	1.41	0.86
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.11	0.86
2:I:1296:ASP:OD2	2:I:1322:SER:N	2.08	0.85
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.58	0.85
1:A:77:ASP:OD1	1:A:77:ASP:N	2.09	0.85
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.10	0.85
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.38	0.85
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.40	0.85
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.38	0.85
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.59	0.85
3:D:339:ARG:HD3	3:D:798:ARG:HH11	1.42	0.84
3:D:418:GLU:HG3	4:E:45:LYS:H	1.40	0.84
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.60	0.84
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.49	0.84
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.58	0.84
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.56	0.84
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.59	0.84
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.58	0.84
1:A:296:GLY:H	1:A:299:SER:HB2	1.43	0.84
1:B:102:LEU:O	1:B:141:SER:HA	1.78	0.83
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.60	0.83
1:A:133:LEU:HD21	1:A:140:ILE:HD11	1.59	0.83
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.59	0.83
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.59	0.83
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.42	0.83
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.12	0.83
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.60	0.82
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.44	0.82
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.60	0.82
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.60	0.82
3:D:425:ARG:HG2	3:D:426:ALA:H	1.42	0.82
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.61	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.25	0.82
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.61	0.82
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.59	0.82
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	1.93	0.82
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.14	0.82
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.13	0.82
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.13	0.82
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.60	0.81
5:L:316:PHE:HZ	5:L:334:SER:HA	1.44	0.81
2:C:703:GLY:N	2:C:705:GLU:OE2	2.11	0.81
3:D:317:THR:HG22	3:D:322:ARG:O	1.81	0.81
2:I:30:ILE:HD12	2:I:30:ILE:H	1.44	0.81
1:G:166:ARG:HH11	1:G:168:ILE:HG12	1.46	0.81
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.63	0.81
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.62	0.80
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.16	0.80
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.61	0.80
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.14	0.80
2:I:17:LYS:NZ	2:I:1154:ASP:HB3	1.96	0.80
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.62	0.80
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.61	0.80
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.28	0.80
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.64	0.80
1:G:229:GLU:HA	1:G:231:PHE:CE2	2.17	0.80
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.64	0.80
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.64	0.80
3:D:339:ARG:HD2	3:D:798:ARG:HD3	1.64	0.79
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.64	0.79
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.28	0.79
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.63	0.79
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.62	0.79
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.64	0.79
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.63	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.64	0.79
2:I:600:THR:HG21	2:I:602:GLU:HG2	1.63	0.78
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.63	0.78
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.64	0.78
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.16	0.78
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.12	0.78
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.17	0.78
1:A:166:ARG:O	1:A:168:ILE:N	2.17	0.78
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.19	0.78
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.16	0.78
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.66	0.78
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.64	0.78
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.66	0.78
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.17	0.78
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.66	0.77
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	1.98	0.77
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.00	0.77
1:H:98:VAL:HG21	1:H:121:VAL:HG23	1.67	0.77
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.49	0.77
5:L:561:MET:HA	5:L:567:MET:HE1	1.65	0.77
5:F:281:ARG:O	5:F:285:ARG:HG3	1.85	0.77
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.65	0.77
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.66	0.77
2:I:227:LYS:O	2:I:245:ARG:NH2	2.18	0.77
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.67	0.76
1:G:218:ARG:NH1	1:H:231:PHE:O	2.18	0.76
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.67	0.76
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.20	0.76
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.66	0.76
2:I:170:VAL:HG21	2:I:172:TYR:CZ	2.20	0.76
1:H:61:ILE:HB	1:H:64:VAL:O	1.85	0.76
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.67	0.76
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.67	0.76
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.14	0.76
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.76
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.67	0.76
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.66	0.76
3:J:425:ARG:HG2	3:J:426:ALA:H	1.51	0.76
3:D:414:GLU:O	4:E:45:LYS:NZ	2.18	0.75
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.68	0.75
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:TYR:HD1	2:C:112:GLY:H	1.31	0.75
3:D:844:THR:OG1	3:D:860:ARG:O	2.02	0.75
2:I:1156:ARG:HH11	2:I:1156:ARG:HB2	1.51	0.75
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.52	0.75
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.21	0.75
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.68	0.75
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.67	0.75
2:I:724:VAL:HG23	2:I:775:GLU:H	1.52	0.75
1:A:92:VAL:O	1:A:148:ARG:NH1	2.18	0.75
3:D:1191:PRO:HB3	3:D:1194:ARG:HH11	1.52	0.75
3:D:1320:ILE:HG23	8:D:2004:4C6:H9	1.68	0.75
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.69	0.75
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.06	0.75
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.68	0.75
5:F:547:VAL:HG13	5:F:598:LEU:HD22	1.69	0.75
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.16	0.75
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.67	0.75
1:H:108:GLY:O	1:H:133:LEU:HB2	1.86	0.74
3:J:128:LEU:HA	3:J:192:MET:HE1	1.69	0.74
1:A:115:ILE:HG22	1:A:116:THR:H	1.52	0.74
3:J:201:LEU:O	3:J:217:LEU:HD11	1.87	0.74
1:A:49:SER:OG	1:A:50:SER:N	2.17	0.74
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.69	0.74
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.18	0.74
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.68	0.74
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.50	0.74
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.23	0.74
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.68	0.74
2:I:892:GLU:OE2	3:J:66:LYS:NZ	2.19	0.74
5:L:281:ARG:O	5:L:285:ARG:HG3	1.88	0.74
1:A:76:GLU:OE2	1:A:76:GLU:N	2.21	0.74
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.69	0.74
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.53	0.74
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.70	0.73
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.52	0.73
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.52	0.73
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.23	0.73
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.68	0.73
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.70	0.73
3:J:846:GLU:HA	3:J:860:ARG:HD2	1.70	0.73
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1281:TYR:CE2	3:D:431:ARG:HB2	2.23	0.73
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.70	0.73
3:D:392:THR:HG21	5:F:606:VAL:HA	1.69	0.73
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.23	0.73
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.24	0.73
2:C:197:ARG:NH1	2:C:201:ARG:O	2.21	0.73
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.70	0.73
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.53	0.73
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.15	0.73
3:J:19:ALA:HB2	3:J:1373:ARG:HH22	1.53	0.73
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.18	0.73
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.69	0.73
2:I:600:THR:HG22	2:I:602:GLU:H	1.53	0.73
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.70	0.73
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.54	0.72
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.19	0.72
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.71	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.21	0.72
3:J:708:ASN:HB3	3:J:712:GLN:O	1.87	0.72
3:D:860:ARG:HB3	3:D:860:ARG:HH11	1.55	0.72
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.54	0.72
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.22	0.72
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.71	0.72
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.52	0.72
1:G:75:GLN:HA	2:I:729:ALA:N	2.05	0.72
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.24	0.72
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.72
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.70	0.72
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.23	0.72
1:H:101:THR:H	1:H:116:THR:HG22	1.54	0.72
1:H:51:MET:HB3	1:H:178:SER:HB2	1.71	0.72
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.53	0.72
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.54	0.72
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.54	0.72
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.72	0.72
2:C:201:ARG:NH2	2:C:370:MET:O	2.21	0.72
1:G:12:ARG:N	1:G:30:PRO:HD2	2.02	0.71
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.72	0.71
1:H:18:GLN:HA	1:H:24:ALA:HA	1.72	0.71
1:A:190:ALA:HB2	1:A:200:LYS:HE3	1.71	0.71
1:A:73:GLY:O	1:A:134:THR:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.71	0.71
3:D:515:ARG:NH2	3:D:717:VAL:O	2.23	0.71
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.73	0.71
5:F:311:THR:HG21	5:F:348:GLU:OE2	1.91	0.71
1:G:61:ILE:HG22	1:G:62:ASP:H	1.55	0.71
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.72	0.71
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.72	0.71
5:F:354:THR:O	5:F:358:VAL:HG23	1.91	0.71
5:F:532:LEU:O	5:F:536:THR:HG23	1.91	0.71
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.24	0.71
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.71	0.71
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.71	0.71
2:I:963:GLU:O	2:I:967:LEU:HB2	1.91	0.71
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.72	0.71
3:D:707:ILE:H	3:D:707:ILE:HD12	1.56	0.71
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.53	0.71
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.72	0.71
1:A:158:ARG:NH2	1:A:172:LEU:HB3	2.05	0.70
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.55	0.70
2:I:123:TYR:OH	2:I:126:GLU:HG3	1.91	0.70
3:J:70:CYS:SG	3:J:71:LEU:N	2.63	0.70
5:L:262:VAL:HG11	5:L:264:LYS:NZ	2.06	0.70
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.73	0.70
2:C:1269:ARG:HD3	3:D:343:LEU:HD11	1.72	0.70
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.07	0.70
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.55	0.70
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.70
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.25	0.70
5:F:320:ILE:HG21	5:F:331:HIS:CE1	2.25	0.70
2:I:499:SER:HA	2:I:502:VAL:HG12	1.74	0.70
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.24	0.70
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.74	0.70
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.72	0.70
3:J:210:SER:O	3:J:214:ARG:HG2	1.91	0.70
3:J:48:THR:O	3:J:50:LYS:N	2.25	0.70
3:D:495:ASN:O	3:D:497:GLU:N	2.23	0.70
2:I:206:ALA:O	2:I:209:ILE:HG22	1.90	0.70
1:A:7:GLU:OE1	1:B:150:ARG:NH1	2.25	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.23	0.70
3:D:805:GLN:O	3:D:807:LEU:N	2.25	0.70
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.72	0.70
5:F:575:GLU:O	5:F:579:GLN:HG2	1.91	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.72	0.70
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.73	0.70
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.25	0.70
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.74	0.69
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.92	0.69
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.72	0.69
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.22	0.69
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.56	0.69
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.74	0.69
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.27	0.69
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.25	0.69
2:C:1269:ARG:CD	3:D:343:LEU:HD11	2.22	0.69
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.74	0.69
3:D:918:ILE:O	3:D:922:SER:OG	2.09	0.69
5:L:386:LEU:O	5:L:389:SER:OG	2.10	0.69
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.74	0.69
3:D:853:THR:HG22	3:D:854:ALA:H	1.56	0.69
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.05	0.69
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.75	0.69
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.73	0.69
2:C:5:TYR:O	2:C:8:LYS:HG2	1.93	0.69
1:G:92:VAL:HA	1:G:120:ASP:O	1.92	0.69
5:L:395:THR:OG1	5:L:396:ASN:N	2.26	0.69
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.75	0.69
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.91	0.69
2:C:615:VAL:HG13	2:C:651:ASP:H	1.58	0.69
2:C:930:ASP:OD2	2:C:931:VAL:N	2.26	0.69
3:D:210:SER:O	3:D:214:ARG:HG2	1.92	0.69
3:D:425:ARG:HG2	3:D:426:ALA:N	2.03	0.69
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.75	0.69
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.57	0.69
1:A:32:GLU:HG2	1:A:198:LEU:HD22	1.75	0.69
1:H:61:ILE:HG12	1:H:171:LEU:HD12	1.75	0.69
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.58	0.69
3:J:259:ARG:HD2	5:L:505:ILE:HD13	1.73	0.69
1:A:113:ALA:O	1:A:115:ILE:N	2.25	0.68
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.73	0.68
2:C:566:GLY:O	2:C:569:ILE:HG13	1.94	0.68
3:D:709:ARG:HD2	3:D:710:ASP:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.75	0.68
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.75	0.68
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.26	0.68
5:F:469:GLN:O	5:F:473:GLU:HB2	1.93	0.68
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.93	0.68
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.07	0.68
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.74	0.68
3:J:902:ASP:OD1	3:J:903:LEU:N	2.26	0.68
1:A:66:HIS:HD2	2:C:874:GLY:HA2	1.59	0.68
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.74	0.68
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.76	0.68
1:H:109:PRO:HA	1:H:132:HIS:HA	1.73	0.68
5:L:233:ASP:O	5:L:236:LYS:HE2	1.93	0.68
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.28	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.76	0.68
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.29	0.68
3:D:1227:HIS:HB2	3:J:1293:GLU:CD	2.14	0.68
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.58	0.68
2:C:1281:TYR:HE2	3:D:431:ARG:HB2	1.59	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.76	0.68
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.76	0.68
3:J:1157:ALA:HB3	3:J:1207:GLY:H	1.59	0.68
1:A:60:GLU:CD	1:A:143:ARG:HH21	1.96	0.67
3:D:75:TYR:HD2	3:D:80:HIS:HD2	1.41	0.67
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.76	0.67
1:H:35:PHE:HA	1:H:38:THR:HG22	1.76	0.67
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.10	0.67
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.75	0.67
2:I:1124:ILE:O	2:I:1128:ILE:HG13	1.94	0.67
3:J:1193:TRP:HB2	3:J:1194:ARG:HH12	1.60	0.67
2:I:871:VAL:O	2:I:944:ARG:NH1	2.27	0.67
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.75	0.67
5:F:163:THR:O	5:F:260:ARG:NH2	2.28	0.67
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.75	0.67
1:A:250:ASP:HA	5:F:605:GLU:HG3	1.77	0.67
2:C:854:ILE:O	2:C:857:VAL:HG22	1.95	0.67
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.76	0.67
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.77	0.67
3:D:339:ARG:HD3	3:D:798:ARG:NH1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.29	0.67
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.77	0.67
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.75	0.67
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.60	0.67
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.28	0.67
4:K:52:ARG:O	4:K:56:GLU:HG2	1.95	0.67
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.77	0.67
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.09	0.67
3:D:515:ARG:O	3:D:545:HIS:HB3	1.94	0.67
1:G:161:SER:O	1:G:163:GLU:N	2.28	0.67
2:I:1197:GLU:HA	2:I:1200:LYS:HD2	1.75	0.67
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.60	0.67
3:J:425:ARG:HG2	3:J:426:ALA:N	2.09	0.67
3:J:797:THR:O	3:J:801:VAL:HG12	1.94	0.67
2:I:1013:GLN:O	2:I:1017:GLN:HG2	1.95	0.66
2:I:998:LEU:HD12	2:I:998:LEU:H	1.59	0.66
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.77	0.66
3:D:510:LEU:O	3:D:514:THR:HG22	1.95	0.66
2:I:499:SER:O	2:I:503:LYS:HB2	1.95	0.66
1:A:31:LEU:HB2	1:A:199:ASP:O	1.95	0.66
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.10	0.66
2:C:303:ASP:HB3	2:C:306:THR:HG23	1.78	0.66
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.77	0.66
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.08	0.66
3:J:45:ASN:HB3	3:J:48:THR:O	1.95	0.66
1:A:135:ASP:O	1:A:138:ALA:N	2.27	0.66
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.77	0.66
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.66
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.77	0.66
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.27	0.66
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.59	0.66
3:J:903:LEU:HB3	3:J:905:ARG:HG3	1.77	0.66
5:L:453:PRO:O	5:L:456:MET:HB2	1.95	0.66
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	1.95	0.66
5:F:276:MET:O	5:F:280:VAL:HG23	1.95	0.66
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.76	0.66
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.31	0.66
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.78	0.66
3:J:853:THR:HG22	3:J:854:ALA:H	1.60	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.77	0.66
5:F:261:LEU:HD12	5:F:261:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4:SER:OG	2:I:5:TYR:N	2.27	0.66
3:J:16:GLU:HG3	3:J:17:PHE:H	1.61	0.66
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.77	0.66
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.77	0.66
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.77	0.66
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.77	0.66
2:C:721:GLY:N	2:C:740:GLU:OE1	2.25	0.66
1:B:196:THR:CG2	3:D:443:GLU:HG3	2.26	0.66
2:I:799:ASN:HB3	2:I:1231:TYR:HD1	1.61	0.66
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.61	0.66
2:C:27:LEU:O	2:C:528:ARG:NH1	2.29	0.65
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.25	0.65
3:J:700:ASN:O	3:J:704:GLU:HB2	1.97	0.65
3:D:594:GLN:HG3	3:D:596:LEU:HD22	1.78	0.65
3:D:709:ARG:HD2	3:D:710:ASP:N	2.11	0.65
5:F:343:LYS:O	5:F:347:ILE:HG13	1.97	0.65
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.76	0.65
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.77	0.65
2:C:1161:LEU:HG	2:C:1161:LEU:O	1.91	0.65
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.11	0.65
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.32	0.65
1:H:69:SER:HB2	1:H:78:ILE:HD11	1.76	0.65
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.78	0.65
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.79	0.65
2:C:1243:MET:HA	3:D:353:SER:HB3	1.78	0.65
2:C:600:THR:HG22	2:C:602:GLU:H	1.61	0.65
2:C:624:ASP:OD1	2:C:625:GLU:N	2.26	0.65
3:J:827:GLU:CB	3:J:832:LYS:HD2	2.27	0.65
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.32	0.65
3:D:709:ARG:O	3:D:711:GLY:N	2.30	0.65
2:C:4:SER:OG	2:C:5:TYR:N	2.30	0.65
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.77	0.65
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.77	0.65
1:H:101:THR:HG22	1:H:116:THR:HB	1.79	0.65
1:H:27:THR:HB	1:H:202:VAL:HG22	1.79	0.65
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.28	0.65
3:J:479:GLU:HG2	4:K:20:VAL:HG11	1.77	0.65
3:J:495:ASN:O	3:J:497:GLU:N	2.30	0.65
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.77	0.65
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.62	0.65
2:C:1017:GLN:O	2:C:1021:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:ILE:HG23	1:H:130:ILE:O	1.97	0.65
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.79	0.65
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.78	0.65
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.31	0.65
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.79	0.65
5:L:343:LYS:O	5:L:347:ILE:HG13	1.96	0.65
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.61	0.65
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.77	0.65
5:F:483:LEU:HD12	5:F:483:LEU:H	1.62	0.65
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.30	0.65
1:G:23:HIS:HB2	1:G:205:MET:O	1.97	0.65
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.78	0.65
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.29	0.65
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.37	0.64
5:F:125:ASP:O	5:F:129:GLN:HG3	1.97	0.64
5:F:466:ILE:CG2	5:F:486:ARG:HG3	2.27	0.64
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.16	0.64
1:H:13:LEU:HA	1:H:28:LEU:HD13	1.79	0.64
1:H:62:ASP:N	1:H:62:ASP:OD1	2.30	0.64
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.30	0.64
3:D:1191:PRO:HB3	3:D:1194:ARG:NH1	2.11	0.64
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	1.96	0.64
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.32	0.64
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.80	0.64
2:I:746:ALA:HA	2:I:974:ARG:HH21	1.62	0.64
1:A:104:LYS:HD3	1:A:114:ASP:OD2	1.98	0.64
2:C:367:TYR:HA	2:C:384:LEU:HD22	1.78	0.64
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.78	0.64
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.98	0.64
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.79	0.64
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.77	0.64
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.64
2:C:40:GLU:HG2	2:C:41:GLN:N	2.12	0.64
1:H:35:PHE:HA	1:H:38:THR:CG2	2.28	0.64
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.79	0.64
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.10	0.64
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.33	0.64
5:L:573:LEU:H	5:L:573:LEU:HD23	1.61	0.64
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.13	0.64
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.80	0.64
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:888:THR:OG1	2:I:914:LYS:HB3	1.97	0.64
2:C:619:ALA:HB1	2:C:657:THR:HA	1.80	0.64
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.29	0.64
5:F:298:PRO:HD2	5:F:326:TRP:CG	2.33	0.64
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.78	0.64
3:J:770:LEU:H	3:J:770:LEU:HD22	1.63	0.64
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.79	0.64
3:D:140:TYR:HB3	5:F:100:MET:SD	2.37	0.64
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.79	0.64
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.80	0.64
3:D:66:LYS:HE2	3:D:69:GLU:OE1	1.97	0.64
5:F:463:LEU:HD21	5:F:487:MET:HG3	1.81	0.64
1:G:45:ARG:NH2	1:H:37:HIS:HB3	2.13	0.64
1:H:9:LEU:HD12	1:H:195:ARG:NH2	2.10	0.64
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.63
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.13	0.63
3:D:327:LEU:HA	3:D:330:MET:HG3	1.81	0.63
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.78	0.63
3:D:60:ARG:HA	3:D:89:GLY:O	1.99	0.63
1:H:102:LEU:O	1:H:141:SER:HA	1.98	0.63
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.33	0.63
2:I:617:ALA:HA	2:I:636:CYS:SG	2.37	0.63
1:B:112:ALA:HA	1:B:115:ILE:HG13	1.80	0.63
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.79	0.63
2:I:705:GLU:HB2	2:I:794:LEU:H	1.62	0.63
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.80	0.63
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.34	0.63
2:I:1065:LYS:HE2	3:J:462:ASP:O	1.98	0.63
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.63	0.63
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.63	0.63
1:A:14:VAL:HG22	1:A:15:ASP:H	1.63	0.63
3:D:1280:VAL:CG2	3:D:1304:ARG:HH21	2.04	0.63
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.34	0.63
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.60	0.63
2:C:510:GLN:NE2	2:C:534:GLY:HA2	2.14	0.63
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.14	0.63
3:J:510:LEU:O	3:J:514:THR:HG22	1.99	0.63
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.81	0.63
3:D:902:ASP:OD1	3:D:903:LEU:N	2.32	0.63
3:J:432:LEU:HD21	3:J:489:ASN:HB3	1.79	0.63
2:C:1255:THR:O	2:C:1257:GLN:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.81	0.63
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.81	0.63
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.79	0.63
5:L:244:THR:O	5:L:247:GLU:HG2	1.99	0.63
1:A:55:ALA:HB3	1:A:177:TYR:HD1	1.61	0.63
2:C:356:THR:HG21	2:C:362:ALA:HA	1.81	0.63
3:D:1179:PRO:HG2	3:D:1183:SER:O	1.99	0.63
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.80	0.63
2:I:857:VAL:HG21	2:I:862:LEU:HD21	1.80	0.63
3:J:102:MET:HE2	3:J:246:PRO:HD3	1.80	0.63
2:C:325:LEU:O	2:C:330:HIS:HB2	1.98	0.62
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.81	0.62
4:E:38:LEU:HB2	4:E:53:GLU:OE1	1.99	0.62
5:F:470:MET:HA	5:F:473:GLU:HB3	1.81	0.62
5:L:245:ALA:O	5:L:249:ILE:HG13	1.99	0.62
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.80	0.62
3:D:491:LEU:HD22	3:D:496:GLY:O	1.99	0.62
3:D:507:VAL:HG11	3:D:598:LYS:HG3	1.81	0.62
3:D:701:LEU:HD12	3:D:723:TYR:HD2	1.64	0.62
2:I:975:ILE:HD13	2:I:998:LEU:HG	1.80	0.62
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.20	0.62
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.11	0.62
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.81	0.62
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.64	0.62
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.80	0.62
2:I:771:VAL:HG21	2:I:783:LEU:HD13	1.82	0.62
3:J:515:ARG:NH2	3:J:717:VAL:O	2.32	0.62
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.81	0.62
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.98	0.62
3:D:271:ARG:HG2	3:D:302:ALA:HB1	1.80	0.62
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.14	0.62
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.35	0.62
5:L:470:MET:O	5:L:478:PRO:HD3	1.99	0.62
1:A:156:SER:HB3	2:C:1059:ARG:NH2	2.08	0.62
1:H:41:ASN:O	1:H:45:ARG:HG3	1.99	0.62
2:I:1192:GLU:O	2:I:1196:LYS:HG2	1.98	0.62
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.30	0.62
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.81	0.62
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.32	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.65	0.62
3:D:432:LEU:HD21	3:D:489:ASN:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:358:ASP:OD2	2:I:361:SER:HB2	2.00	0.62
2:I:498:ILE:H	2:I:498:ILE:HD12	1.65	0.62
3:J:600:ALA:O	3:J:603:LYS:HG2	1.99	0.62
2:C:744:GLY:C	2:C:746:ALA:H	2.03	0.62
3:D:197:GLU:O	3:D:201:LEU:HG	1.99	0.62
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.81	0.62
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.35	0.62
1:A:54:CYS:HA	1:A:148:ARG:HA	1.82	0.62
2:C:138:ILE:O	2:C:139:ASN:ND2	2.33	0.62
2:C:421:SER:H	2:C:424:ASP:HB2	1.64	0.62
1:H:9:LEU:HB3	1:H:32:GLU:HG2	1.81	0.62
2:I:490:GLN:HA	2:I:493:ILE:HG23	1.82	0.62
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.34	0.62
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.82	0.62
5:L:544:THR:HG22	5:L:607:LEU:HD11	1.81	0.62
1:A:145:LYS:HZ2	1:A:147:GLN:HG3	1.64	0.62
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.15	0.62
2:C:377:THR:HB	2:C:380:ALA:H	1.65	0.62
2:C:561:ILE:O	2:C:680:LEU:HD12	2.00	0.62
2:C:796:LEU:HD12	2:C:796:LEU:H	1.64	0.62
3:D:339:ARG:CD	3:D:798:ARG:HD3	2.30	0.62
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.82	0.62
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.82	0.62
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.15	0.62
3:D:248:ASP:O	3:D:251:PRO:HG3	2.00	0.61
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.33	0.61
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.30	0.61
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.80	0.61
1:G:93:GLN:H	1:G:120:ASP:HB3	1.63	0.61
2:I:356:THR:HG21	2:I:362:ALA:HA	1.82	0.61
2:I:560:PRO:O	3:J:780:ARG:NH2	2.32	0.61
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.81	0.61
3:D:203:GLU:O	3:D:207:GLU:HG2	1.99	0.61
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.15	0.61
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.65	0.61
2:I:519:ASN:O	2:I:523:GLU:HG3	1.99	0.61
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.32	0.61
3:D:1344:LEU:O	3:D:1346:GLY:N	2.27	0.61
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.29	0.61
3:D:661:VAL:CG1	3:D:685:ILE:HD11	2.30	0.61
1:G:14:VAL:HG22	1:G:15:ASP:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.83	0.61
2:I:582:ASN:HB3	2:I:586:PHE:H	1.65	0.61
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.31	0.61
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.83	0.61
5:F:311:THR:HB	5:F:345:GLN:HG2	1.81	0.61
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.34	0.61
2:I:232:ILE:HD12	2:I:330:HIS:O	2.00	0.61
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.00	0.61
5:L:515:GLU:HG2	5:L:516:ASP:H	1.66	0.61
2:C:448:LEU:HB2	2:C:553:THR:HB	1.81	0.61
1:G:156:SER:HB2	2:I:1059:ARG:HH22	1.65	0.61
1:H:101:THR:H	1:H:116:THR:CG2	2.14	0.61
2:I:518:ASN:OD1	2:I:518:ASN:N	2.33	0.61
3:D:244:VAL:HA	3:D:269:TYR:OH	2.01	0.61
1:H:151:GLY:O	1:H:177:TYR:HB2	1.99	0.61
2:I:360:LEU:O	2:I:364:VAL:HG23	1.99	0.61
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.82	0.61
3:J:812:ASP:HB2	3:J:911:LYS:HE3	1.83	0.61
5:L:465:ARG:HD2	5:L:468:ARG:HH22	1.65	0.61
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.82	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.66	0.61
2:C:149:LEU:HD12	2:C:452:ARG:O	2.01	0.61
2:C:55:SER:OG	2:C:465:ARG:NH1	2.34	0.61
3:D:632:ALA:O	3:D:635:SER:OG	2.18	0.61
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.83	0.61
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
2:I:596:ASP:CG	2:I:597:GLY:H	2.05	0.61
3:J:514:THR:HG21	3:J:596:LEU:HG	1.82	0.61
5:L:299:LYS:HA	5:L:302:PHE:CB	2.28	0.61
5:L:414:LYS:HD3	5:L:434:TRP:HZ3	1.66	0.61
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.82	0.61
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.83	0.61
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.33	0.61
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.82	0.61
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.15	0.61
5:F:244:THR:O	5:F:247:GLU:HG2	2.00	0.60
5:F:573:LEU:H	5:F:573:LEU:HD23	1.66	0.60
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.82	0.60
3:J:751:ASP:HB3	3:J:753:SER:H	1.66	0.60
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.82	0.60
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:582:ASN:HB3	2:C:586:PHE:H	1.66	0.60
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.22	0.60
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.18	0.60
1:G:8:PHE:O	1:G:9:LEU:HB2	2.00	0.60
2:I:797:GLY:O	2:I:1231:TYR:OH	2.19	0.60
2:I:798:GLN:HB2	2:I:828:PHE:CE1	2.35	0.60
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.16	0.60
3:J:215:LYS:O	3:J:218:THR:HG22	2.01	0.60
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.31	0.60
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.35	0.60
1:H:49:SER:O	1:H:151:GLY:HA2	2.00	0.60
3:J:267:ASP:HA	3:J:270:ARG:HH21	1.66	0.60
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.01	0.60
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.83	0.60
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.00	0.60
3:J:551:ARG:HA	3:J:568:SER:O	2.01	0.60
2:C:1191:LYS:O	2:C:1195:ILE:HG13	1.99	0.60
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.66	0.60
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.83	0.60
5:F:466:ILE:HG23	5:F:486:ARG:HG3	1.83	0.60
2:I:941:LYS:HD3	2:I:949:GLU:OE1	2.01	0.60
5:L:557:LYS:HG3	5:L:561:MET:HE1	1.83	0.60
1:B:73:GLY:CA	1:B:134:THR:HG22	2.27	0.60
2:C:148:GLN:NE2	2:C:533:LEU:O	2.26	0.60
3:D:224:LEU:O	3:D:227:PHE:N	2.34	0.60
3:D:427:PRO:HB2	3:D:429:LEU:HD22	1.84	0.60
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.18	0.60
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.83	0.60
3:J:649:LYS:O	3:J:653:ILE:HG13	2.01	0.60
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.83	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.33	0.60
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.82	0.60
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.17	0.60
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.42	0.60
5:F:130:VAL:HB	5:F:365:MET:HG3	1.83	0.60
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.83	0.60
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.84	0.60
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.02	0.60
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.60
2:I:971:LEU:HD21	2:I:1014:LEU:O	2.02	0.60
3:J:473:THR:HG23	3:J:476:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.01	0.60
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.83	0.60
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.35	0.60
3:D:27:PRO:O	3:D:31:ARG:HG3	2.02	0.60
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.17	0.60
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.67	0.60
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.83	0.60
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.84	0.60
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.32	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.83	0.59
3:D:825:VAL:HG22	3:D:833:GLU:H	1.67	0.59
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.67	0.59
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.83	0.59
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.67	0.59
3:J:405:GLU:O	3:J:408:VAL:HG22	2.02	0.59
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.84	0.59
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.17	0.59
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.14	0.59
1:G:195:ARG:HG3	1:G:198:LEU:HG	1.84	0.59
2:I:169:LYS:O	2:I:170:VAL:HG22	2.02	0.59
2:I:528:ARG:NH2	2:I:576:SER:O	2.35	0.59
2:I:57:PHE:CD1	2:I:58:PRO:HA	2.37	0.59
3:J:619:ILE:O	3:J:623:GLN:HG2	2.03	0.59
5:L:465:ARG:HB3	5:L:468:ARG:HH12	1.67	0.59
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.83	0.59
3:D:421:VAL:CG1	3:D:439:PRO:HG3	2.32	0.59
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.83	0.59
2:I:462:ASN:O	2:I:466:VAL:HG23	2.02	0.59
3:J:1163:VAL:HG21	3:J:1175:LEU:HD21	1.83	0.59
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.84	0.59
1:A:49:SER:HG	1:A:50:SER:HG	1.51	0.59
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.03	0.59
5:F:299:LYS:O	5:F:303:ILE:HG12	2.02	0.59
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.84	0.59
5:L:290:LEU:HD22	5:L:333:VAL:HG21	1.83	0.59
1:A:71:LYS:HD3	1:A:72:GLU:N	2.17	0.59
1:B:47:LEU:O	1:B:180:VAL:HG21	2.02	0.59
2:C:41:GLN:NE2	2:C:73:TYR:O	2.34	0.59
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.59
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.83	0.59
5:L:390:ILE:O	5:L:393:LYS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.59
2:I:12:ARG:NH2	2:I:698:PRO:O	2.27	0.59
3:J:418:GLU:H	4:K:45:LYS:NZ	2.01	0.59
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.84	0.59
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.83	0.59
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.36	0.59
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.64	0.59
2:I:685:MET:HA	2:I:688:GLN:HE21	1.66	0.59
1:A:253:LEU:HA	1:A:278:ILE:HG13	1.85	0.59
2:C:62:TYR:O	2:C:64:GLY:N	2.36	0.59
2:I:384:LEU:O	2:I:388:LEU:HG	2.03	0.59
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.85	0.59
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.36	0.59
3:D:1191:PRO:CB	3:D:1194:ARG:HH11	2.16	0.59
5:F:245:ALA:O	5:F:249:ILE:HG13	2.03	0.59
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.67	0.59
5:L:139:GLU:HG2	5:L:351:THR:HA	1.84	0.59
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.85	0.59
1:A:296:GLY:N	1:A:299:SER:HB2	2.16	0.59
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.03	0.59
2:C:705:GLU:HB2	2:C:794:LEU:H	1.68	0.59
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.84	0.59
3:D:854:ALA:HB2	3:J:1372:ARG:CG	2.33	0.59
2:I:168:GLY:O	2:I:170:VAL:N	2.24	0.59
3:J:735:ALA:O	3:J:739:GLN:HG3	2.03	0.59
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.85	0.59
5:L:320:ILE:HG23	5:L:327:SER:O	2.02	0.59
5:L:348:GLU:HA	5:L:353:LEU:O	2.03	0.59
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.85	0.59
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.58
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.83	0.58
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.38	0.58
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.36	0.58
2:C:486:THR:HG23	2:C:487:LEU:N	2.18	0.58
3:J:733:SER:O	3:J:737:ILE:HG12	2.04	0.58
1:B:35:PHE:HA	1:B:38:THR:HG22	1.84	0.58
3:D:26:SER:HA	3:D:236:TRP:NE1	2.19	0.58
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.84	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE1	1.86	0.58
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.03	0.58
1:A:236:ASP:HA	1:B:14:VAL:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.36	0.58
3:D:678:ARG:O	3:D:682:VAL:HG23	2.03	0.58
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.85	0.58
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.69	0.58
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.85	0.58
3:J:689:ALA:O	3:J:693:VAL:HG23	2.03	0.58
1:B:101:THR:H	1:B:116:THR:CG2	2.15	0.58
2:C:517:GLN:O	2:C:517:GLN:HG2	2.02	0.58
2:C:998:LEU:HD12	2:C:998:LEU:H	1.68	0.58
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.24	0.58
3:D:490:ILE:HA	3:D:500:ILE:CG1	2.33	0.58
5:F:379:MET:O	5:F:383:ASN:ND2	2.37	0.58
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.85	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58
4:K:32:VAL:O	4:K:34:GLY:N	2.34	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.85	0.58
5:L:230:VAL:O	5:L:234:THR:HG23	2.03	0.58
1:B:49:SER:O	1:B:151:GLY:HA2	2.04	0.58
2:C:323:ALA:O	2:C:327:GLN:HG3	2.04	0.58
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.84	0.58
5:F:226:ALA:O	5:F:229:VAL:HG22	2.03	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.85	0.58
3:J:1167:LYS:CE	3:J:1174:ARG:HD2	2.34	0.58
3:J:155:GLU:CB	3:J:158:GLN:HB2	2.25	0.58
2:I:1269:ARG:NE	3:J:343:LEU:HD21	2.17	0.58
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.69	0.58
5:L:561:MET:HA	5:L:567:MET:CE	2.33	0.58
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.85	0.58
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.19	0.58
3:D:48:THR:C	3:D:50:LYS:H	2.06	0.58
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	1.85	0.58
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.34	0.58
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.38	0.58
2:C:643:SER:HG	2:C:645:PHE:HE1	1.52	0.58
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.19	0.58
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.58
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.85	0.58
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.36	0.58
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.34	0.58
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:515:GLU:HG2	5:L:516:ASP:N	2.18	0.58
1:B:101:THR:H	1:B:116:THR:HG21	1.69	0.58
2:C:70:TYR:HA	2:C:100:LEU:HD23	1.85	0.58
2:C:696:ASP:O	2:C:697:LYS:HB3	2.03	0.58
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.38	0.58
3:D:374:LEU:HD23	3:D:412:LEU:HD12	1.85	0.58
3:J:57:PHE:CE1	3:J:252:LEU:HB2	2.38	0.58
3:J:810:THR:HG23	3:J:811:GLU:H	1.69	0.58
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.85	0.58
3:D:161:THR:H	3:D:164:GLN:HB2	1.69	0.58
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.85	0.58
1:H:50:SER:HA	1:H:150:ARG:O	2.04	0.58
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.34	0.58
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.69	0.58
2:I:80:PHE:HZ	2:I:1038:GLN:HE22	1.52	0.58
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.86	0.58
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.04	0.58
2:C:685:MET:HA	2:C:688:GLN:HE21	1.69	0.57
3:D:215:LYS:HE3	3:D:216:LYS:HG3	1.86	0.57
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.85	0.57
1:G:12:ARG:H	1:G:30:PRO:CD	2.09	0.57
5:L:357:GLN:O	5:L:361:ILE:HG13	2.04	0.57
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.84	0.57
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.85	0.57
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.70	0.57
3:D:474:LEU:HA	3:D:477:GLN:HG3	1.85	0.57
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.43	0.57
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.19	0.57
3:D:268:LEU:HG	3:D:324:LEU:HD22	1.86	0.57
3:D:438:GLU:OE2	3:D:481:ARG:NH2	2.28	0.57
3:D:787:ALA:O	3:D:790:THR:HB	2.04	0.57
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.86	0.57
2:I:519:ASN:ND2	2:I:689:ALA:O	2.37	0.57
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.34	0.57
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.40	0.57
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.69	0.57
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.86	0.57
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.86	0.57
3:D:161:THR:HG23	3:D:164:GLN:H	1.69	0.57
3:D:653:ILE:HG23	3:D:692:ARG:CZ	2.35	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.33	0.57
2:I:800:MET:O	2:I:1229:TYR:HA	2.04	0.57
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.85	0.57
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.85	0.57
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.34	0.57
3:D:279:LEU:HD12	3:D:295:GLU:HG3	1.85	0.57
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.35	0.57
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.69	0.57
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.40	0.57
1:A:234:LEU:N	1:B:218:ARG:HH12	2.02	0.57
2:C:1160:ASP:HB2	2:C:1161:LEU:HD12	1.86	0.57
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.68	0.57
1:G:189:ALA:HB1	1:G:191:ARG:CZ	2.35	0.57
1:H:100:LEU:HD23	1:H:116:THR:O	2.05	0.57
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.86	0.57
1:A:71:LYS:HB3	1:A:74:VAL:HG13	1.86	0.57
2:C:211:ARG:NH1	2:C:357:ASN:O	2.38	0.57
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.04	0.57
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.87	0.57
5:F:494:ILE:O	5:F:498:LEU:HB2	2.05	0.57
1:G:47:LEU:O	1:G:180:VAL:HG11	2.04	0.57
1:H:64:VAL:HG12	1:H:66:HIS:H	1.68	0.57
2:I:32:LEU:HD23	2:I:130:MET:SD	2.45	0.57
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.05	0.57
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.28	0.57
5:L:288:MET:HG2	5:L:299:LYS:HE2	1.86	0.57
2:I:5:TYR:O	2:I:8:LYS:HG2	2.04	0.57
3:J:26:SER:HA	3:J:236:TRP:NE1	2.20	0.57
5:L:474:MET:O	5:L:476:ARG:N	2.28	0.57
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.69	0.57
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.39	0.57
5:F:484:ALA:O	5:F:491:GLU:HB2	2.05	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.86	0.57
3:J:147:ILE:HG13	3:J:147:ILE:O	2.05	0.57
3:J:79:LYS:HB2	5:L:569:THR:H	1.70	0.57
5:L:148:TYR:OH	5:L:218:ARG:HA	2.04	0.57
5:L:465:ARG:CD	5:L:468:ARG:HH22	2.18	0.57
3:D:45:ASN:HB3	3:D:48:THR:O	2.04	0.57
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.86	0.57
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.02	0.57
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:O	1:A:108:GLY:N	2.38	0.56
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.85	0.56
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.69	0.56
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.19	0.56
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.20	0.56
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.86	0.56
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.86	0.56
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.45	0.56
2:I:157:PHE:O	2:I:443:ASP:N	2.36	0.56
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.27	0.56
2:I:5:TYR:HD1	2:I:8:LYS:HD3	1.70	0.56
1:A:112:ALA:O	1:A:115:ILE:HG13	2.05	0.56
1:B:35:PHE:HA	1:B:38:THR:CG2	2.35	0.56
2:C:541:GLU:OE1	2:C:541:GLU:N	2.36	0.56
2:C:898:GLU:OE1	2:C:898:GLU:N	2.30	0.56
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.87	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.86	0.56
8:J:2004:4C6:O	8:J:2004:4C6:H20	2.04	0.56
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.68	0.56
5:L:456:MET:O	5:L:460:ILE:HG13	2.05	0.56
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.88	0.56
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.71	0.56
1:G:195:ARG:HD2	1:G:196:THR:H	1.69	0.56
1:H:216:ALA:O	1:H:220:ALA:N	2.37	0.56
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.87	0.56
3:J:522:GLY:O	3:J:525:MET:HG2	2.06	0.56
3:J:749:LYS:HG2	3:J:753:SER:O	2.05	0.56
4:K:54:ILE:HD13	4:K:59:ILE:HG22	1.87	0.56
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.06	0.56
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.87	0.56
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.35	0.56
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.87	0.56
1:G:224:LEU:CD2	1:G:228:LEU:HD22	2.35	0.56
2:I:1269:ARG:HD3	3:J:343:LEU:CD2	2.24	0.56
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.21	0.56
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.05	0.56
3:J:393:THR:HG23	3:J:396:ALA:H	1.71	0.56
2:C:359:ARG:CZ	2:C:363:LEU:HD11	2.36	0.56
2:C:498:ILE:H	2:C:498:ILE:HD12	1.70	0.56
2:C:778:GLU:O	2:C:781:ASP:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:ARG:HB2	2:C:997:TRP:CZ3	2.41	0.56
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.41	0.56
1:H:60:GLU:HG3	1:H:143:ARG:O	2.06	0.56
2:I:1247:SER:HB3	3:J:375:GLU:O	2.05	0.56
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.87	0.56
5:L:277:MET:SD	5:L:359:LYS:HG2	2.46	0.56
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.86	0.56
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.86	0.56
1:H:78:ILE:O	1:H:82:LEU:HG	2.06	0.56
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.88	0.56
2:I:149:LEU:HD12	2:I:452:ARG:O	2.06	0.56
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.87	0.56
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.34	0.56
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.86	0.56
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.51	0.56
1:A:219:ARG:O	1:A:222:THR:HB	2.06	0.56
2:C:486:THR:HG23	2:C:487:LEU:H	1.70	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.56
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.06	0.56
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.21	0.56
3:D:797:THR:O	3:D:801:VAL:HG12	2.05	0.56
1:G:166:ARG:NH1	1:G:168:ILE:HG12	2.19	0.56
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.70	0.56
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.69	0.56
3:J:805:GLN:NE2	3:J:1348:LYS:HD3	2.21	0.56
5:L:314:THR:O	5:L:318:ALA:HB3	2.06	0.56
1:A:318:LEU:O	1:A:320:ASN:N	2.38	0.56
1:B:88:LEU:HD12	1:B:89:ALA:H	1.71	0.56
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.87	0.56
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.41	0.56
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.87	0.56
3:D:1226:VAL:HG21	3:J:1292:LEU:HA	1.86	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.88	0.56
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.88	0.56
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.87	0.56
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.40	0.56
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.30	0.56
2:I:1131:MET:HB3	2:I:1141:LEU:HD11	1.88	0.56
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.06	0.56
2:I:1225:VAL:HG12	3:J:636:GLY:O	2.06	0.56
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.88	0.56
2:C:76:GLY:O	2:C:94:ALA:HB1	2.05	0.56
3:D:619:ILE:O	3:D:623:GLN:HG2	2.05	0.56
5:F:561:MET:HA	5:F:567:MET:HE1	1.86	0.56
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.35	0.56
3:J:1167:LYS:HD3	3:J:1174:ARG:HH11	1.71	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
3:J:844:THR:HG21	3:J:858:VAL:HG21	1.87	0.56
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.21	0.56
1:A:212:ASP:O	1:A:215:GLU:HB3	2.06	0.55
1:B:219:ARG:HA	1:B:222:THR:HB	1.87	0.55
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.87	0.55
3:D:707:ILE:HD12	3:D:707:ILE:N	2.20	0.55
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.87	0.55
5:F:320:ILE:HG23	5:F:327:SER:O	2.05	0.55
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.20	0.55
3:D:210:SER:HB2	3:D:213:LYS:CB	2.32	0.55
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.89	0.55
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.42	0.55
5:F:513:ASP:C	5:F:515:GLU:H	2.09	0.55
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.70	0.55
2:C:1207:SER:C	2:C:1209:GLN:H	2.08	0.55
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.72	0.55
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.88	0.55
2:I:425:ILE:O	2:I:429:MET:HG3	2.05	0.55
3:J:1320:ILE:HG23	8:J:2004:4C6:H9	1.87	0.55
3:J:418:GLU:HG3	4:K:45:LYS:H	1.72	0.55
1:A:194:GLN:OE1	1:A:195:ARG:N	2.40	0.55
1:B:81:ILE:O	1:B:85:LEU:HG	2.05	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.21	0.55
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.89	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55
3:D:810:THR:HG23	3:D:811:GLU:H	1.71	0.55
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.22	0.55
1:H:102:LEU:HD11	1:H:130:ILE:HG21	1.88	0.55
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.22	0.55
5:L:280:VAL:O	5:L:284:GLU:HG3	2.06	0.55
1:A:145:LYS:NZ	1:A:147:GLN:HG3	2.21	0.55
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.86	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:ASP:OD1	2:C:324:LYS:HE3	2.05	0.55
2:C:1281:TYR:HE2	3:D:431:ARG:CB	2.20	0.55
3:D:54:ASP:OD1	3:D:54:ASP:N	2.39	0.55
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.34	0.55
5:L:346:GLN:HA	5:L:349:GLU:OE2	2.07	0.55
1:A:47:LEU:O	1:A:180:VAL:HG11	2.07	0.55
1:A:253:LEU:HA	1:A:278:ILE:CG1	2.37	0.55
1:A:282:VAL:O	1:A:315:GLY:N	2.40	0.55
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.88	0.55
3:D:327:LEU:O	3:D:330:MET:HB2	2.06	0.55
3:D:557:LYS:HA	3:D:563:LEU:HA	1.89	0.55
3:D:638:SER:OG	3:D:639:VAL:N	2.39	0.55
5:F:465:ARG:CD	5:F:468:ARG:HH22	2.20	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
2:I:431:LYS:O	2:I:435:ILE:HG13	2.07	0.55
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.47	0.55
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.88	0.55
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.22	0.55
3:J:598:LYS:O	3:J:601:ILE:HG22	2.06	0.55
5:L:340:ALA:HA	5:L:343:LYS:HZ3	1.72	0.55
2:C:9:LYS:HD2	2:C:791:LEU:HD11	1.89	0.55
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.05	0.55
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.87	0.55
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.07	0.55
5:F:230:VAL:O	5:F:234:THR:HG23	2.05	0.55
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.40	0.55
5:F:372:ALA:O	5:F:376:LYS:HG3	2.07	0.55
3:J:1140:ARG:HH21	3:J:1236:GLU:HG3	1.71	0.55
3:J:580:TRP:HH2	3:J:587:LEU:O	1.89	0.55
3:J:638:SER:OG	3:J:639:VAL:N	2.39	0.55
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.72	0.55
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.36	0.55
3:D:1193:TRP:HB2	3:D:1194:ARG:CZ	2.37	0.55
3:D:799:ARG:HG2	3:D:1309:ILE:HD12	1.89	0.55
3:D:161:THR:CG2	3:D:164:GLN:H	2.20	0.55
3:D:102:MET:HE2	3:D:246:PRO:HD3	1.89	0.55
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.72	0.55
1:G:190:ALA:CB	1:G:200:LYS:HB2	2.20	0.55
1:H:134:THR:HG23	1:H:135:ASP:H	1.70	0.55
2:I:888:THR:HG23	2:I:916:SER:OG	2.07	0.55
3:J:197:GLU:O	3:J:201:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.15	0.55
4:K:62:GLN:O	4:K:66:VAL:HG23	2.07	0.55
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.87	0.55
1:B:12:ARG:O	1:B:13:LEU:HB3	2.06	0.55
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	0.55
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.89	0.55
3:D:535:ARG:O	3:D:539:SER:OG	2.24	0.55
3:D:514:THR:O	3:D:595:ALA:HA	2.07	0.55
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.40	0.55
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.40	0.55
5:F:137:TYR:O	5:F:141:ILE:HG12	2.06	0.55
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.55
2:I:715:THR:HG23	2:I:717:VAL:HG23	1.89	0.55
2:I:715:THR:OG1	2:I:782:VAL:HG12	2.06	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.22	0.55
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.89	0.55
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.22	0.55
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.89	0.55
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.42	0.55
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.88	0.55
2:C:494:ASN:HB3	2:C:497:PRO:HG2	1.89	0.54
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.88	0.54
5:F:143:TYR:CE2	5:F:147:GLN:HG3	2.43	0.54
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.07	0.54
2:C:1142:ARG:NH1	2:C:1165:SER:HA	2.15	0.54
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.07	0.54
3:J:1262:ARG:HD2	3:J:1279:GLN:NE2	2.21	0.54
5:L:470:MET:HA	5:L:473:GLU:HB3	1.88	0.54
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.88	0.54
5:F:400:GLN:HB2	5:F:403:ASP:OD2	2.07	0.54
1:G:76:GLU:OE1	1:G:132:HIS:N	2.36	0.54
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.72	0.54
2:I:971:LEU:HD22	2:I:1018:TYR:CD1	2.43	0.54
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.42	0.54
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.88	0.54
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.89	0.54
3:J:517:CYS:HA	3:J:716:GLN:NE2	2.21	0.54
3:D:79:LYS:HE3	3:D:80:HIS:HA	1.90	0.54
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.89	0.54
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.54
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1167:LYS:HD3	3:J:1174:ARG:NH1	2.22	0.54
1:A:133:LEU:HD11	1:A:140:ILE:HG12	1.89	0.54
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.90	0.54
3:D:848:VAL:O	3:D:857:LEU:HD12	2.08	0.54
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.43	0.54
5:F:343:LYS:H	5:F:343:LYS:HD2	1.72	0.54
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.90	0.54
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.89	0.54
2:I:896:THR:HB	2:I:897:PRO:HD2	1.89	0.54
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.90	0.54
3:J:694:SER:O	3:J:698:MET:HB2	2.07	0.54
5:L:511:ILE:HG13	5:L:512:GLY:H	1.73	0.54
1:B:92:VAL:CG1	1:B:95:LYS:HB3	2.37	0.54
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.22	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.40	0.54
1:G:10:LYS:NZ	1:H:229:GLU:OE1	2.36	0.54
1:H:65:LEU:HD22	1:H:171:LEU:HD21	1.89	0.54
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.89	0.54
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.22	0.54
3:J:850:LYS:HB2	3:J:852:GLY:O	2.07	0.54
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.23	0.54
5:L:577:GLY:O	5:L:581:ASP:N	2.40	0.54
1:A:124:VAL:HG11	1:A:210:THR:HG23	1.89	0.54
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.72	0.54
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.89	0.54
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.90	0.54
3:D:560:ASN:ND2	3:D:560:ASN:O	2.40	0.54
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.08	0.54
3:J:279:LEU:HD12	3:J:295:GLU:HG3	1.89	0.54
3:J:793:SER:O	3:J:797:THR:HG23	2.08	0.54
4:K:71:GLU:O	4:K:75:GLN:HG3	2.08	0.54
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.90	0.54
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.89	0.54
3:D:48:THR:HB	3:D:50:LYS:HG3	1.90	0.54
2:I:131:THR:HG22	2:I:132:ASP:H	1.71	0.54
2:I:930:ASP:OD2	2:I:931:VAL:N	2.40	0.54
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.89	0.54
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.90	0.54
1:A:135:ASP:O	1:A:137:ASN:N	2.41	0.54
3:D:903:LEU:HB3	3:D:905:ARG:H	1.71	0.54
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:122:SER:O	3:J:126:LEU:HG	2.07	0.54
2:I:1305:TYR:CD2	5:L:531:PRO:HB2	2.43	0.54
1:A:137:ASN:N	1:A:137:ASN:OD1	2.41	0.54
1:A:310:ARG:HA	1:A:310:ARG:NE	2.23	0.54
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.89	0.54
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.43	0.54
3:D:871:LEU:HA	3:D:874:GLU:HG3	1.89	0.54
2:I:1131:MET:HB3	2:I:1141:LEU:CD1	2.37	0.54
2:I:389:PHE:HD1	2:I:395:TYR:HE1	1.54	0.54
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.43	0.54
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.43	0.54
3:J:1167:LYS:HZ3	3:J:1170:LYS:HB2	1.71	0.54
2:C:759:SER:OG	2:C:763:THR:N	2.41	0.53
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	1.89	0.53
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.90	0.53
1:H:37:HIS:CD2	2:I:1216:ARG:HD2	2.43	0.53
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.43	0.53
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.42	0.53
5:F:225:ARG:O	5:F:229:VAL:HG13	2.08	0.53
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.43	0.53
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.42	0.53
2:C:1236:ASN:HB2	2:C:1238:LEU:HD11	1.90	0.53
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.43	0.53
2:C:976:ARG:HB2	2:C:997:TRP:HZ3	1.73	0.53
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.91	0.53
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.38	0.53
1:G:39:LEU:HD21	1:H:224:LEU:HD11	1.89	0.53
2:I:615:VAL:HG13	2:I:651:ASP:H	1.72	0.53
3:J:697:MET:HG3	3:J:698:MET:N	2.23	0.53
3:J:647:PRO:HG3	3:J:697:MET:N	2.23	0.53
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.42	0.53
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.89	0.53
3:D:223:LEU:O	3:D:226:ALA:HB3	2.09	0.53
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.91	0.53
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.88	0.53
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.09	0.53
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.91	0.53
3:J:363:LEU:HD21	3:J:487:THR:HG22	1.90	0.53
2:C:1192:GLU:OE2	3:D:764:ARG:HD3	2.09	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.53
1:H:182:ARG:HD3	1:H:206:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ASP:HB3	1:H:141:SER:O	2.08	0.53
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.44	0.53
5:L:377:LYS:O	5:L:381:GLU:HG3	2.09	0.53
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.91	0.53
1:A:263:THR:HG22	1:A:302:GLU:HG2	1.89	0.53
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.90	0.53
3:D:54:ASP:HB2	3:D:61:ILE:HD11	1.90	0.53
5:F:395:THR:OG1	5:F:396:ASN:N	2.42	0.53
2:I:1243:MET:HA	3:J:353:SER:HB3	1.90	0.53
3:J:773:PHE:O	3:J:776:THR:HB	2.09	0.53
5:L:306:PHE:CE1	5:L:310:GLU:HG3	2.44	0.53
1:A:319:GLU:O	1:A:320:ASN:HB2	2.08	0.53
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.09	0.53
3:D:751:ASP:HB3	3:D:753:SER:H	1.73	0.53
5:F:233:ASP:O	5:F:236:LYS:HE2	2.07	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.53
1:H:215:GLU:OE1	1:H:219:ARG:NH1	2.41	0.53
1:G:156:SER:HB2	2:I:1059:ARG:NH2	2.24	0.53
3:J:322:ARG:HB2	3:J:322:ARG:HH11	1.72	0.53
3:J:720:ASN:OD1	3:J:722:ILE:HG22	2.09	0.53
3:J:845:ALA:O	3:J:860:ARG:NE	2.40	0.53
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.43	0.53
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.91	0.53
2:C:425:ILE:O	2:C:429:MET:HG3	2.09	0.53
3:D:500:ILE:O	3:D:500:ILE:HG22	2.08	0.53
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.26	0.53
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.09	0.53
1:H:82:LEU:O	1:H:86:LYS:HG3	2.09	0.53
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.39	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.91	0.53
3:J:660:GLU:O	3:J:664:ILE:HG12	2.08	0.53
3:J:709:ARG:HD2	3:J:710:ASP:N	2.24	0.53
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.89	0.53
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.91	0.53
3:D:211:GLU:O	3:D:215:LYS:HB3	2.08	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.08	0.53
5:F:166:VAL:HG23	5:F:258:GLN:O	2.09	0.53
1:G:154:PRO:HG2	1:G:157:THR:OG1	2.08	0.53
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.22	0.53
1:H:98:VAL:HG11	1:H:121:VAL:CG2	2.39	0.53
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:588:PRO:O	3:J:591:ILE:HG22	2.09	0.53
3:J:761:ALA:H	3:J:771:GLN:HE22	1.56	0.53
3:J:903:LEU:HD22	3:J:909:ILE:HD12	1.91	0.53
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.90	0.53
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.53
2:C:150:HIS:CE1	2:C:454:ARG:HE	2.27	0.53
2:C:720:ARG:CZ	2:C:736:VAL:HG21	2.38	0.53
5:F:316:PHE:HZ	5:F:334:SER:HA	1.74	0.53
1:G:195:ARG:CG	1:G:198:LEU:HG	2.38	0.53
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.91	0.53
2:I:692:THR:OG1	2:I:827:ARG:O	2.27	0.53
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.90	0.53
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.08	0.53
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.53
3:J:903:LEU:HB3	3:J:905:ARG:H	1.74	0.53
3:D:600:ALA:O	3:D:603:LYS:HG2	2.09	0.52
3:D:733:SER:O	3:D:737:ILE:HG12	2.09	0.52
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.74	0.52
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.90	0.52
2:I:1238:LEU:H	2:I:1238:LEU:HD12	1.74	0.52
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.23	0.52
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.08	0.52
3:J:156:ARG:HH12	3:J:157:GLN:NE2	2.07	0.52
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.91	0.52
3:J:537:TYR:CZ	3:J:544:LEU:HD22	2.44	0.52
3:J:872:LEU:O	3:J:877:VAL:HG12	2.09	0.52
5:L:419:PHE:HD1	5:L:430:TYR:CD2	2.27	0.52
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.74	0.52
2:C:98:VAL:O	2:C:121:GLU:HA	2.08	0.52
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.44	0.52
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.91	0.52
3:D:705:THR:OG1	3:D:718:SER:HA	2.09	0.52
1:G:60:GLU:HB2	1:G:170:ARG:CG	2.39	0.52
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.09	0.52
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.29	0.52
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.52
3:J:903:LEU:CB	3:J:905:ARG:HG3	2.39	0.52
1:A:190:ALA:CB	1:A:200:LYS:HB2	2.39	0.52
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.38	0.52
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.92	0.52
2:C:565:GLU:HG2	2:C:565:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.44	0.52
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.35	0.52
3:D:706:VAL:HG12	3:D:715:LYS:HB2	1.91	0.52
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.92	0.52
1:G:76:GLU:OE2	1:G:76:GLU:N	2.42	0.52
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.24	0.52
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.10	0.52
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.73	0.52
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.91	0.52
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.92	0.52
1:A:44:ARG:NH2	2:C:1091:GLY:O	2.42	0.52
3:D:347:VAL:HG12	3:D:348:ASP:O	2.09	0.52
3:D:529:GLY:HA2	3:D:551:ARG:O	2.09	0.52
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.91	0.52
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.90	0.52
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.90	0.52
5:F:557:LYS:O	5:F:561:MET:HB2	2.09	0.52
1:H:92:VAL:HG13	1:H:120:ASP:O	2.10	0.52
2:I:517:GLN:O	2:I:517:GLN:HG2	2.09	0.52
2:I:521:LEU:O	2:I:525:THR:HB	2.09	0.52
3:J:436:ALA:HB3	3:J:485:MET:HA	1.91	0.52
5:L:460:ILE:O	5:L:463:LEU:HB2	2.10	0.52
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.52
5:L:608:ARG:O	5:L:611:LEU:N	2.30	0.52
1:A:102:LEU:HD23	1:A:115:ILE:HA	1.91	0.52
1:A:73:GLY:HA2	2:C:726:TYR:OH	2.10	0.52
2:C:466:VAL:O	2:C:470:ARG:HG2	2.09	0.52
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.45	0.52
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.90	0.52
1:G:36:GLY:C	1:G:187:VAL:HG11	2.30	0.52
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.91	0.52
2:I:143:ARG:NH2	2:I:512:SER:O	2.42	0.52
3:J:363:LEU:HG	3:J:363:LEU:O	2.10	0.52
2:C:169:LYS:HE2	2:C:190:PRO:O	2.09	0.52
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.93	0.52
3:D:1160:SER:HA	3:D:1204:VAL:O	2.10	0.52
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.34	0.52
3:D:490:ILE:HA	3:D:500:ILE:HG12	1.91	0.52
3:D:84:ILE:HG22	3:D:91:GLU:HB3	1.90	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.91	0.52
2:I:159:SER:O	2:I:160:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.23	0.52
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.74	0.52
3:J:1168:GLU:O	3:J:1170:LYS:N	2.43	0.52
3:J:266:ASN:O	3:J:270:ARG:HB2	2.10	0.52
1:A:233:ASP:O	1:A:234:LEU:HG	2.09	0.52
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.92	0.52
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	1.90	0.52
3:D:772:TYR:O	3:D:775:SER:HB3	2.10	0.52
4:E:60:ASN:OD1	4:E:63:ILE:HD13	2.09	0.52
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.37	0.52
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.23	0.52
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.91	0.52
2:I:320:ASP:OD1	2:I:324:LYS:HE3	2.08	0.52
2:I:796:LEU:H	2:I:796:LEU:HD12	1.74	0.52
3:J:1265:THR:HG22	3:J:1277:GLY:CA	2.34	0.52
5:L:288:MET:HA	5:L:302:PHE:CZ	2.45	0.52
2:I:908:GLU:OE1	5:L:611:LEU:HD22	2.09	0.52
1:A:195:ARG:HG2	1:A:198:LEU:HD11	1.91	0.52
1:B:56:VAL:HG11	1:B:144:ILE:HD11	1.92	0.52
2:C:637:ARG:HA	2:C:642:SER:HA	1.92	0.52
2:C:667:LEU:CD2	2:C:704:MET:HB2	2.40	0.52
5:F:354:THR:OG1	5:F:356:GLU:HB3	2.10	0.52
2:I:158:ASP:OD1	2:I:159:SER:N	2.42	0.52
2:I:721:GLY:N	2:I:740:GLU:OE1	2.38	0.52
2:I:757:THR:O	2:I:765:ILE:HG23	2.10	0.52
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.10	0.52
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.52
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.52
2:C:182:SER:O	2:C:395:TYR:HE1	1.93	0.52
2:C:550:VAL:HG11	3:D:776:THR:CG2	2.39	0.52
1:A:66:HIS:CD2	2:C:874:GLY:HA2	2.44	0.52
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.52
5:F:569:THR:OG1	5:F:570:ASP:N	2.43	0.52
3:J:1344:LEU:O	3:J:1346:GLY:N	2.40	0.52
3:J:611:ILE:HB	3:J:612:LEU:HD12	1.92	0.52
3:J:705:THR:OG1	3:J:718:SER:HA	2.10	0.52
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.90	0.52
5:L:261:LEU:HD12	5:L:261:LEU:H	1.75	0.52
5:L:262:VAL:HG11	5:L:264:LYS:HZ1	1.72	0.52
5:L:421:TYR:CE2	5:L:422:ARG:HG3	2.44	0.52
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.73	0.52
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.25	0.52
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.92	0.52
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.20	0.52
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.92	0.52
2:C:635:THR:HG23	2:C:644:LEU:HD22	1.92	0.52
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.91	0.52
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.92	0.52
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.91	0.52
2:I:1082:ILE:HD12	2:I:1082:ILE:H	1.75	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:CA	2.40	0.52
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.25	0.52
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.42	0.52
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.91	0.52
3:J:48:THR:C	3:J:50:LYS:H	2.13	0.52
4:K:49:ILE:O	4:K:53:GLU:HG3	2.10	0.52
5:L:313:ASP:CG	5:L:338:HIS:HE2	2.13	0.52
1:B:75:GLN:HG2	1:B:76:GLU:OE1	2.10	0.51
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.90	0.51
3:D:227:PHE:O	3:D:230:SER:HB3	2.10	0.51
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.35	0.51
3:D:537:TYR:CE2	3:D:544:LEU:HD22	2.45	0.51
3:D:598:LYS:O	3:D:601:ILE:HG22	2.09	0.51
3:D:825:VAL:C	3:D:826:ILE:HG13	2.30	0.51
5:F:348:GLU:HA	5:F:353:LEU:O	2.10	0.51
5:F:465:ARG:HA	5:F:468:ARG:NH2	2.24	0.51
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.25	0.51
2:I:362:ALA:O	2:I:366:ILE:HG13	2.10	0.51
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.91	0.51
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.45	0.51
5:L:135:ALA:HB1	5:L:253:SER:HB3	1.91	0.51
1:A:55:ALA:HB3	1:A:177:TYR:CD1	2.44	0.51
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.43	0.51
1:B:99:ILE:HD12	1:B:145:LYS:HB2	1.90	0.51
1:B:151:GLY:O	1:B:177:TYR:HB2	2.10	0.51
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.92	0.51
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.10	0.51
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.92	0.51
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.25	0.51
3:J:1149:ARG:NH2	3:J:1153:PRO:HG2	2.26	0.51
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:419:HIS:HB2	4:K:45:LYS:HE2	1.92	0.51
3:J:503:SER:H	3:J:506:VAL:HG11	1.75	0.51
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.45	0.51
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.11	0.51
2:C:1247:SER:HB3	3:D:375:GLU:O	2.10	0.51
5:F:471:LEU:HD23	5:F:476:ARG:O	2.09	0.51
1:G:13:LEU:H	1:G:13:LEU:HD23	1.74	0.51
1:H:73:GLY:CA	1:H:134:THR:HG22	2.33	0.51
2:I:277:LEU:HD23	2:I:282:VAL:HG21	1.92	0.51
2:I:228:VAL:HB	2:I:335:THR:OG1	2.11	0.51
2:I:448:LEU:HB2	2:I:553:THR:HB	1.93	0.51
1:A:187:VAL:O	1:A:187:VAL:HG23	2.10	0.51
1:A:218:ARG:HG3	1:B:231:PHE:O	2.09	0.51
1:A:134:THR:HG23	2:C:726:TYR:CE1	2.45	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.92	0.51
5:F:325:PRO:HG2	5:F:326:TRP:CD1	2.45	0.51
1:G:197:ASP:O	1:G:198:LEU:HD23	2.09	0.51
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.46	0.51
2:I:468:LEU:O	2:I:471:VAL:HG12	2.09	0.51
3:J:1349:GLU:O	3:J:1353:VAL:HG12	2.11	0.51
3:J:412:LEU:O	3:J:415:VAL:HG22	2.09	0.51
3:J:697:MET:O	3:J:701:LEU:N	2.32	0.51
3:J:825:VAL:CG1	3:J:833:GLU:HB3	2.40	0.51
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.45	0.51
5:L:121:LYS:O	5:L:124:GLU:HB2	2.11	0.51
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.74	0.51
2:C:1269:ARG:HG2	3:D:343:LEU:HD11	1.93	0.51
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.17	0.51
5:F:426:LYS:HD3	5:F:428:SER:HB2	1.93	0.51
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.92	0.51
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.41	0.51
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.26	0.51
2:I:696:ASP:O	2:I:697:LYS:HB3	2.09	0.51
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.93	0.51
3:J:1170:LYS:C	3:J:1172:LYS:H	2.13	0.51
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.25	0.51
3:J:102:MET:CE	3:J:246:PRO:HD3	2.41	0.51
5:L:372:ALA:O	5:L:376:LYS:HG3	2.11	0.51
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.93	0.51
2:C:1006:GLU:O	2:C:1010:GLN:N	2.44	0.51
2:C:106:GLU:O	2:C:109:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1134:GLN:O	2:C:1135:GLN:HG2	2.09	0.51
2:C:147:SER:OG	2:C:455:SER:HB3	2.10	0.51
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.41	0.51
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.10	0.51
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.11	0.51
3:D:102:MET:CE	3:D:246:PRO:HD3	2.40	0.51
1:G:219:ARG:HA	1:G:222:THR:HB	1.92	0.51
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.41	0.51
2:C:268:ARG:HD2	2:C:270:THR:CG2	2.40	0.51
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.11	0.51
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.92	0.51
3:D:432:LEU:HD21	3:D:489:ASN:CB	2.40	0.51
2:I:1174:GLU:O	2:I:1177:ARG:HG2	2.11	0.51
2:I:494:ASN:HB3	2:I:497:PRO:HG2	1.91	0.51
2:I:582:ASN:HB3	2:I:586:PHE:N	2.25	0.51
3:J:680:ASN:O	3:J:683:ILE:HG22	2.09	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.46	0.51
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.44	0.51
3:D:266:ASN:O	3:D:270:ARG:HB2	2.10	0.51
3:D:702:GLN:HG3	3:D:723:TYR:OH	2.09	0.51
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.92	0.51
2:I:1012:GLU:O	2:I:1016:GLU:HG3	2.10	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.46	0.51
5:L:247:GLU:O	5:L:251:LYS:HG3	2.10	0.51
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.93	0.51
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.11	0.51
3:J:420:PRO:O	3:J:471:PRO:HD2	2.11	0.51
3:J:615:LYS:HE2	3:J:616:PRO:HD3	1.92	0.51
3:J:857:LEU:HD13	3:J:858:VAL:HG13	1.92	0.51
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.93	0.51
2:C:42:ASP:O	2:C:44:GLU:N	2.36	0.51
2:C:882:ILE:HD12	2:C:882:ILE:H	1.76	0.51
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.93	0.51
1:G:56:VAL:HG21	1:G:144:ILE:HG23	1.91	0.51
2:I:1158:LYS:HG3	2:I:1159:VAL:N	2.25	0.51
3:J:557:LYS:HA	3:J:563:LEU:HA	1.93	0.51
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.26	0.51
1:A:228:LEU:O	1:A:231:PHE:N	2.42	0.50
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.10	0.50
1:A:318:LEU:HD23	1:A:321:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.26	0.50
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.46	0.50
2:C:4:SER:HB3	2:C:7:GLU:CG	2.34	0.50
2:C:600:THR:HG22	2:C:601:ASP:N	2.26	0.50
2:C:987:GLU:O	2:C:991:LYS:HE3	2.10	0.50
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.43	0.50
3:D:147:ILE:HG13	3:D:147:ILE:O	2.11	0.50
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.50
2:I:168:GLY:C	2:I:170:VAL:H	2.13	0.50
2:I:465:ARG:O	2:I:469:VAL:HG13	2.11	0.50
2:I:561:ILE:HD11	2:I:665:ALA:HB1	1.93	0.50
4:K:59:ILE:HG23	4:K:64:LEU:HD21	1.93	0.50
5:L:124:GLU:O	5:L:128:ASN:HB2	2.11	0.50
1:A:152:TYR:CE2	1:A:154:PRO:HB3	2.46	0.50
2:C:802:VAL:CG2	2:C:1098:LEU:HD22	2.41	0.50
3:D:1227:HIS:HA	3:D:1230:THR:CG2	2.39	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:847:ASP:HB3	3:D:859:PRO:HA	1.94	0.50
5:F:572:THR:HG23	5:F:575:GLU:HG3	1.94	0.50
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.76	0.50
2:I:557:ARG:NH2	2:I:608:ALA:HA	2.26	0.50
2:I:959:ASP:O	2:I:963:GLU:HG2	2.11	0.50
3:J:1280:VAL:O	3:J:1284:ARG:N	2.37	0.50
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.92	0.50
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.74	0.50
1:A:12:ARG:H	1:A:30:PRO:HD2	1.76	0.50
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.44	0.50
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.26	0.50
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.93	0.50
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.92	0.50
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.11	0.50
3:D:11:GLN:HE21	3:D:15:GLU:CD	2.15	0.50
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.50
3:D:45:ASN:O	3:D:46:TYR:HD2	1.94	0.50
5:F:142:THR:O	5:F:146:GLU:HG3	2.12	0.50
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.46	0.50
3:J:277:ASN:HA	3:J:280:LYS:HG3	1.92	0.50
3:J:923:ILE:O	3:J:926:PRO:HD2	2.11	0.50
3:D:793:SER:O	3:D:797:THR:HG23	2.10	0.50
5:F:585:GLU:O	5:F:589:GLN:HG3	2.11	0.50
2:I:486:THR:HG23	2:I:487:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:998:LEU:HD12	2:I:998:LEU:N	2.26	0.50
3:J:514:THR:HG21	3:J:596:LEU:HB2	1.94	0.50
5:L:234:THR:O	5:L:245:ALA:HB2	2.11	0.50
5:L:347:ILE:HB	5:L:355:ILE:HD11	1.93	0.50
2:C:93:SER:OG	2:C:126:GLU:OE1	2.26	0.50
3:D:261:ALA:HA	5:F:505:ILE:H	1.76	0.50
3:D:702:GLN:O	3:D:718:SER:N	2.37	0.50
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.41	0.50
3:D:849:LEU:CB	3:D:853:THR:HG23	2.41	0.50
1:H:51:MET:HB3	1:H:178:SER:CB	2.41	0.50
2:I:156:PHE:CZ	2:I:158:ASP:HB2	2.47	0.50
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.26	0.50
5:L:551:LEU:CD2	5:L:597:LYS:HD2	2.41	0.50
1:A:113:ALA:C	1:A:115:ILE:H	2.14	0.50
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.76	0.50
2:C:60:GLN:O	2:C:476:LYS:HE2	2.11	0.50
2:C:886:LYS:HB3	2:C:917:SER:HA	1.93	0.50
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.12	0.50
3:D:21:LYS:NZ	3:D:23:ALA:HB2	2.26	0.50
3:D:80:HIS:CB	3:D:83:VAL:HG11	2.41	0.50
3:D:849:LEU:HA	3:D:855:ASP:O	2.10	0.50
2:I:607:SER:OG	2:I:609:ILE:HG13	2.12	0.50
3:J:761:ALA:H	3:J:771:GLN:NE2	2.09	0.50
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.93	0.50
5:L:108:VAL:HG11	5:L:381:GLU:O	2.11	0.50
1:A:71:LYS:HD3	1:A:72:GLU:H	1.76	0.50
2:C:345:PRO:O	2:C:349:GLU:HG2	2.12	0.50
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.77	0.50
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.24	0.50
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.92	0.50
3:D:697:MET:SD	3:D:741:ALA:HB3	2.51	0.50
3:D:770:LEU:HD22	3:D:770:LEU:H	1.77	0.50
5:F:414:LYS:O	5:F:417:ASP:N	2.43	0.50
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.41	0.50
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.93	0.50
1:H:88:LEU:HD21	1:H:115:ILE:HD11	1.92	0.50
2:I:250:THR:HA	2:I:268:ARG:HA	1.94	0.50
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.93	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.76	0.50
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.94	0.50
1:A:274:ALA:O	1:A:275:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.93	0.50
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.77	0.50
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.47	0.50
2:C:884:VAL:HG21	2:C:1050:VAL:HB	1.93	0.50
2:C:897:PRO:HB2	2:C:898:GLU:OE1	2.12	0.50
3:D:1353:VAL:HG13	3:D:1355:ARG:HG2	1.94	0.50
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.94	0.50
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.27	0.50
5:F:606:VAL:O	5:F:609:SER:OG	2.30	0.50
1:G:47:LEU:HB3	1:G:183:ILE:HD13	1.94	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.93	0.50
2:I:494:ASN:OD1	5:L:471:LEU:HD13	2.11	0.50
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.57	0.50
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.93	0.50
1:A:250:ASP:CB	5:F:601:PRO:HB3	2.42	0.49
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.94	0.49
5:F:134:VAL:HG13	5:F:273:MET:HE3	1.93	0.49
5:F:298:PRO:HD2	5:F:326:TRP:CD1	2.48	0.49
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.27	0.49
2:I:1129:ASN:CB	2:I:1177:ARG:HB2	2.41	0.49
2:I:1156:ARG:NH1	2:I:1156:ARG:HB2	2.23	0.49
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.12	0.49
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.38	0.49
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.42	0.49
3:J:905:ARG:CZ	3:J:910:ASN:HD21	2.25	0.49
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.47	0.49
2:C:303:ASP:HB3	2:C:306:THR:CG2	2.42	0.49
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.12	0.49
4:E:72:GLN:O	4:E:76:GLU:HG3	2.12	0.49
1:G:45:ARG:CD	2:I:1083:GLU:HB3	2.42	0.49
2:I:138:ILE:O	2:I:139:ASN:ND2	2.44	0.49
3:J:515:ARG:O	3:J:545:HIS:HB3	2.12	0.49
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.77	0.49
4:K:3:ARG:NE	4:K:3:ARG:HA	2.27	0.49
5:L:341:LEU:CD2	5:L:344:LEU:HD23	2.42	0.49
1:A:295:LEU:HD23	1:A:299:SER:HB2	1.94	0.49
2:C:104:ILE:O	2:C:113:THR:HA	2.11	0.49
3:D:1359:ALA:O	3:D:1363:TYR:N	2.44	0.49
3:D:647:PRO:HG3	3:D:697:MET:CB	2.42	0.49
3:D:660:GLU:O	3:D:663:GLU:HB2	2.11	0.49
3:D:901:ARG:HA	3:D:908:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.77	0.49
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.48	0.49
3:D:1299:GLY:HA2	3:J:1301:THR:CG2	2.42	0.49
3:J:156:ARG:HH12	3:J:157:GLN:HE21	1.59	0.49
3:J:825:VAL:HG22	3:J:833:GLU:H	1.78	0.49
5:L:289:LYS:HG2	5:L:293:GLU:OE1	2.13	0.49
5:L:574:GLU:N	5:L:574:GLU:OE1	2.45	0.49
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.94	0.49
3:D:292:VAL:O	3:D:296:LYS:HG3	2.12	0.49
3:J:363:LEU:HB2	3:J:450:HIS:CE1	2.48	0.49
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.41	0.49
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.94	0.49
5:L:379:MET:HG2	5:L:416:VAL:HG22	1.94	0.49
2:C:1268:GLN:HE22	3:D:352:ARG:NE	2.10	0.49
2:C:696:ASP:CB	2:C:798:GLN:HG2	2.32	0.49
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.45	0.49
2:I:26:TYR:OH	2:I:28:LEU:HD12	2.13	0.49
2:I:933:VAL:HG11	2:I:945:ALA:HB2	1.94	0.49
2:I:96:LEU:HD23	2:I:124:MET:HG3	1.93	0.49
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.11	0.49
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.28	0.49
2:C:617:ALA:HA	2:C:636:CYS:SG	2.52	0.49
3:D:1167:LYS:CD	3:D:1174:ARG:HD2	2.41	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.12	0.49
3:D:161:THR:HG22	3:D:164:GLN:CB	2.41	0.49
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.95	0.49
3:D:849:LEU:HD22	3:D:849:LEU:H	1.77	0.49
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.11	0.49
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.95	0.49
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.34	0.49
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.76	0.49
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.94	0.49
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.12	0.49
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.28	0.49
2:C:122:VAL:CG1	2:C:493:ILE:HD13	2.42	0.49
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.94	0.49
2:C:292:ILE:HG22	2:C:317:LEU:HB2	1.94	0.49
2:C:448:LEU:HA	2:C:448:LEU:HD23	1.57	0.49
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.93	0.49
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.46	0.49
3:J:290:ILE:HD12	3:J:290:ILE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.39	0.49
5:L:325:PRO:HG2	5:L:326:TRP:CD1	2.47	0.49
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.42	0.49
1:B:115:ILE:HG22	1:B:116:THR:N	2.28	0.49
2:C:1131:MET:HE2	2:C:1141:LEU:HA	1.94	0.49
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.48	0.49
2:C:891:GLY:O	2:C:892:GLU:HG3	2.13	0.49
5:F:326:TRP:O	5:F:330:LEU:HG	2.12	0.49
5:F:390:ILE:HD12	5:F:435:ILE:HG21	1.95	0.49
1:H:56:VAL:HG21	1:H:144:ILE:HD11	1.94	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
2:I:619:ALA:HB1	2:I:657:THR:HA	1.94	0.49
2:I:698:PRO:HA	2:I:1231:TYR:CD1	2.48	0.49
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.77	0.49
3:J:16:GLU:HG3	3:J:17:PHE:CD2	2.45	0.49
3:J:56:LEU:H	3:J:56:LEU:HD12	1.78	0.49
1:A:59:VAL:HG21	1:A:85:LEU:HD12	1.95	0.49
1:B:108:GLY:O	1:B:133:LEU:HB2	2.12	0.49
2:C:1246:ARG:NH1	2:C:1249:GLY:HA3	2.27	0.49
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.63	0.49
2:I:60:GLN:O	2:I:476:LYS:HE2	2.12	0.49
3:J:901:ARG:HA	3:J:908:ILE:HA	1.94	0.49
5:L:262:VAL:HG11	5:L:264:LYS:HZ2	1.75	0.49
5:L:469:GLN:O	5:L:473:GLU:HB2	2.13	0.49
5:L:585:GLU:HA	5:L:588:ARG:HD2	1.95	0.49
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.12	0.49
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.95	0.49
2:C:421:SER:N	2:C:424:ASP:OD2	2.45	0.49
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.43	0.49
5:F:465:ARG:HA	5:F:468:ARG:CZ	2.42	0.49
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.13	0.49
2:I:848:GLU:CG	2:I:888:THR:HG22	2.43	0.49
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.39	0.49
3:J:358:GLY:N	3:J:359:PRO:HD3	2.28	0.49
3:J:517:CYS:HB2	3:J:716:GLN:OE1	2.13	0.49
2:I:560:PRO:HG3	3:J:773:PHE:CE2	2.48	0.49
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.78	0.48
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.43	0.48
5:F:503:GLU:OE1	5:F:504:PRO:HD2	2.13	0.48
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.27	0.48
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.78	0.48
1:A:234:LEU:HD12	1:B:218:ARG:NH1	2.28	0.48
1:A:77:ASP:O	1:A:80:GLU:N	2.46	0.48
2:C:70:TYR:HA	2:C:100:LEU:CD2	2.42	0.48
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.94	0.48
2:C:510:GLN:CD	2:C:534:GLY:HA2	2.34	0.48
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.28	0.48
3:D:1286:LYS:HA	3:D:1289:ASN:HB2	1.95	0.48
3:D:201:LEU:O	3:D:217:LEU:HD11	2.13	0.48
3:D:204:GLU:HB3	3:D:217:LEU:HD21	1.94	0.48
1:G:166:ARG:N	1:G:167:PRO:HD2	2.28	0.48
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.28	0.48
2:I:243:PRO:O	2:I:246:LEU:HD12	2.13	0.48
2:I:470:ARG:HA	2:I:473:ARG:HD2	1.95	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.48
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.48
3:J:554:GLU:HA	3:J:580:TRP:HZ2	1.78	0.48
3:J:81:ARG:C	3:J:83:VAL:H	2.16	0.48
3:J:848:VAL:HG11	3:J:877:VAL:HG21	1.94	0.48
1:A:82:LEU:HB3	1:A:173:VAL:HG12	1.95	0.48
1:B:63:GLY:CA	1:B:71:LYS:HE3	2.36	0.48
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.43	0.48
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.96	0.48
2:C:487:LEU:H	2:C:487:LEU:HD23	1.79	0.48
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.14	0.48
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.94	0.48
3:D:1227:HIS:CA	3:D:1230:THR:HG22	2.42	0.48
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
2:I:971:LEU:HD22	2:I:1018:TYR:HD1	1.79	0.48
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.48
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.48	0.48
3:J:615:LYS:O	3:J:619:ILE:HG22	2.13	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
5:L:283:GLN:O	5:L:287:ILE:HG13	2.14	0.48
5:L:577:GLY:HA3	5:L:583:THR:CG2	2.32	0.48
2:C:488:MET:O	2:C:490:GLN:N	2.44	0.48
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.95	0.48
2:C:1101:LEU:O	3:D:731:ARG:HD3	2.14	0.48
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.14	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	1.94	0.48
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:30:ILE:CD1	2:I:30:ILE:H	2.17	0.48
2:I:528:ARG:HD3	2:I:663:VAL:HG21	1.96	0.48
2:I:632:ASP:O	2:I:647:ARG:HB2	2.13	0.48
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.78	0.48
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.48	0.48
3:J:48:THR:HB	3:J:50:LYS:HG3	1.96	0.48
1:A:27:THR:C	1:A:28:LEU:HD12	2.33	0.48
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.48	0.48
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.93	0.48
2:C:553:THR:O	2:C:557:ARG:HD2	2.12	0.48
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.14	0.48
2:C:615:VAL:HG11	2:C:649:GLN:O	2.13	0.48
3:D:1165:PHE:CD1	3:D:1165:PHE:N	2.81	0.48
1:G:226:GLU:O	1:G:229:GLU:HG3	2.13	0.48
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	2.14	0.48
2:I:1282:GLY:O	2:I:1284:ALA:N	2.47	0.48
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.28	0.48
2:I:646:SER:HB3	2:I:649:GLN:CG	2.44	0.48
2:I:655:VAL:N	2:I:659:GLN:OE1	2.46	0.48
2:I:850:ILE:O	2:I:850:ILE:HG22	2.13	0.48
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.78	0.48
1:A:227:GLN:CG	1:B:39:LEU:HD11	2.41	0.48
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.79	0.48
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.96	0.48
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.95	0.48
3:D:810:THR:HG23	3:D:811:GLU:N	2.28	0.48
2:C:906:PHE:HE2	5:F:608:ARG:HH11	1.61	0.48
1:G:231:PHE:CD1	1:G:231:PHE:O	2.66	0.48
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.48
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.96	0.48
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.48
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.42	0.48
3:D:537:TYR:CZ	3:D:544:LEU:HD22	2.49	0.48
3:D:683:ILE:CD1	3:D:754:ILE:HG23	2.43	0.48
3:D:83:VAL:O	3:D:91:GLU:HA	2.13	0.48
4:E:39:VAL:HG21	4:E:56:GLU:HG3	1.95	0.48
5:F:507:MET:O	5:F:519:LEU:HB3	2.14	0.48
1:G:142:MET:HG3	1:G:144:ILE:HG13	1.95	0.48
1:G:77:ASP:O	1:G:81:ILE:HG13	2.13	0.48
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.29	0.48
2:I:1192:GLU:OE2	3:J:764:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:478:LEU:HD13	4:K:24:ALA:HA	1.96	0.48
5:L:343:LYS:HD2	5:L:343:LYS:H	1.79	0.48
1:B:46:ILE:HD12	1:B:224:LEU:HB2	1.95	0.48
2:C:13:LYS:O	2:C:1183:ALA:N	2.45	0.48
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.47	0.48
3:D:363:LEU:HB2	3:D:450:HIS:CE1	2.49	0.48
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.48
3:D:83:VAL:HG13	3:D:92:VAL:CG1	2.44	0.48
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.42	0.48
2:I:607:SER:N	2:I:610:GLU:HB2	2.28	0.48
2:I:646:SER:HB3	2:I:649:GLN:CD	2.34	0.48
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.49	0.48
5:L:316:PHE:O	5:L:320:ILE:HG13	2.14	0.48
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.43	0.48
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.78	0.48
2:C:617:ALA:HB3	2:C:653:MET:CB	2.44	0.48
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.14	0.48
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.96	0.48
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.48	0.48
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.79	0.48
5:F:292:VAL:HG21	5:F:299:LYS:CG	2.44	0.48
5:F:511:ILE:CG1	5:F:512:GLY:H	2.27	0.48
1:H:13:LEU:O	1:H:13:LEU:HD12	2.14	0.48
2:I:369:MET:SD	2:I:370:MET:SD	3.12	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.94	0.48
2:I:897:PRO:HD3	3:J:77:ARG:HH22	1.78	0.48
3:J:744:ARG:HH11	3:J:763:PHE:HZ	1.61	0.48
5:L:130:VAL:HG23	5:L:266:PHE:HZ	1.79	0.48
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.49	0.48
1:B:92:VAL:HG12	1:B:95:LYS:HB3	1.96	0.48
2:C:169:LYS:HD3	2:C:190:PRO:HA	1.96	0.48
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.48	0.48
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.44	0.48
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	1.96	0.48
3:D:215:LYS:CE	3:D:216:LYS:HG3	2.43	0.48
5:F:577:GLY:CA	5:F:583:THR:HG23	2.34	0.48
2:I:1322:SER:HB3	3:J:345:LYS:HZ1	1.79	0.48
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.45	0.48
1:A:252:ILE:HG22	1:A:278:ILE:CD1	2.44	0.47
2:C:1142:ARG:HD3	2:C:1161:LEU:HD13	1.96	0.47
2:C:189:ASP:OD1	2:C:193:ASN:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:SER:O	2:C:431:LYS:NZ	2.46	0.47
2:C:62:TYR:C	2:C:64:GLY:H	2.18	0.47
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.46	0.47
3:D:1162:ILE:O	3:D:1178:THR:N	2.47	0.47
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.49	0.47
3:D:252:LEU:HD23	3:D:262:THR:HB	1.96	0.47
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.49	0.47
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.96	0.47
5:F:348:GLU:CG	5:F:354:THR:HA	2.44	0.47
2:I:885:GLY:HA2	2:I:917:SER:CB	2.41	0.47
2:I:976:ARG:HB2	2:I:997:TRP:CZ3	2.48	0.47
3:J:490:ILE:HA	3:J:500:ILE:CG1	2.43	0.47
3:J:647:PRO:HG3	3:J:697:MET:CA	2.44	0.47
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.47
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.97	0.47
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.30	0.47
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.40	0.47
3:D:58:CYS:SG	3:D:60:ARG:HB3	2.55	0.47
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.47	0.47
3:D:75:TYR:CD2	3:D:80:HIS:HD2	2.27	0.47
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.12	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.95	0.47
1:H:11:PRO:O	1:H:12:ARG:HG3	2.14	0.47
2:I:383:SER:O	2:I:387:ASN:HB2	2.14	0.47
2:I:38:PHE:HB2	2:I:457:GLY:O	2.13	0.47
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.97	0.47
2:I:667:LEU:HD23	2:I:704:MET:HB2	1.95	0.47
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.47	0.47
3:J:1319:PHE:O	3:J:1322:ALA:HB3	2.14	0.47
3:J:517:CYS:CA	3:J:716:GLN:HE22	2.25	0.47
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.78	0.47
3:J:259:ARG:HD2	5:L:505:ILE:CD1	2.40	0.47
1:A:12:ARG:HG2	1:A:13:LEU:H	1.80	0.47
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.14	0.47
2:C:39:ILE:O	2:C:39:ILE:HG23	2.14	0.47
2:C:519:ASN:HB3	2:C:522:SER:CB	2.44	0.47
2:C:522:SER:O	2:C:525:THR:HG22	2.13	0.47
3:D:630:ALA:O	3:D:633:ALA:HB3	2.15	0.47
1:H:110:VAL:HG23	1:H:133:LEU:HD13	1.97	0.47
1:H:67:GLU:O	1:H:78:ILE:HB	2.14	0.47
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1142:ARG:NH1	2:I:1169:VAL:HG21	2.29	0.47
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.96	0.47
2:I:202:ARG:NH1	2:I:369:MET:HA	2.29	0.47
2:I:153:PRO:HB2	2:I:401:GLY:HA2	1.96	0.47
2:I:10:ARG:NH2	2:I:791:LEU:HB2	2.28	0.47
3:J:510:LEU:HA	3:J:513:MET:HE2	1.96	0.47
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.96	0.47
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.95	0.47
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.61	0.47
2:C:395:TYR:HB3	2:C:419:ILE:CG2	2.45	0.47
2:C:493:ILE:HG12	2:C:493:ILE:O	2.13	0.47
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.39	0.47
1:G:156:SER:CB	2:I:1059:ARG:HH22	2.26	0.47
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.03	0.47
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.97	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.45	0.47
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.29	0.47
2:I:568:ASN:HB2	2:I:571:LEU:HB2	1.95	0.47
2:I:849:GLU:HB2	2:I:851:THR:HG22	1.96	0.47
2:I:932:GLN:HB3	2:I:934:PHE:CE2	2.50	0.47
3:J:133:ARG:O	3:J:137:ARG:HB2	2.15	0.47
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.96	0.47
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.21	0.47
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.96	0.47
3:J:709:ARG:HD2	3:J:710:ASP:H	1.78	0.47
5:L:362:ASN:HA	5:L:365:MET:HB2	1.96	0.47
5:L:392:LYS:O	5:L:395:THR:HG22	2.14	0.47
5:L:558:VAL:HG23	5:L:580:PHE:HE2	1.79	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.46	0.47
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.96	0.47
2:C:1269:ARG:CG	3:D:343:LEU:HD11	2.43	0.47
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.79	0.47
2:I:670:PHE:CD1	2:I:1113:LEU:HD23	2.49	0.47
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.21	0.47
2:I:1299:ASN:O	2:I:1303:LYS:HG2	2.15	0.47
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.97	0.47
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.96	0.47
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.97	0.47
5:L:311:THR:O	5:L:341:LEU:HD21	2.14	0.47
1:A:58:GLU:HG2	1:A:158:ARG:NH2	2.25	0.47
1:A:11:PRO:HD2	1:B:227:GLN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.96	0.47
2:C:785:ASP:OD2	2:C:791:LEU:N	2.46	0.47
2:C:861:ALA:HB1	2:C:882:ILE:CD1	2.45	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.47
2:C:1281:TYR:OH	3:D:431:ARG:O	2.32	0.47
3:D:810:THR:O	3:D:911:LYS:HE2	2.14	0.47
4:E:15:ASN:HB3	4:E:18:ASP:H	1.80	0.47
1:H:79:LEU:O	1:H:82:LEU:HB2	2.14	0.47
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.97	0.47
5:L:454:VAL:O	5:L:458:GLU:HG3	2.15	0.47
5:L:585:GLU:O	5:L:589:GLN:HG3	2.14	0.47
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.44	0.47
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.47
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.62	0.47
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.14	0.47
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	1.97	0.47
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.27	0.47
3:J:418:GLU:HB3	4:K:48:VAL:HG23	1.97	0.47
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.96	0.47
2:C:670:PHE:CD1	2:C:1113:LEU:HD23	2.50	0.47
2:C:256:GLU:OE2	2:C:261:VAL:HG22	2.14	0.47
2:C:785:ASP:HB3	2:C:789:THR:O	2.13	0.47
3:D:1327:GLU:OE2	3:D:1329:THR:HB	2.14	0.47
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.48	0.47
3:D:514:THR:HG21	3:D:596:LEU:HG	1.97	0.47
5:F:583:THR:O	5:F:584:ARG:HB2	2.14	0.47
2:I:802:VAL:CG2	2:I:1098:LEU:HD13	2.45	0.47
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.83	0.47
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.95	0.47
2:C:667:LEU:HD23	2:C:704:MET:HB2	1.96	0.47
2:C:857:VAL:HG21	2:C:862:LEU:HD21	1.97	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.70	0.47
3:D:322:ARG:HH11	3:D:322:ARG:HB2	1.79	0.47
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:CB	2.44	0.47
2:I:964:LEU:HD13	2:I:1021:LEU:O	2.14	0.47
3:J:1162:ILE:HD12	3:J:1163:VAL:H	1.80	0.47
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.97	0.47
3:J:658:GLU:O	3:J:661:VAL:HG22	2.14	0.47
5:L:415:ALA:O	5:L:419:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.97	0.47
1:A:263:THR:HG23	1:A:266:SER:H	1.78	0.47
2:C:1028:LYS:O	2:C:1032:LYS:HB2	2.15	0.47
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.78	0.47
2:C:62:TYR:C	2:C:64:GLY:N	2.68	0.47
2:C:980:VAL:HA	2:C:984:VAL:HA	1.97	0.47
3:D:124:ILE:HG23	3:D:189:LEU:HD21	1.96	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:412:LEU:HD23	3:D:416:ILE:HG12	1.96	0.47
3:D:518:VAL:HB	3:D:707:ILE:HD13	1.97	0.47
1:G:73:GLY:HA2	1:G:134:THR:HG22	1.96	0.47
2:I:337:PHE:CE2	2:I:343:HIS:CD2	3.03	0.47
3:J:481:ARG:O	4:K:6:VAL:HG11	2.15	0.47
2:C:210:LEU:O	2:C:215:TYR:HB2	2.15	0.47
3:D:746:LEU:HG	3:D:758:PRO:HG3	1.96	0.47
3:D:870:ASP:O	3:D:874:GLU:N	2.44	0.47
1:G:190:ALA:C	1:G:191:ARG:HD3	2.36	0.47
2:I:1014:LEU:O	2:I:1018:TYR:HB2	2.15	0.47
2:I:519:ASN:HB3	2:I:522:SER:HB2	1.97	0.47
2:I:551:HIS:CE1	2:I:553:THR:OG1	2.68	0.47
2:I:561:ILE:O	2:I:680:LEU:HD12	2.15	0.47
2:I:1223:ARG:HG3	3:J:635:SER:O	2.15	0.47
3:J:850:LYS:HB3	3:J:851:PRO:CD	2.42	0.47
1:A:310:ARG:HA	1:A:310:ARG:HE	1.79	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.97	0.46
3:D:647:PRO:HG3	3:D:697:MET:CA	2.45	0.46
2:C:490:GLN:HG3	5:F:472:GLN:CG	2.43	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.50	0.46
2:I:324:LYS:O	2:I:327:GLN:NE2	2.48	0.46
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.33	0.46
2:I:975:ILE:O	2:I:979:LEU:HB2	2.15	0.46
3:J:189:LEU:HB3	3:J:234:PRO:CB	2.43	0.46
3:J:691:ASP:O	3:J:695:LYS:HG2	2.15	0.46
3:J:707:ILE:HD12	3:J:707:ILE:H	1.80	0.46
5:L:288:MET:CG	5:L:299:LYS:HE2	2.45	0.46
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.46
2:C:632:ASP:O	2:C:647:ARG:HB2	2.15	0.46
2:C:879:GLY:HA2	2:C:920:VAL:HG12	1.97	0.46
2:C:746:ALA:CB	2:C:974:ARG:HE	2.28	0.46
3:D:1156:LEU:N	3:D:1156:LEU:HD22	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.97	0.46
3:D:19:ALA:H	3:D:1344:LEU:HD12	1.80	0.46
3:D:905:ARG:HH12	4:E:10:VAL:CG1	2.28	0.46
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.97	0.46
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.97	0.46
1:G:166:ARG:O	1:G:168:ILE:N	2.48	0.46
1:H:201:LEU:HG	1:H:203:ILE:CD1	2.46	0.46
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.46
2:I:985:GLU:CG	2:I:988:LYS:HD2	2.46	0.46
2:I:98:VAL:C	2:I:121:GLU:HA	2.34	0.46
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.97	0.46
3:J:68:TYR:C	3:J:92:VAL:HG23	2.34	0.46
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.28	0.46
1:B:106:GLY:O	1:B:133:LEU:HB3	2.15	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.50	0.46
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.30	0.46
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.76	0.46
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.96	0.46
3:D:744:ARG:HG3	3:D:744:ARG:O	2.15	0.46
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.44	0.46
5:F:311:THR:HG21	5:F:348:GLU:CD	2.35	0.46
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.15	0.46
5:F:97:PRO:HA	5:F:100:MET:HG3	1.98	0.46
1:G:22:THR:OG1	1:G:23:HIS:N	2.48	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.15	0.46
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.47	0.46
3:J:1281:GLU:O	3:J:1285:VAL:HB	2.16	0.46
3:J:233:LYS:H	3:J:236:TRP:HE3	1.63	0.46
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.46
3:J:683:ILE:HD11	3:J:754:ILE:HG21	1.98	0.46
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.73	0.46
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.98	0.46
5:L:129:GLN:HB2	5:L:368:GLY:HA3	1.98	0.46
1:B:153:VAL:O	1:B:175:ALA:N	2.22	0.46
2:C:1252:SER:HB3	2:C:1255:THR:O	2.16	0.46
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.67	0.46
4:E:71:GLU:O	4:E:75:GLN:HG3	2.15	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.45	0.46
3:J:801:VAL:O	3:J:805:GLN:HB2	2.15	0.46
5:L:114:GLU:HG3	5:L:115:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:253:SER:O	5:L:257:LYS:HG3	2.15	0.46
5:L:346:GLN:O	5:L:346:GLN:HG2	2.14	0.46
2:C:229:ILE:CD1	2:C:334:GLU:HG2	2.46	0.46
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.80	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.45	0.46
3:D:367:GLY:HA3	3:D:448:GLN:CB	2.38	0.46
3:D:702:GLN:HA	3:D:723:TYR:CE2	2.50	0.46
3:D:848:VAL:HG13	3:D:857:LEU:CD1	2.46	0.46
5:F:287:ILE:O	5:F:291:CYS:SG	2.70	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
2:I:582:ASN:O	2:I:585:GLY:N	2.47	0.46
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.44	0.46
2:I:921:PRO:HB2	2:I:924:VAL:HG22	1.97	0.46
3:J:103:GLY:C	3:J:244:VAL:HG22	2.36	0.46
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.13	0.46
3:D:1284:ARG:NH2	3:J:1292:LEU:HD11	2.30	0.46
3:J:293:ARG:O	3:J:296:LYS:N	2.49	0.46
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.51	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.15	0.46
1:B:191:ARG:O	1:B:191:ARG:HG2	2.15	0.46
2:C:1247:SER:OG	2:C:1248:THR:N	2.49	0.46
2:C:600:THR:HG22	2:C:601:ASP:H	1.81	0.46
3:D:1163:VAL:HG21	3:D:1175:LEU:HD21	1.98	0.46
3:D:647:PRO:CG	3:D:697:MET:HB3	2.42	0.46
3:D:847:ASP:N	3:D:847:ASP:OD1	2.42	0.46
5:F:461:ASN:O	5:F:465:ARG:HG2	2.15	0.46
2:I:1023:HIS:O	2:I:1027:LYS:HG2	2.15	0.46
2:I:124:MET:HE2	2:I:493:ILE:HD11	1.98	0.46
2:I:553:THR:O	2:I:557:ARG:HD2	2.16	0.46
3:J:245:LEU:O	3:J:250:ARG:NE	2.46	0.46
3:J:848:VAL:H	3:J:858:VAL:HG22	1.81	0.46
5:L:108:VAL:HG11	5:L:381:GLU:C	2.35	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.26	0.46
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.53	0.46
1:A:296:GLY:H	1:A:299:SER:CB	2.20	0.46
2:C:953:LEU:HD13	2:C:1036:ILE:HD12	1.97	0.46
2:C:1142:ARG:HH11	2:C:1161:LEU:CD1	2.28	0.46
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.46	0.46
2:C:867:GLU:HG3	2:C:867:GLU:H	1.17	0.46
2:C:95:PRO:CA	2:C:126:GLU:HG2	2.46	0.46
3:D:710:ASP:OD1	3:D:711:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.46	0.46
2:I:1180:MET:HA	2:I:1181:PRO:HD3	1.78	0.46
2:I:1255:THR:O	2:I:1257:GLN:N	2.48	0.46
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.46
2:I:738:GLU:HA	2:I:741:MET:CE	2.46	0.46
2:I:811:ASN:N	2:I:811:ASN:OD1	2.48	0.46
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.97	0.46
3:J:1157:ALA:HB3	3:J:1207:GLY:N	2.28	0.46
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.15	0.46
3:J:1319:PHE:CD1	3:J:1319:PHE:C	2.89	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.15	0.46
5:L:372:ALA:O	5:L:375:ALA:HB3	2.16	0.46
1:B:57:THR:OG1	1:B:147:GLN:HB3	2.16	0.46
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.97	0.46
2:C:91:THR:HB	2:C:138:ILE:O	2.16	0.46
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.97	0.46
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.46
3:D:1197:ASN:HB2	3:D:1212:ASP:OD2	2.16	0.46
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.80	0.46
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.81	0.46
3:D:318:GLY:C	3:D:320:ASN:H	2.19	0.46
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.46
5:F:383:ASN:O	5:F:386:LEU:HB3	2.15	0.46
2:I:106:GLU:O	2:I:109:ALA:HB2	2.16	0.46
2:I:1139:ALA:O	2:I:1143:GLU:HB2	2.16	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
3:J:596:LEU:HD11	3:J:604:MET:CE	2.45	0.46
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.97	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.16	0.46
1:B:217:ILE:HA	1:B:220:ALA:HB3	1.96	0.46
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.16	0.46
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.96	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
3:D:123:ARG:NH1	3:D:1334:GLU:HG3	2.31	0.46
2:C:1269:ARG:HD3	3:D:343:LEU:HD21	1.96	0.46
3:D:708:ASN:HB3	3:D:712:GLN:O	2.16	0.46
5:F:226:ALA:O	5:F:230:VAL:HG12	2.15	0.46
5:F:316:PHE:O	5:F:320:ILE:HG13	2.15	0.46
5:F:489:MET:O	5:F:491:GLU:N	2.49	0.46
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.51	0.46
1:H:217:ILE:HA	1:H:220:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.98	0.46
2:I:886:LYS:CE	2:I:916:SER:HB3	2.46	0.46
3:J:267:ASP:OD1	3:J:271:ARG:NH2	2.49	0.46
5:L:288:MET:O	5:L:292:VAL:HG23	2.16	0.46
5:L:138:PRO:HD2	5:L:353:LEU:HD11	1.98	0.46
2:C:131:THR:HG22	2:C:132:ASP:H	1.81	0.46
2:C:730:SER:O	2:C:753:LEU:HB2	2.15	0.46
2:C:976:ARG:HD2	2:C:989:LEU:CD2	2.46	0.46
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.46
3:D:137:ARG:CG	3:D:142:GLU:HB2	2.45	0.46
3:D:58:CYS:SG	3:D:59:ALA:N	2.89	0.46
3:D:744:ARG:O	3:D:759:ILE:HB	2.15	0.46
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.46
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.46	0.46
2:I:290:GLU:HG2	2:I:319:LEU:HD12	1.97	0.46
3:J:1298:VAL:O	3:J:1298:VAL:HG13	2.16	0.46
3:J:452:LEU:HD11	3:J:625:MET:HB2	1.98	0.46
3:J:491:LEU:HD22	3:J:496:GLY:O	2.16	0.46
3:J:514:THR:HG21	3:J:596:LEU:CG	2.46	0.46
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.41	0.46
3:J:825:VAL:C	3:J:826:ILE:HG13	2.36	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.51	0.46
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.13	0.46
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.16	0.46
1:B:38:THR:HG23	1:B:39:LEU:N	2.32	0.45
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.51	0.45
2:C:744:GLY:O	2:C:746:ALA:N	2.48	0.45
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.80	0.45
2:C:811:ASN:N	2:C:811:ASN:OD1	2.48	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.50	0.45
3:D:45:ASN:O	3:D:46:TYR:HB3	2.15	0.45
3:D:627:THR:HG23	3:D:628:GLY:N	2.31	0.45
3:D:860:ARG:CB	3:D:860:ARG:HH11	2.26	0.45
5:F:222:ALA:O	5:F:226:ALA:N	2.45	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.45	0.45
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.41	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.80	0.45
2:I:1296:ASP:OD2	2:I:1321:GLU:N	2.49	0.45
2:I:91:THR:HB	2:I:138:ILE:O	2.16	0.45
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.49	0.45
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:805:GLN:HE22	3:J:1348:LYS:HD3	1.80	0.45
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.73	0.45
3:J:844:THR:HG23	3:J:864:LEU:HD21	1.98	0.45
3:J:93:THR:HG22	3:J:94:GLN:H	1.80	0.45
3:J:474:LEU:HB2	4:K:28:ARG:NH1	2.31	0.45
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.31	0.45
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.68	0.45
1:A:321:TRP:CD2	1:A:322:PRO:HB3	2.50	0.45
1:B:62:ASP:HB3	1:B:141:SER:O	2.15	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.46	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.65	0.45
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.75	0.45
2:C:960:LEU:HD11	2:C:1028:LYS:HE2	1.97	0.45
3:D:521:LYS:HB3	3:D:541:LEU:O	2.16	0.45
2:I:1212:LEU:HD11	2:I:1227:VAL:HG11	1.98	0.45
2:I:1292:THR:HG22	2:I:1293:VAL:N	2.31	0.45
2:I:175:ARG:HD3	2:I:183:TRP:CE3	2.52	0.45
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.97	0.45
3:J:1327:GLU:OE1	3:J:1330:ARG:HB2	2.17	0.45
3:J:267:ASP:HA	3:J:270:ARG:NH2	2.28	0.45
5:L:474:MET:C	5:L:476:ARG:H	2.15	0.45
1:A:189:ALA:HB1	1:A:191:ARG:NH2	2.31	0.45
2:C:210:LEU:HB2	2:C:220:ILE:HD11	1.97	0.45
2:C:30:ILE:HD12	2:C:30:ILE:H	1.82	0.45
2:C:800:MET:HG3	2:C:1096:ILE:CD1	2.46	0.45
2:C:83:GLN:O	2:C:87:ILE:HG13	2.17	0.45
2:C:883:LEU:HB3	2:C:1052:VAL:HG21	1.99	0.45
3:D:210:SER:OG	3:D:213:LYS:HD2	2.16	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
3:D:58:CYS:SG	3:D:60:ARG:N	2.87	0.45
5:F:290:LEU:O	5:F:333:VAL:HG11	2.16	0.45
5:F:386:LEU:O	5:F:390:ILE:HG13	2.17	0.45
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.72	0.45
2:I:1196:LYS:O	2:I:1200:LYS:HG3	2.17	0.45
2:I:486:THR:HG23	2:I:487:LEU:N	2.31	0.45
5:L:557:LYS:HG3	5:L:561:MET:CE	2.46	0.45
1:A:47:LEU:O	1:A:180:VAL:HG21	2.17	0.45
2:C:1307:ASN:O	2:C:1311:GLY:N	2.50	0.45
2:C:15:PHE:CD2	2:C:1190:ALA:HB2	2.51	0.45
3:D:247:PRO:HA	3:D:250:ARG:CZ	2.47	0.45
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:298:MET:SD	5:F:402:LEU:HB3	2.57	0.45
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.81	0.45
2:I:95:PRO:HB3	2:I:123:TYR:CE1	2.51	0.45
2:I:119:GLU:CG	2:I:489:PRO:HD2	2.43	0.45
2:I:814:ASP:N	2:I:814:ASP:OD1	2.49	0.45
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.99	0.45
5:L:310:GLU:O	5:L:344:LEU:HD21	2.16	0.45
2:C:106:GLU:HG3	2:C:107:ARG:N	2.32	0.45
2:C:117:ILE:H	2:C:117:ILE:HG12	1.59	0.45
2:C:1117:LEU:HD21	2:C:1182:ILE:HD12	1.99	0.45
2:C:1230:MET:HG2	2:C:1232:MET:HG3	1.99	0.45
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.98	0.45
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.81	0.45
2:C:826:ASP:O	2:C:829:THR:HB	2.16	0.45
2:C:87:ILE:H	2:C:87:ILE:HG13	1.51	0.45
3:D:311:ARG:NH2	3:D:1329:THR:HG21	2.32	0.45
3:D:490:ILE:HA	3:D:500:ILE:HG13	1.98	0.45
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.95	0.45
1:G:166:ARG:O	1:G:167:PRO:C	2.55	0.45
2:I:974:ARG:HD3	2:I:1010:GLN:HE21	1.82	0.45
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.82	0.45
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.98	0.45
3:J:193:ASP:HB3	3:J:196:GLN:HG2	1.98	0.45
3:J:398:LYS:O	3:J:402:GLU:HB2	2.16	0.45
3:J:532:GLU:HB2	3:J:535:ARG:NH2	2.30	0.45
3:J:811:GLU:O	3:J:895:CYS:HA	2.16	0.45
3:J:861:ASN:HD22	3:J:883:ARG:HH11	1.63	0.45
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.51	0.45
1:A:237:VAL:O	1:B:13:LEU:HA	2.17	0.45
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.97	0.45
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.99	0.45
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.16	0.45
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.47	0.45
3:D:1350:ASN:OD1	3:D:1355:ARG:HD2	2.17	0.45
3:D:405:GLU:O	3:D:408:VAL:HG22	2.17	0.45
2:I:361:SER:O	2:I:364:VAL:HB	2.16	0.45
2:I:516:ASP:HB3	2:I:522:SER:HG	1.81	0.45
2:I:526:HIS:O	2:I:529:ARG:HB2	2.17	0.45
3:J:73:GLY:O	3:J:76:LYS:HG3	2.17	0.45
5:L:565:ILE:HG22	5:L:566:ASP:OD1	2.16	0.45
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.52	0.45
2:C:615:VAL:HG13	2:C:651:ASP:N	2.29	0.45
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.42	0.45
3:D:276:ASN:O	3:D:280:LYS:HG2	2.17	0.45
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.80	0.45
3:D:491:LEU:HA	3:D:491:LEU:HD23	1.72	0.45
3:D:98:ARG:O	3:D:247:PRO:HD2	2.17	0.45
5:F:96:ASP:O	5:F:99:ARG:N	2.42	0.45
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.98	0.45
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.17	0.45
2:I:1306:LYS:HE2	5:L:535:ALA:HA	1.97	0.45
3:J:451:PRO:HD2	3:J:625:MET:SD	2.57	0.45
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.17	0.45
2:I:898:GLU:CB	5:L:540:LEU:HD22	2.46	0.45
5:L:583:THR:HG22	5:L:584:ARG:N	2.32	0.45
2:C:239:MET:N	2:C:285:ILE:O	2.48	0.45
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.32	0.45
3:D:327:LEU:HD23	3:D:327:LEU:HA	1.74	0.45
3:D:47:ARG:NH1	5:F:500:ILE:HD11	2.31	0.45
1:G:166:ARG:HD2	1:G:166:ARG:C	2.37	0.45
1:G:51:MET:HA	1:G:52:PRO:HD3	1.80	0.45
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.82	0.45
1:G:150:ARG:NH1	1:H:7:GLU:O	2.42	0.45
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.98	0.45
2:I:1262:LYS:C	2:I:1264:GLN:H	2.20	0.45
2:I:1340:GLU:HG2	3:J:21:LYS:HB2	1.98	0.45
2:I:976:ARG:O	2:I:980:VAL:HG23	2.17	0.45
3:J:35:PHE:HE1	3:J:101:ARG:HH11	1.64	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.31	0.45
3:J:596:LEU:HD11	3:J:604:MET:HE1	1.98	0.45
3:J:474:LEU:CD2	4:K:28:ARG:HG2	2.47	0.45
1:A:31:LEU:HD12	1:A:201:LEU:HB2	1.99	0.45
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.99	0.45
1:A:312:LEU:H	1:A:312:LEU:HD12	1.81	0.45
1:A:60:GLU:HG3	1:A:169:GLY:O	2.17	0.45
1:A:90:VAL:O	1:A:210:THR:HG21	2.17	0.45
2:C:1146:GLN:HG2	2:C:1160:ASP:OD1	2.16	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.17	0.45
2:C:796:LEU:HD12	2:C:796:LEU:N	2.30	0.45
2:C:871:VAL:O	2:C:944:ARG:NH1	2.50	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:342:LEU:O	3:D:343:LEU:C	2.54	0.45
3:D:513:MET:CE	3:D:579:LEU:HD13	2.47	0.45
1:H:65:LEU:HD22	1:H:171:LEU:HD11	1.99	0.45
2:I:272:ARG:HD3	2:I:273:HIS:CD2	2.52	0.45
2:I:682:GLY:O	2:I:686:GLN:HB2	2.17	0.45
3:J:193:ASP:HB3	3:J:196:GLN:CG	2.46	0.45
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.97	0.45
3:J:510:LEU:HD12	3:J:628:GLY:HA2	1.99	0.45
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.98	0.45
1:A:282:VAL:HG22	1:A:316:MET:SD	2.56	0.45
2:C:688:GLN:OE1	2:C:1237:HIS:CE1	2.69	0.45
2:C:1276:TRP:HA	2:C:1279:GLU:OE1	2.17	0.45
2:C:353:VAL:O	2:C:355:PRO:HD3	2.17	0.45
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.31	0.45
3:D:1250:ASP:O	3:D:1251:LYS:C	2.55	0.45
3:D:478:LEU:HG	4:E:47:THR:HG23	1.98	0.45
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.45
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.86	0.45
1:G:50:SER:HG	1:H:35:PHE:HE1	1.64	0.45
2:I:1287:LEU:HD23	2:I:1288:GLN:N	2.32	0.45
2:I:658:GLN:O	2:I:661:VAL:HG22	2.17	0.45
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.99	0.45
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.41	0.45
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.17	0.45
2:I:618:GLN:OE1	3:J:769:VAL:HB	2.16	0.45
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.40	0.45
1:A:285:THR:OG1	1:A:286:GLU:N	2.50	0.44
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.17	0.44
2:C:202:ARG:NH1	2:C:368:ARG:HH22	2.14	0.44
2:C:865:LEU:HD23	2:C:871:VAL:HA	1.99	0.44
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.32	0.44
3:D:427:PRO:HB2	3:D:429:LEU:CD2	2.47	0.44
3:D:853:THR:HG22	3:D:854:ALA:N	2.29	0.44
1:G:14:VAL:HG13	1:G:27:THR:HB	1.98	0.44
2:I:106:GLU:HG3	2:I:107:ARG:N	2.31	0.44
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
3:J:1149:ARG:HH21	3:J:1153:PRO:HG2	1.80	0.44
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.72	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.71	0.44
5:L:292:VAL:HG21	5:L:299:LYS:CG	2.47	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.32	0.44
2:C:18:ARG:HG2	2:C:1188:ASP:OD1	2.17	0.44
2:C:557:ARG:HB3	2:C:587:LEU:HD13	2.00	0.44
2:C:814:ASP:N	2:C:814:ASP:OD1	2.50	0.44
2:C:950:GLU:O	2:C:953:LEU:HB3	2.16	0.44
3:D:1146:GLU:HG2	3:D:1148:ARG:NH2	2.33	0.44
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.83	0.44
3:D:343:LEU:HD13	3:D:344:GLY:N	2.33	0.44
3:D:357:VAL:HB	3:D:358:GLY:H	1.67	0.44
3:D:412:LEU:O	3:D:415:VAL:HG22	2.17	0.44
3:D:518:VAL:N	3:D:716:GLN:HE22	2.15	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HG3	1.99	0.44
5:F:572:THR:O	5:F:576:VAL:HG23	2.18	0.44
2:I:981:ALA:HB1	2:I:1007:LYS:HZ3	1.81	0.44
2:I:670:PHE:CE1	2:I:1184:THR:HG21	2.52	0.44
1:G:77:ASP:CG	2:I:755:LYS:HZ1	2.18	0.44
2:I:945:ALA:O	2:I:949:GLU:HB2	2.17	0.44
3:J:1291:GLU:HG2	3:J:1297:LYS:NZ	2.32	0.44
3:J:845:ALA:HB3	3:J:846:GLU:HG2	1.99	0.44
5:L:362:ASN:HA	5:L:365:MET:CB	2.46	0.44
1:A:285:THR:O	1:A:289:LEU:HG	2.18	0.44
1:B:6:THR:OG1	1:B:7:GLU:N	2.50	0.44
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.17	0.44
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.80	0.44
2:C:858:GLY:O	2:C:862:LEU:HG	2.18	0.44
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.00	0.44
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.98	0.44
3:D:416:ILE:HA	3:D:416:ILE:HD12	1.72	0.44
3:D:45:ASN:O	3:D:46:TYR:CD2	2.69	0.44
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.98	0.44
5:F:130:VAL:HA	5:F:133:SER:HB2	1.98	0.44
1:G:200:LYS:HB2	1:G:200:LYS:HE2	1.60	0.44
1:H:34:GLY:O	1:H:38:THR:HG22	2.18	0.44
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.82	0.44
2:I:269:ILE:HD12	2:I:269:ILE:H	1.81	0.44
2:I:153:PRO:HB2	2:I:401:GLY:CA	2.48	0.44
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.86	0.44
2:C:1082:ILE:CD1	2:C:1082:ILE:H	2.29	0.44
2:C:202:ARG:HH11	2:C:369:MET:HB2	1.83	0.44
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.52	0.44
3:D:1283:SER:O	3:D:1286:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.47	0.44
3:D:48:THR:C	3:D:50:LYS:N	2.67	0.44
3:D:56:LEU:HD12	3:D:56:LEU:H	1.82	0.44
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.52	0.44
3:D:291:ILE:CD1	5:F:409:ASN:HB3	2.47	0.44
2:I:1210:ILE:HG22	2:I:1211:ARG:N	2.32	0.44
2:I:812:PHE:N	2:I:815:SER:OG	2.50	0.44
3:J:1219:ASP:O	3:J:1222:ARG:N	2.50	0.44
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.32	0.44
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	1.98	0.44
3:J:327:LEU:HA	3:J:327:LEU:HD23	1.65	0.44
3:J:490:ILE:HA	3:J:500:ILE:HG13	2.00	0.44
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.69	0.44
3:J:844:THR:OG1	3:J:860:ARG:O	2.14	0.44
5:L:511:ILE:CG1	5:L:512:GLY:H	2.30	0.44
5:L:584:ARG:HD2	5:L:584:ARG:HA	1.68	0.44
1:A:219:ARG:O	1:A:223:ILE:HG13	2.17	0.44
2:C:5:TYR:CD2	2:C:778:GLU:HB2	2.53	0.44
2:C:616:ILE:HG22	2:C:617:ALA:O	2.18	0.44
2:C:895:LEU:HD11	2:C:900:LYS:HG3	1.99	0.44
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.80	0.44
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.66	0.44
3:D:26:SER:OG	3:D:28:ASP:N	2.50	0.44
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.53	0.44
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.83	0.44
3:D:469:HIS:O	3:D:471:PRO:HD3	2.18	0.44
3:D:53:ARG:HA	3:D:54:ASP:HA	1.72	0.44
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.98	0.44
2:I:178:PRO:HB3	2:I:395:TYR:CE2	2.53	0.44
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.44
3:J:510:LEU:HD22	3:J:601:ILE:CD1	2.48	0.44
3:J:513:MET:HE3	3:J:579:LEU:HD22	1.99	0.44
3:J:736:GLN:O	3:J:739:GLN:N	2.44	0.44
5:L:139:GLU:CG	5:L:351:THR:HA	2.46	0.44
5:L:363:ARG:O	5:L:367:ILE:HG13	2.17	0.44
5:L:476:ARG:HD2	5:L:477:GLU:H	1.83	0.44
1:B:192:VAL:O	1:B:195:ARG:N	2.50	0.44
2:C:708:VAL:CG1	2:C:794:LEU:HD22	2.47	0.44
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.82	0.44
3:D:128:LEU:HA	3:D:192:MET:HE1	2.00	0.44
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:710:ASP:CG	3:D:711:GLY:H	2.20	0.44
3:D:827:GLU:CB	3:D:832:LYS:HD2	2.48	0.44
3:D:94:GLN:HB2	3:D:96:LYS:HB2	1.99	0.44
4:E:62:GLN:O	4:E:66:VAL:HG23	2.16	0.44
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
2:C:898:GLU:HB3	5:F:544:THR:HG21	1.99	0.44
1:G:14:VAL:HG22	1:G:15:ASP:N	2.33	0.44
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.99	0.44
1:G:75:GLN:HA	2:I:729:ALA:H	1.81	0.44
1:H:224:LEU:O	1:H:228:LEU:HG	2.17	0.44
2:I:617:ALA:HB3	2:I:653:MET:CB	2.48	0.44
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.50	0.44
3:J:761:ALA:N	3:J:771:GLN:HE22	2.15	0.44
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.18	0.44
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.44
2:C:866:ASP:OD2	2:C:869:GLY:N	2.51	0.44
2:C:903:ARG:NE	2:C:910:ALA:HB2	2.32	0.44
3:D:442:ILE:HD13	3:D:442:ILE:HA	1.81	0.44
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.44
5:F:484:ALA:C	5:F:491:GLU:HB2	2.38	0.44
2:I:1122:LYS:NZ	2:I:1178:LYS:O	2.41	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.99	0.44
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.81	0.44
2:I:157:PHE:CD1	2:I:174:ALA:HB2	2.53	0.44
3:J:161:THR:H	3:J:164:GLN:HB2	1.83	0.44
2:I:1223:ARG:HD3	3:J:637:ALA:HA	1.98	0.44
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.18	0.44
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.50	0.44
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.99	0.44
2:C:494:ASN:HB3	2:C:497:PRO:CG	2.48	0.44
2:C:960:LEU:O	2:C:963:GLU:HB2	2.18	0.44
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.33	0.44
3:D:279:LEU:HD11	3:D:296:LYS:HG2	2.00	0.44
3:D:532:GLU:O	3:D:536:LEU:HB2	2.17	0.44
3:D:660:GLU:O	3:D:664:ILE:HG12	2.18	0.44
3:D:849:LEU:HB2	3:D:853:THR:HG23	1.99	0.44
5:F:390:ILE:O	5:F:393:LYS:HB2	2.18	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.99	0.44
5:F:466:ILE:HG21	5:F:486:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.81	0.44
2:I:1132:LEU:HD13	2:I:1177:ARG:HD2	2.00	0.44
2:I:614:TYR:CD1	2:I:652:TYR:CE1	3.06	0.44
2:I:870:ILE:CG2	2:I:944:ARG:HD3	2.47	0.44
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.82	0.44
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.80	0.44
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.44
5:L:114:GLU:HG3	5:L:115:GLY:N	2.32	0.44
5:L:297:MET:HA	5:L:326:TRP:HB3	2.00	0.44
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.82	0.44
1:A:317:ARG:O	1:A:318:LEU:HD13	2.18	0.44
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.48	0.44
1:B:54:CYS:O	1:B:90:VAL:HB	2.18	0.44
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.44
2:C:484:LEU:HB2	2:C:485:ASP:H	1.62	0.44
3:D:169:LEU:HA	3:D:169:LEU:HD23	1.82	0.44
3:D:172:PHE:HB3	3:D:175:GLU:OE2	2.17	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
3:D:847:ASP:CA	3:D:860:ARG:H	2.31	0.44
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.18	0.44
2:I:867:GLU:H	2:I:867:GLU:HG3	1.61	0.44
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.48	0.44
3:J:238:ILE:HD13	3:J:238:ILE:HA	1.74	0.44
3:J:416:ILE:HD12	3:J:416:ILE:HA	1.70	0.44
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.44
3:J:59:ALA:HA	3:J:63:GLY:O	2.18	0.44
5:L:226:ALA:O	5:L:230:VAL:HG12	2.18	0.44
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.83	0.44
5:L:575:GLU:O	5:L:579:GLN:HG2	2.17	0.44
1:A:295:LEU:CD2	1:A:300:LEU:HB2	2.48	0.43
1:A:319:GLU:OE2	1:A:319:GLU:HA	2.18	0.43
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.43
2:C:198:ILE:O	2:C:201:ARG:HB2	2.18	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.48	0.43
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.00	0.43
3:D:678:ARG:HD3	3:D:682:VAL:CG2	2.48	0.43
3:D:707:ILE:HD11	3:D:716:GLN:CG	2.46	0.43
3:D:772:TYR:O	3:D:775:SER:N	2.51	0.43
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.33	0.43
1:H:115:ILE:HG22	1:H:116:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:ASN:ND2	1:H:129:VAL:O	2.50	0.43
1:H:86:LYS:HG2	1:H:173:VAL:CG1	2.48	0.43
2:I:600:THR:CG2	2:I:602:GLU:HG2	2.41	0.43
2:I:971:LEU:O	2:I:1014:LEU:HD23	2.18	0.43
3:J:123:ARG:HD3	3:J:123:ARG:HA	1.91	0.43
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.99	0.43
3:J:525:MET:O	3:J:548:VAL:HG13	2.18	0.43
3:J:858:VAL:HG11	3:J:872:LEU:HD21	2.00	0.43
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.48	0.43
4:K:39:VAL:HG21	4:K:56:GLU:HG3	2.00	0.43
3:J:298:MET:SD	5:L:406:GLN:HG3	2.58	0.43
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.00	0.43
1:B:57:THR:O	1:B:173:VAL:N	2.47	0.43
2:C:1308:ILE:HD12	2:C:1308:ILE:HG23	1.72	0.43
3:D:799:ARG:HD2	3:D:1146:GLU:OE1	2.17	0.43
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.42	0.43
3:D:316:ILE:HA	3:D:323:PRO:HA	2.00	0.43
3:D:61:ILE:HB	3:D:62:PHE:CD2	2.53	0.43
3:D:660:GLU:HB3	3:D:685:ILE:CD1	2.23	0.43
3:D:846:GLU:HA	3:D:860:ARG:HD3	2.00	0.43
3:D:919:ALA:CB	3:D:1255:VAL:HG21	2.47	0.43
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.43
5:F:316:PHE:CZ	5:F:334:SER:HA	2.52	0.43
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.99	0.43
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	2.01	0.43
2:I:158:ASP:CG	2:I:159:SER:H	2.21	0.43
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.53	0.43
2:I:466:VAL:O	2:I:469:VAL:HG22	2.17	0.43
2:I:987:GLU:HG2	2:I:991:LYS:HE3	2.00	0.43
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.99	0.43
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.17	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.53	0.43
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.43
5:L:148:TYR:O	5:L:151:VAL:N	2.41	0.43
5:L:166:VAL:HG23	5:L:258:GLN:HA	2.00	0.43
5:L:276:MET:O	5:L:280:VAL:HG23	2.18	0.43
5:L:316:PHE:HZ	5:L:334:SER:CA	2.22	0.43
5:L:412:LEU:CD1	5:L:435:ILE:HD11	2.42	0.43
2:C:15:PHE:HA	2:C:1155:VAL:HG11	2.01	0.43
2:C:218:GLU:HG3	2:C:299:LYS:HA	2.00	0.43
2:C:490:GLN:HG3	5:F:472:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:761:GLN:O	2:C:762:ASN:HB2	2.16	0.43
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.00	0.43
3:D:80:HIS:ND1	3:D:80:HIS:N	2.66	0.43
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.43
1:H:125:LYS:HB3	1:H:125:LYS:HE2	1.77	0.43
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.52	0.43
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.34	0.43
2:I:882:ILE:HG13	2:I:919:ARG:NH1	2.33	0.43
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.15	0.43
3:J:69:GLU:HG3	3:J:76:LYS:HG2	2.00	0.43
5:L:292:VAL:HG21	5:L:299:LYS:HG3	2.00	0.43
2:C:599:VAL:HG21	2:C:623:LEU:HD13	2.00	0.43
2:C:811:ASN:HD22	2:C:1098:LEU:C	2.21	0.43
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	0.43
2:C:985:GLU:O	2:C:989:LEU:N	2.42	0.43
2:C:987:GLU:HG2	2:C:991:LYS:CE	2.46	0.43
3:D:1171:GLY:O	3:D:1193:TRP:HZ3	2.02	0.43
3:D:452:LEU:HA	3:D:452:LEU:HD23	1.84	0.43
3:D:395:LYS:HG2	5:F:536:THR:HG21	2.01	0.43
2:C:902:LEU:HD12	5:F:607:LEU:HD23	2.01	0.43
2:I:1083:GLU:HG3	2:I:1083:GLU:H	1.58	0.43
2:I:1164:PHE:O	2:I:1166:ASP:N	2.51	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.48	0.43
2:I:184:LEU:HD12	2:I:184:LEU:HA	1.64	0.43
2:I:377:THR:HG22	2:I:379:GLU:OE2	2.19	0.43
2:I:600:THR:HG22	2:I:601:ASP:N	2.33	0.43
2:I:972:PHE:HD2	2:I:975:ILE:HD12	1.84	0.43
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.01	0.43
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.00	0.43
3:J:500:ILE:O	3:J:500:ILE:HG22	2.18	0.43
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.54	0.43
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.00	0.43
3:J:905:ARG:HH11	4:K:16:ARG:HB2	1.83	0.43
4:K:19:LEU:CD1	4:K:54:ILE:HG21	2.48	0.43
5:L:576:VAL:O	5:L:580:PHE:HB2	2.19	0.43
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.17	0.43
1:B:152:TYR:CD1	1:B:176:CYS:HA	2.53	0.43
2:C:1110:GLY:O	2:C:1114:GLU:HB2	2.19	0.43
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.19	0.43
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.49	0.43
2:C:318:SER:O	2:C:322:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:CG2	2.48	0.43
3:D:193:ASP:HB3	3:D:196:GLN:CG	2.48	0.43
3:D:363:LEU:HG	3:D:363:LEU:O	2.17	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.31	0.43
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.39	0.43
5:F:573:LEU:HD13	5:F:588:ARG:CZ	2.48	0.43
3:J:128:LEU:HD23	3:J:192:MET:CE	2.47	0.43
3:J:1319:PHE:HD1	3:J:1319:PHE:C	2.22	0.43
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.34	0.43
3:J:899:TYR:CE1	3:J:1251:LYS:HD2	2.52	0.43
5:L:213:ASP:HB2	5:L:216:LEU:HB3	1.99	0.43
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.19	0.43
2:C:1268:GLN:HE22	3:D:352:ARG:CD	2.31	0.43
2:C:1282:GLY:HA3	4:E:17:PHE:HE1	1.82	0.43
2:C:30:ILE:N	2:C:30:ILE:HD12	2.34	0.43
2:C:202:ARG:HH12	2:C:368:ARG:HH22	1.66	0.43
3:D:1171:GLY:C	3:D:1193:TRP:HZ3	2.21	0.43
3:D:1355:ARG:NH2	3:D:1369:ARG:HH12	2.17	0.43
3:D:262:THR:OG1	3:D:263:SER:N	2.52	0.43
3:D:848:VAL:HG13	3:D:857:LEU:HD13	2.00	0.43
5:F:227:GLN:HG3	5:F:252:LEU:HA	2.00	0.43
2:I:107:ARG:HA	2:I:108:GLU:HA	1.71	0.43
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.29	0.43
3:J:1371:ARG:O	3:J:1371:ARG:HG2	2.16	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.71	0.43
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.19	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.19	0.43
3:J:768:ASN:HD21	3:J:770:LEU:HD23	1.84	0.43
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.41	0.43
5:L:449:THR:OG1	5:L:503:GLU:OE1	2.36	0.43
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.43
2:C:211:ARG:HA	2:C:215:TYR:O	2.18	0.43
3:D:516:ASP:HA	3:D:545:HIS:HB2	2.00	0.43
3:D:588:PRO:HB2	3:D:590:SER:OG	2.19	0.43
2:I:1204:LEU:HB3	2:I:1205:PRO:HD2	2.00	0.43
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.00	0.43
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.01	0.43
4:K:13:ILE:HD11	4:K:54:ILE:HG23	2.01	0.43
5:L:414:LYS:HD3	5:L:434:TRP:CZ3	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD22	1:A:275:ILE:HG21	2.00	0.43
1:A:78:ILE:HA	1:A:81:ILE:HG13	2.00	0.43
2:C:324:LYS:C	2:C:327:GLN:HE21	2.16	0.43
2:C:600:THR:HG21	2:C:602:GLU:HG2	2.00	0.43
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.99	0.43
2:C:739:ASP:N	2:C:739:ASP:OD1	2.45	0.43
2:C:738:GLU:HA	2:C:741:MET:CE	2.48	0.43
3:D:1175:LEU:HD12	3:D:1175:LEU:HA	1.86	0.43
3:D:1184:ASP:N	3:D:1185:PRO:HD3	2.33	0.43
3:D:1279:GLN:NE2	3:D:1317:GLU:OE2	2.52	0.43
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.49	0.43
3:D:825:VAL:HG22	3:D:833:GLU:N	2.32	0.43
1:H:219:ARG:HA	1:H:222:THR:HB	2.01	0.43
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.34	0.43
2:I:170:VAL:CG2	2:I:172:TYR:CZ	2.99	0.43
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.83	0.43
2:I:805:MET:HE3	2:I:805:MET:HB2	1.74	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:CD2	2.47	0.43
3:J:19:ALA:H	3:J:1344:LEU:HD12	1.84	0.43
3:J:528:THR:HG22	3:J:532:GLU:HB3	1.99	0.43
3:J:592:VAL:HA	3:J:596:LEU:HD21	2.01	0.43
3:J:75:TYR:OH	3:J:86:GLU:OE2	2.35	0.43
5:L:414:LYS:O	5:L:417:ASP:N	2.51	0.43
5:L:561:MET:HB2	5:L:561:MET:HE3	1.52	0.43
1:A:166:ARG:O	1:A:167:PRO:C	2.52	0.43
1:A:66:HIS:O	1:A:66:HIS:ND1	2.49	0.43
2:C:95:PRO:HA	2:C:126:GLU:HA	2.01	0.43
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.54	0.43
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.86	0.43
3:D:278:ARG:O	3:D:282:LEU:HG	2.19	0.43
3:D:303:VAL:O	3:D:306:LEU:HB3	2.19	0.43
3:D:797:THR:HG22	3:D:924:GLY:HA3	2.00	0.43
5:F:139:GLU:HG2	5:F:351:THR:HA	2.01	0.43
5:F:467:SER:O	5:F:471:LEU:N	2.52	0.43
1:G:107:ILE:HG12	1:G:135:ASP:O	2.19	0.43
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.99	0.43
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.33	0.43
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.51	0.43
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.19	0.43
2:I:1305:TYR:CG	5:L:531:PRO:HB2	2.53	0.43
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.00	0.43
3:J:223:LEU:O	3:J:226:ALA:HB3	2.18	0.43
3:J:654:ILE:O	3:J:658:GLU:HB2	2.18	0.43
5:L:227:GLN:HG3	5:L:252:LEU:HA	2.00	0.43
5:L:250:LEU:O	5:L:254:GLU:HG2	2.19	0.43
5:L:141:ILE:HD13	5:L:256:PHE:CD1	2.54	0.43
5:L:343:LYS:HA	5:L:346:GLN:HB3	2.01	0.43
5:L:397:ARG:HB3	5:L:443:ILE:HD13	2.00	0.43
5:L:96:ASP:OD2	5:L:98:VAL:HG13	2.19	0.43
1:A:300:LEU:HD13	1:A:304:LYS:HE2	2.00	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.01	0.43
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.76	0.43
2:C:250:THR:HA	2:C:268:ARG:HA	2.01	0.43
2:C:744:GLY:C	2:C:746:ALA:N	2.71	0.43
3:D:309:ASN:OD1	3:D:314:ARG:HA	2.18	0.43
3:D:681:LYS:O	3:D:685:ILE:HG23	2.19	0.43
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.43	0.43
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.43
3:D:762:ASN:OD1	3:D:765:GLU:HG3	2.19	0.43
1:H:65:LEU:CD2	1:H:171:LEU:HD21	2.47	0.43
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.01	0.43
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.54	0.43
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.22	0.43
2:I:125:GLY:CA	2:I:499:SER:HB2	2.45	0.43
2:I:854:ILE:HD11	2:I:885:GLY:HA3	2.00	0.43
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.01	0.43
3:J:404:GLU:HG2	3:J:409:TRP:CZ2	2.54	0.43
3:J:545:HIS:CD2	3:J:719:PHE:HE1	2.37	0.43
5:L:312:SER:OG	5:L:313:ASP:N	2.52	0.43
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.60	0.42
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.20	0.42
2:C:38:PHE:HB2	2:C:457:GLY:O	2.19	0.42
2:C:69:GLN:HG2	2:C:101:ARG:O	2.19	0.42
2:C:819:SER:HB3	2:C:1085:MET:SD	2.59	0.42
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	2.00	0.42
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	2.01	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
3:D:1199:PHE:HB2	3:D:1202:GLU:CB	2.46	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.19	0.42
3:D:847:ASP:CB	3:D:860:ARG:H	2.32	0.42
3:D:84:ILE:H	3:D:84:ILE:HG13	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:872:LEU:HD22	3:D:877:VAL:HG11	2.01	0.42
3:J:1167:LYS:O	3:J:1168:GLU:HG2	2.18	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.54	0.42
3:J:825:VAL:HG11	3:J:833:GLU:HB3	2.00	0.42
1:B:134:THR:HG23	1:B:135:ASP:N	2.34	0.42
2:C:63:SER:C	2:C:65:ASN:H	2.21	0.42
3:D:1252:HIS:O	3:D:1255:VAL:HG22	2.20	0.42
3:D:198:CYS:HA	3:D:221:ILE:CD1	2.49	0.42
3:D:427:PRO:O	3:D:429:LEU:HD22	2.19	0.42
1:B:48:LEU:CD2	3:D:535:ARG:HG3	2.48	0.42
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.42
1:G:18:GLN:HG3	1:G:24:ALA:HB2	2.02	0.42
1:G:31:LEU:HA	1:G:31:LEU:HD23	1.67	0.42
1:H:33:ARG:HD3	1:H:197:ASP:OD2	2.18	0.42
2:I:17:LYS:HZ3	2:I:17:LYS:HG3	1.30	0.42
2:I:315:MET:HB2	2:I:315:MET:HE3	1.92	0.42
2:I:47:TYR:OH	2:I:398:SER:HB2	2.19	0.42
2:I:734:ILE:O	2:I:748:ILE:HB	2.18	0.42
2:I:870:ILE:HG22	2:I:944:ARG:HH11	1.81	0.42
3:J:912:GLY:HA2	3:J:1363:TYR:CD1	2.53	0.42
3:J:521:LYS:NZ	3:J:540:GLY:O	2.51	0.42
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.54	0.42
3:J:641:ILE:HD13	3:J:644:MET:CE	2.48	0.42
3:J:742:GLY:O	3:J:762:ASN:HB3	2.19	0.42
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
5:L:357:GLN:HA	5:L:360:ASP:HB2	2.01	0.42
2:C:1002:LEU:HD23	2:C:1003:THR:O	2.19	0.42
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.84	0.42
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.59	0.42
2:C:301:TYR:CE2	2:C:333:ILE:HA	2.53	0.42
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.54	0.42
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.49	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.55	0.42
3:D:140:TYR:O	3:D:297:ARG:NH1	2.52	0.42
3:D:193:ASP:CG	3:D:196:GLN:HG2	2.39	0.42
3:D:519:ASN:HA	3:D:523:GLU:OE1	2.19	0.42
3:D:817:HIS:CE1	3:D:860:ARG:NH2	2.87	0.42
4:E:49:ILE:O	4:E:53:GLU:HG3	2.19	0.42
5:F:98:VAL:O	5:F:102:MET:HB2	2.18	0.42
5:F:486:ARG:HG2	5:F:486:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HD13	1:G:173:VAL:HG12	2.01	0.42
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.42
1:H:178:SER:HA	1:H:179:PRO:HD3	1.76	0.42
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.34	0.42
3:J:1175:LEU:HD12	3:J:1175:LEU:HA	1.84	0.42
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.02	0.42
3:J:271:ARG:HB2	3:J:271:ARG:HE	1.40	0.42
3:J:382:TYR:CE1	3:J:398:LYS:HA	2.53	0.42
3:J:810:THR:HG22	3:J:894:VAL:H	1.84	0.42
5:L:338:HIS:HA	5:L:341:LEU:HB2	2.00	0.42
5:L:280:VAL:HG21	5:L:358:VAL:HG11	2.01	0.42
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.54	0.42
1:B:87:GLY:O	1:B:128:HIS:NE2	2.52	0.42
2:C:1230:MET:HE3	2:C:1230:MET:HB2	1.91	0.42
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.80	0.42
2:C:972:PHE:HB3	2:C:994:ARG:HH21	1.81	0.42
3:D:1183:SER:CB	3:D:1185:PRO:HD3	2.50	0.42
3:D:128:LEU:HA	3:D:192:MET:CE	2.50	0.42
3:D:98:ARG:O	3:D:248:ASP:HB2	2.19	0.42
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.40	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.76	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA3	2.00	0.42
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	2.01	0.42
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.60	0.42
2:I:671:LEU:HD23	2:I:1186:VAL:HG11	2.02	0.42
2:I:719:LYS:N	2:I:751:TYR:OH	2.52	0.42
2:I:800:MET:HE3	2:I:800:MET:HB3	1.87	0.42
2:I:976:ARG:CD	2:I:989:LEU:HD23	2.41	0.42
3:D:1301:THR:CG2	3:J:1301:THR:HG23	2.50	0.42
3:J:168:ALA:O	3:J:172:PHE:HD2	2.03	0.42
3:J:26:SER:O	3:J:30:ILE:HG13	2.19	0.42
3:J:809:VAL:HG12	3:J:911:LYS:HA	2.00	0.42
5:L:220:LYS:O	5:L:223:GLU:HB3	2.20	0.42
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.78	0.42
1:A:82:LEU:HB3	1:A:173:VAL:CG1	2.50	0.42
1:B:154:PRO:HD2	1:B:157:THR:OG1	2.20	0.42
2:C:614:TYR:CE1	2:C:652:TYR:HE1	2.37	0.42
3:D:253:VAL:HG21	5:F:523:ILE:HG21	2.01	0.42
3:D:42:GLU:HG2	3:D:52:GLU:HG2	2.00	0.42
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.54	0.42
3:D:872:LEU:O	3:D:877:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:811:GLU:O	3:D:895:CYS:HA	2.20	0.42
1:G:222:THR:O	1:G:226:GLU:HB2	2.19	0.42
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.19	0.42
2:I:1106:ARG:HB3	2:I:1108:ASN:ND2	2.34	0.42
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.19	0.42
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.42
2:I:845:LEU:H	2:I:845:LEU:HG	1.49	0.42
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.52	0.42
3:J:894:VAL:HG22	3:J:1258:ARG:HH11	1.85	0.42
3:J:1273:ASP:HB3	3:J:1276:GLU:CD	2.40	0.42
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.85	0.42
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.53	0.42
3:J:735:ALA:O	3:J:738:ARG:HB3	2.19	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.35	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.34	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.20	0.42
1:A:150:ARG:HH11	1:B:6:THR:N	2.18	0.42
1:A:315:GLY:C	1:A:316:MET:HG3	2.39	0.42
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.99	0.42
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.01	0.42
1:B:196:THR:HG22	1:B:197:ASP:N	2.35	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.20	0.42
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.83	0.42
2:C:98:VAL:HB	2:C:124:MET:HE3	2.00	0.42
2:C:138:ILE:HG22	2:C:139:ASN:N	2.35	0.42
2:C:168:GLY:O	2:C:170:VAL:N	2.34	0.42
2:C:202:ARG:HH11	2:C:369:MET:CB	2.31	0.42
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.34	0.42
2:C:885:GLY:HA2	2:C:917:SER:HB3	2.02	0.42
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.54	0.42
1:G:58:GLU:CD	1:G:145:LYS:HE3	2.39	0.42
1:G:224:LEU:HD22	1:H:228:LEU:CD1	2.49	0.42
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.42
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.71	0.42
2:I:147:SER:HB2	2:I:529:ARG:O	2.20	0.42
2:I:812:PHE:HZ	3:J:503:SER:CB	2.32	0.42
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.50	0.42
3:J:885:VAL:HG22	3:J:885:VAL:H	1.49	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HD3	2.01	0.42
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.55	0.42
1:A:182:ARG:O	1:A:183:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:N	2.34	0.42
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	2.19	0.42
2:C:317:LEU:HD11	2:C:333:ILE:HG21	2.02	0.42
2:C:960:LEU:HD13	2:C:960:LEU:HA	1.75	0.42
3:D:641:ILE:HD13	3:D:644:MET:CE	2.49	0.42
3:D:689:ALA:O	3:D:692:ARG:HB2	2.19	0.42
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.01	0.42
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.91	0.42
1:H:48:LEU:HG	1:H:183:ILE:HD11	2.01	0.42
2:I:23:ASP:N	2:I:23:ASP:OD1	2.38	0.42
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.87	0.42
2:I:672:GLU:HG3	2:I:672:GLU:H	1.27	0.42
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.49	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.20	0.42
5:L:112:THR:O	5:L:116:GLU:HG3	2.19	0.42
5:L:399:LEU:HG	5:L:403:ASP:HB3	2.02	0.42
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.49	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.30	0.42
2:C:150:HIS:CD2	2:C:150:HIS:N	2.87	0.42
2:C:39:ILE:O	2:C:40:GLU:HB2	2.20	0.42
2:C:88:ARG:HB3	2:C:90:VAL:HG23	2.01	0.42
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.42
3:D:372:MET:O	3:D:376:LEU:HD12	2.20	0.42
3:D:710:ASP:CG	3:D:711:GLY:N	2.73	0.42
5:F:111:LEU:HA	5:F:111:LEU:HD23	1.77	0.42
5:F:117:ILE:HA	5:F:120:ALA:HB3	2.00	0.42
5:F:253:SER:O	5:F:257:LYS:HG3	2.20	0.42
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
2:I:210:LEU:HB2	2:I:220:ILE:HD11	2.02	0.42
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.32	0.42
2:I:697:LYS:HA	2:I:795:ALA:HB2	2.02	0.42
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.50	0.42
2:I:830:THR:HG23	2:I:832:HIS:NE2	2.35	0.42
2:I:943:LYS:O	2:I:947:GLU:HG3	2.20	0.42
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.50	0.42
3:J:521:LYS:HD2	3:J:541:LEU:O	2.18	0.42
5:L:292:VAL:HA	5:L:297:MET:O	2.19	0.42
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.51	0.42
2:I:856:ASN:CB	5:L:613:ASP:HA	2.50	0.42
2:C:48:GLY:H	2:C:51:ALA:HB3	1.84	0.42
2:C:615:VAL:HG22	2:C:650:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.02	0.42
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.23	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.02	0.42
3:D:718:SER:OG	3:D:720:ASN:HB3	2.20	0.42
3:D:903:LEU:HB3	3:D:905:ARG:N	2.35	0.42
3:D:63:GLY:HA3	3:D:98:ARG:HG3	2.01	0.42
5:F:414:LYS:HD3	5:F:434:TRP:CZ3	2.55	0.42
5:F:448:ARG:HE	5:F:448:ARG:HB3	1.70	0.42
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.70	0.42
5:F:499:LYS:HA	5:F:502:LYS:HE2	2.00	0.42
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.02	0.42
1:G:40:GLY:HA2	1:G:201:LEU:HD21	2.02	0.42
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.54	0.42
2:I:421:SER:H	2:I:424:ASP:HB2	1.85	0.42
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.48	0.42
2:I:971:LEU:HG	2:I:1014:LEU:HD23	2.01	0.42
3:J:1173:ARG:HH21	3:J:1196:LEU:HD21	1.85	0.42
3:J:423:LEU:HB3	3:J:466:MET:CE	2.50	0.42
3:J:422:LEU:O	3:J:468:VAL:HA	2.19	0.42
3:J:701:LEU:HD12	3:J:723:TYR:HD2	1.85	0.42
3:J:835:LEU:HG	3:J:839:VAL:CG2	2.49	0.42
3:J:857:LEU:HD12	3:J:858:VAL:H	1.84	0.42
3:J:885:VAL:HG12	3:J:894:VAL:CG1	2.50	0.42
1:A:46:ILE:CG2	1:A:223:ILE:HD12	2.50	0.42
2:C:1164:PHE:C	2:C:1166:ASP:H	2.23	0.42
2:C:622:ASN:O	2:C:630:VAL:HB	2.20	0.42
3:D:1162:ILE:HD12	3:D:1163:VAL:H	1.85	0.42
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.34	0.42
3:D:823:THR:HA	3:D:835:LEU:HD13	2.02	0.42
3:D:915:ILE:HA	3:D:918:ILE:HG23	2.01	0.42
1:G:115:ILE:HG22	1:G:116:THR:N	2.35	0.42
1:H:47:LEU:O	1:H:180:VAL:HG21	2.20	0.42
2:I:1134:GLN:NE2	2:I:1136:GLN:OE1	2.53	0.42
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.42
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.90	0.42
2:I:836:LEU:HD21	2:I:921:PRO:HD3	2.01	0.42
3:J:116:PHE:O	3:J:123:ARG:HB2	2.20	0.42
3:J:537:TYR:CE2	3:J:544:LEU:HD22	2.54	0.42
3:J:54:ASP:HB3	3:J:60:ARG:HH11	1.85	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.50	0.42
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:54:ILE:HA	4:K:59:ILE:O	2.20	0.42
5:L:418:LYS:HD2	5:L:434:TRP:CH2	2.55	0.42
1:A:73:GLY:C	1:A:134:THR:HG22	2.41	0.41
1:A:231:PHE:HE1	1:B:28:LEU:HD23	1.85	0.41
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.50	0.41
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.28	0.41
2:C:202:ARG:NH1	2:C:369:MET:HB2	2.35	0.41
2:C:6:THR:HG21	2:C:782:VAL:HG23	2.01	0.41
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	2.33	0.41
3:D:358:GLY:N	3:D:359:PRO:HD3	2.35	0.41
5:F:313:ASP:CG	5:F:338:HIS:HE2	2.23	0.41
5:F:504:PRO:C	5:F:505:ILE:HD12	2.40	0.41
1:H:10:LYS:HA	1:H:11:PRO:HD3	1.82	0.41
2:I:1121:ALA:HB2	2:I:1182:ILE:CD1	2.49	0.41
2:I:1276:TRP:HA	2:I:1279:GLU:OE1	2.19	0.41
2:I:170:VAL:HG21	2:I:172:TYR:OH	2.19	0.41
2:I:397:LEU:O	2:I:398:SER:OG	2.22	0.41
2:I:525:THR:HG21	2:I:687:ARG:CD	2.50	0.41
2:I:62:TYR:O	2:I:64:GLY:N	2.53	0.41
2:I:898:GLU:HB3	5:L:540:LEU:CD2	2.45	0.41
3:J:1250:ASP:O	3:J:1251:LYS:C	2.58	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.73	0.41
3:J:641:ILE:HD13	3:J:644:MET:HE3	2.01	0.41
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.50	0.41
3:J:88:CYS:O	3:J:90:VAL:N	2.53	0.41
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.66	0.41
5:L:117:ILE:HG23	5:L:421:TYR:CE1	2.55	0.41
1:A:27:THR:O	1:A:28:LEU:HD12	2.20	0.41
1:A:98:VAL:HG22	1:A:100:LEU:HD12	2.02	0.41
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.87	0.41
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.02	0.41
2:C:1192:GLU:O	2:C:1195:ILE:HB	2.20	0.41
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.86	0.41
2:C:455:SER:HA	2:C:459:MET:HE2	2.02	0.41
2:C:494:ASN:HB3	2:C:497:PRO:CD	2.50	0.41
2:C:632:ASP:HB2	2:C:633:LEU:HD23	2.02	0.41
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.41
2:C:1281:TYR:CD2	3:D:431:ARG:HB2	2.55	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.19	0.41
3:D:712:GLN:HG2	3:D:712:GLN:H	1.51	0.41
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.41
5:F:470:MET:O	5:F:478:PRO:HD3	2.20	0.41
1:H:73:GLY:HA2	1:H:134:THR:CG2	2.36	0.41
2:I:820:GLU:N	2:I:1080:ASN:O	2.53	0.41
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.55	0.41
2:I:698:PRO:HA	2:I:1231:TYR:CE1	2.54	0.41
2:I:202:ARG:HG3	2:I:202:ARG:H	1.73	0.41
2:I:718:ALA:HB2	2:I:783:LEU:HD23	2.01	0.41
2:I:920:VAL:HG13	2:I:921:PRO:HD2	2.01	0.41
3:J:491:LEU:HD23	3:J:498:PRO:HA	2.00	0.41
3:J:64:PRO:O	3:J:95:THR:OG1	2.33	0.41
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.02	0.41
3:J:85:CYS:SG	3:J:86:GLU:N	2.93	0.41
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.60	0.41
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.85	0.41
5:L:165:PHE:HE1	5:L:259:PHE:CD2	2.37	0.41
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.02	0.41
1:A:36:GLY:C	1:A:187:VAL:HG11	2.40	0.41
1:A:18:GLN:HA	1:A:24:ALA:CB	2.49	0.41
1:A:8:PHE:HE1	1:A:32:GLU:OE1	2.04	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.41
2:C:671:LEU:HD23	2:C:1186:VAL:CG1	2.50	0.41
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.41
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.70	0.41
3:D:278:ARG:HG2	3:D:278:ARG:O	2.20	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.83	0.41
5:F:320:ILE:O	5:F:327:SER:HB3	2.21	0.41
1:G:189:ALA:HB1	1:G:191:ARG:NH2	2.35	0.41
1:G:44:ARG:HG3	1:G:183:ILE:CG2	2.45	0.41
2:I:971:LEU:HD11	2:I:1014:LEU:O	2.19	0.41
2:I:15:PHE:CE1	2:I:1194:GLU:HB3	2.56	0.41
2:I:237:LEU:HA	2:I:237:LEU:HD13	1.72	0.41
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.84	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41
3:J:1162:ILE:HD12	3:J:1163:VAL:N	2.35	0.41
3:J:293:ARG:O	3:J:294:ASN:C	2.57	0.41
3:J:515:ARG:NH2	3:J:717:VAL:HG23	2.34	0.41
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:271:ASN:O	5:L:275:VAL:HG23	2.20	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.19	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.83	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.84	0.41
2:C:658:GLN:O	2:C:660:VAL:N	2.54	0.41
2:C:12:ARG:NE	2:C:793:GLU:OE1	2.39	0.41
2:C:896:THR:HB	2:C:897:PRO:HD2	2.02	0.41
3:D:646:ILE:HG12	3:D:646:ILE:H	1.58	0.41
3:D:701:LEU:HD12	3:D:723:TYR:CD2	2.51	0.41
3:D:723:TYR:CE1	3:D:727:ASP:HB2	2.55	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.54	0.41
5:F:344:LEU:O	5:F:355:ILE:HD11	2.19	0.41
1:G:190:ALA:HA	1:G:200:LYS:HE2	2.02	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.02	0.41
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.33	0.41
2:I:571:LEU:HD23	2:I:571:LEU:HA	1.62	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.65	0.41
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.73	0.41
2:I:550:VAL:CG1	3:J:777:HIS:HA	2.50	0.41
3:J:796:LEU:HA	3:J:796:LEU:HD12	1.64	0.41
5:L:157:ARG:HB3	5:L:160:ASP:OD2	2.19	0.41
5:L:381:GLU:O	5:L:384:LEU:HG	2.20	0.41
1:A:22:THR:O	1:A:207:THR:N	2.37	0.41
1:A:92:VAL:HG11	1:A:98:VAL:HG11	2.03	0.41
1:B:51:MET:HB3	1:B:178:SER:HB2	2.01	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.02	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HG2	2.02	0.41
2:C:848:GLU:CG	2:C:888:THR:HG22	2.50	0.41
2:C:850:ILE:O	2:C:850:ILE:HG22	2.21	0.41
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.02	0.41
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.55	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.02	0.41
3:D:654:ILE:O	3:D:658:GLU:N	2.49	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.20	0.41
3:D:832:LYS:NZ	3:D:1243:LEU:HD12	2.35	0.41
5:F:124:GLU:O	5:F:128:ASN:HB2	2.21	0.41
5:F:388:ILE:O	5:F:392:LYS:HG3	2.21	0.41
1:G:102:LEU:HD23	1:G:115:ILE:CG1	2.45	0.41
1:H:134:THR:HG23	1:H:135:ASP:N	2.34	0.41
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.21	0.41
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.36	0.41
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.55	0.41
2:I:49:LEU:HB2	2:I:73:TYR:CZ	2.56	0.41
2:I:836:LEU:HD11	2:I:1054:LEU:HD22	2.02	0.41
3:J:116:PHE:O	3:J:124:ILE:HG13	2.20	0.41
3:J:138:VAL:HG21	3:J:145:VAL:HB	2.02	0.41
3:J:616:PRO:HA	3:J:619:ILE:HG22	2.03	0.41
3:J:825:VAL:HG13	3:J:833:GLU:HB3	2.02	0.41
4:K:44:ASP:HB2	4:K:49:ILE:HG13	2.01	0.41
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.03	0.41
1:A:295:LEU:HD22	1:A:300:LEU:HB2	2.02	0.41
1:A:54:CYS:HB3	1:A:148:ARG:HD3	2.02	0.41
1:A:56:VAL:CG2	1:A:144:ILE:HG23	2.51	0.41
1:B:108:GLY:HA2	1:B:109:PRO:HD3	1.83	0.41
1:B:98:VAL:HG11	1:B:121:VAL:HG22	2.03	0.41
2:C:626:GLU:HB2	2:C:628:HIS:CE1	2.56	0.41
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.02	0.41
2:C:921:PRO:HB2	2:C:924:VAL:HG22	2.03	0.41
3:D:368:LEU:CD2	3:D:373:ALA:HB2	2.48	0.41
5:F:281:ARG:HH11	5:F:281:ARG:HD2	1.71	0.41
5:F:519:LEU:C	5:F:519:LEU:HD23	2.41	0.41
5:F:583:THR:HG22	5:F:584:ARG:N	2.35	0.41
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.78	0.41
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.20	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:O	2.19	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.03	0.41
2:I:209:ILE:HD13	2:I:209:ILE:HG21	1.84	0.41
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.41
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.86	0.41
3:J:678:ARG:O	3:J:682:VAL:HG23	2.20	0.41
3:J:860:ARG:HD2	3:J:860:ARG:HA	1.89	0.41
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.94	0.41
1:A:18:GLN:HA	1:A:24:ALA:HB2	2.03	0.41
1:A:260:LEU:HB2	1:A:262:LEU:HG	2.02	0.41
1:B:15:ASP:O	1:B:27:THR:HG23	2.21	0.41
2:C:297:VAL:HG12	2:C:315:MET:O	2.20	0.41
2:C:421:SER:H	2:C:424:ASP:CB	2.33	0.41
2:C:136:PHE:HE2	2:C:456:VAL:HG11	1.85	0.41
2:C:906:PHE:HE2	5:F:608:ARG:NH1	2.19	0.41
3:D:1178:THR:HA	3:D:1179:PRO:HD3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1266:ILE:HD12	3:D:1274:PHE:N	2.36	0.41
3:D:1345:ARG:HG2	3:D:1370:MET:CE	2.51	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.36	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41
5:F:310:GLU:O	5:F:344:LEU:HD21	2.21	0.41
1:G:49:SER:HB3	2:I:1083:GLU:OE2	2.21	0.41
1:H:203:ILE:HD12	1:H:203:ILE:N	2.36	0.41
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.50	0.41
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.19	0.41
2:I:1323:PHE:CE1	2:I:1327:LEU:HD11	2.56	0.41
2:I:385:PHE:CE2	2:I:390:PHE:HE2	2.38	0.41
2:I:511:LEU:HA	2:I:511:LEU:HD23	1.77	0.41
3:J:903:LEU:CD2	3:J:909:ILE:HD12	2.51	0.41
3:J:395:LYS:CG	5:L:536:THR:HG21	2.45	0.41
5:L:607:LEU:O	5:L:610:PHE:HB2	2.21	0.41
1:A:102:LEU:O	1:A:141:SER:HA	2.20	0.41
1:A:173:VAL:HG23	1:A:174:ASP:O	2.21	0.41
1:A:216:ALA:O	1:A:218:ARG:N	2.54	0.41
1:A:321:TRP:CE2	1:A:322:PRO:HB3	2.56	0.41
2:C:1281:TYR:CD2	2:C:1281:TYR:N	2.88	0.41
2:C:1288:GLN:O	2:C:1292:THR:HB	2.20	0.41
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.56	0.41
2:C:594:VAL:HG22	2:C:599:VAL:HG22	2.03	0.41
2:C:59:ILE:HG21	2:C:59:ILE:HD13	1.75	0.41
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.36	0.41
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.83	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.55	0.41
3:D:555:TYR:HB3	3:D:563:LEU:HD23	2.02	0.41
5:F:474:MET:O	5:F:476:ARG:N	2.48	0.41
1:G:31:LEU:HB2	1:G:199:ASP:O	2.21	0.41
1:G:51:MET:HB3	1:G:51:MET:HE3	1.93	0.41
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.56	0.41
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.56	0.41
2:I:211:ARG:NE	2:I:354:ASP:OD2	2.35	0.41
2:I:487:LEU:HD23	2:I:487:LEU:H	1.85	0.41
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.35	0.41
2:I:95:PRO:HB3	2:I:123:TYR:HE1	1.85	0.41
3:J:335:GLN:CB	3:J:336:GLY:HA3	2.51	0.41
2:I:1274:GLU:HG3	3:J:428:THR:OG1	2.19	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:H	1:A:174:ASP:HA	1.86	0.41
1:A:208:ASN:OD1	1:A:208:ASN:N	2.53	0.41
1:A:318:LEU:HD22	1:A:318:LEU:N	2.36	0.41
2:C:1250:SER:HB3	2:C:1259:LEU:O	2.21	0.41
2:C:420:LEU:HD23	2:C:420:LEU:HA	1.76	0.41
2:C:62:TYR:HE1	2:C:476:LYS:O	2.03	0.41
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.51	0.41
3:D:1347:LEU:O	3:D:1348:LYS:C	2.59	0.41
5:F:483:LEU:N	5:F:483:LEU:HD12	2.34	0.41
1:H:100:LEU:HD11	1:H:121:VAL:CG2	2.50	0.41
1:G:39:LEU:CD2	1:H:224:LEU:HD11	2.51	0.41
2:I:161:LYS:HA	2:I:170:VAL:HA	2.03	0.41
2:I:207:THR:HG21	2:I:351:LEU:HG	2.02	0.41
2:I:590:PRO:HG3	2:I:605:TYR:CE1	2.55	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.76	0.41
3:J:357:VAL:HB	3:J:358:GLY:H	1.75	0.41
3:J:504:GLN:HG3	3:J:505:ASP:H	1.86	0.41
3:J:527:LEU:HB3	3:J:532:GLU:CG	2.51	0.41
3:J:722:ILE:HD11	3:J:740:LEU:HD23	2.01	0.41
3:J:842:ARG:HB3	3:J:882:VAL:HG11	2.02	0.41
4:K:15:ASN:O	4:K:16:ARG:HB3	2.21	0.41
5:L:227:GLN:CG	5:L:252:LEU:HA	2.50	0.41
5:L:166:VAL:HG23	5:L:258:GLN:O	2.21	0.41
5:L:573:LEU:CD1	5:L:588:ARG:HE	2.33	0.41
1:B:192:VAL:O	1:B:194:GLN:N	2.53	0.41
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.56	0.41
2:C:757:THR:O	2:C:765:ILE:HG23	2.21	0.41
3:D:601:ILE:HG21	3:D:601:ILE:HD13	1.78	0.41
3:D:840:LEU:HD12	3:D:864:LEU:O	2.20	0.41
1:G:178:SER:HA	1:G:179:PRO:HD3	1.91	0.41
1:H:95:LYS:HZ3	1:H:98:VAL:HG23	1.84	0.41
2:I:519:ASN:HB3	2:I:522:SER:CB	2.51	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:CG	2.51	0.41
3:J:1372:ARG:HE	3:J:1372:ARG:HB2	1.64	0.41
3:J:156:ARG:NH1	3:J:157:GLN:NE2	2.69	0.41
3:J:294:ASN:O	3:J:298:MET:HG3	2.21	0.41
3:J:805:GLN:HB3	3:J:806:ASP:H	1.73	0.41
5:L:291:CYS:HB3	5:L:297:MET:SD	2.61	0.41
5:L:138:PRO:HB2	5:L:351:THR:O	2.20	0.41
5:L:96:ASP:O	5:L:98:VAL:N	2.54	0.41
1:A:107:ILE:H	1:A:107:ILE:HG13	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:OE1	1:A:172:LEU:HD21	2.21	0.41
1:B:38:THR:HG23	1:B:39:LEU:H	1.85	0.41
1:B:48:LEU:CD1	1:B:183:ILE:HD11	2.50	0.41
2:C:22:LEU:HD22	2:C:23:ASP:N	2.36	0.41
2:C:369:MET:O	2:C:372:PRO:HD3	2.21	0.41
2:C:666:SER:OG	2:C:704:MET:HG3	2.21	0.41
1:A:134:THR:HG21	2:C:727:VAL:O	2.21	0.41
3:D:307:LEU:HD23	3:D:307:LEU:HA	1.81	0.41
3:D:339:ARG:O	3:D:340:GLN:HG2	2.20	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.21	0.41
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.36	0.41
5:F:465:ARG:HB3	5:F:468:ARG:HH12	1.86	0.41
5:F:95:THR:O	5:F:96:ASP:C	2.59	0.41
1:G:134:THR:HG23	1:G:135:ASP:N	2.36	0.41
2:I:211:ARG:NH2	2:I:351:LEU:HD22	2.36	0.41
2:I:405:PHE:CE2	2:I:409:LEU:HD12	2.56	0.41
2:I:569:ILE:C	2:I:571:LEU:H	2.23	0.41
2:I:974:ARG:HD2	2:I:1014:LEU:CD2	2.51	0.41
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.95	0.41
3:J:234:PRO:HD2	3:J:235:GLU:OE2	2.21	0.41
3:J:369:PRO:HB3	3:J:444:GLY:O	2.20	0.41
3:J:440:VAL:O	3:J:442:ILE:HG12	2.21	0.41
5:L:463:LEU:HA	5:L:463:LEU:HD23	1.73	0.41
1:A:182:ARG:HG2	1:A:183:ILE:N	2.36	0.40
1:B:133:LEU:HD11	1:B:140:ILE:HG21	2.03	0.40
2:C:1303:LYS:HD3	2:C:1303:LYS:HA	1.78	0.40
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.03	0.40
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.36	0.40
3:D:113:HIS:ND1	3:D:113:HIS:C	2.74	0.40
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.36	0.40
3:D:277:ASN:HA	3:D:280:LYS:HG3	2.03	0.40
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.03	0.40
3:D:664:ILE:HG22	3:D:678:ARG:HG2	2.02	0.40
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.52	0.40
1:G:26:VAL:HG22	1:G:203:ILE:HB	2.04	0.40
1:H:6:THR:O	1:H:6:THR:HG22	2.21	0.40
2:I:197:ARG:HH12	2:I:203:LYS:HB2	1.86	0.40
2:I:402:ARG:HG2	2:I:416:GLY:H	1.86	0.40
2:I:559:CYS:CB	2:I:662:SER:HB3	2.50	0.40
2:I:663:VAL:H	2:I:663:VAL:HG22	1.51	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.96	0.40
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.03	0.40
3:J:481:ARG:O	3:J:485:MET:HB2	2.20	0.40
5:L:409:ASN:O	5:L:413:MET:HG3	2.22	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
1:A:83:LEU:HB3	2:C:694:ARG:NH2	2.36	0.40
2:C:1146:GLN:O	2:C:1150:ASP:OD2	2.39	0.40
2:C:121:GLU:HG3	2:C:121:GLU:H	1.57	0.40
2:C:271:ALA:O	2:C:275:ARG:HG3	2.21	0.40
2:C:62:TYR:CE1	2:C:476:LYS:HB3	2.56	0.40
2:C:530:ILE:O	2:C:572:ILE:O	2.40	0.40
3:D:1327:GLU:HG2	3:D:1328:THR:N	2.35	0.40
3:D:1357:ILE:O	3:D:1362:GLY:HA3	2.21	0.40
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.03	0.40
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.40
3:D:466:MET:HB3	3:D:466:MET:HE2	1.98	0.40
3:D:489:ASN:HA	3:D:904:ALA:HB1	2.03	0.40
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.90	0.40
5:F:599:ARG:O	5:F:604:SER:HB2	2.21	0.40
1:G:75:GLN:HG3	1:G:76:GLU:OE2	2.21	0.40
1:G:45:ARG:CG	1:H:38:THR:HB	2.36	0.40
1:H:86:LYS:HD2	1:H:174:ASP:HB2	2.03	0.40
2:I:136:PHE:CE1	2:I:506:PHE:HE2	2.40	0.40
2:I:564:PRO:HG2	2:I:568:ASN:O	2.20	0.40
2:I:85:CYS:SG	2:I:92:TYR:HA	2.61	0.40
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.86	0.40
3:J:1233:ILE:HG22	3:J:1234:VAL:N	2.36	0.40
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.77	0.40
5:L:164:GLY:O	5:L:260:ARG:HB2	2.20	0.40
2:C:9:LYS:O	2:C:1175:ASN:ND2	2.53	0.40
2:C:1064:ASP:OD1	2:C:1239:VAL:HG12	2.22	0.40
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	2.03	0.40
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.56	0.40
2:C:616:ILE:HG13	2:C:652:TYR:HB2	2.03	0.40
2:C:656:SER:OG	2:C:658:GLN:HB2	2.21	0.40
2:C:800:MET:HB3	2:C:800:MET:HE3	1.81	0.40
2:C:72:SER:O	2:C:98:VAL:HG13	2.21	0.40
3:D:1353:VAL:O	3:D:1353:VAL:HG22	2.22	0.40
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.86	0.40
2:C:1281:TYR:OH	3:D:434:ILE:O	2.39	0.40
3:D:57:PHE:CD2	3:D:57:PHE:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:406:GLN:NE2	5:F:406:GLN:HA	2.36	0.40
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.74	0.40
1:H:100:LEU:HB3	1:H:115:ILE:HG22	2.02	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.03	0.40
2:I:579:ALA:O	2:I:580:GLN:HG3	2.21	0.40
2:I:606:LEU:HD23	2:I:611:GLU:HA	2.04	0.40
2:I:726:TYR:CZ	2:I:728:ASP:HB2	2.56	0.40
2:I:517:GLN:NE2	2:I:759:SER:HA	2.37	0.40
2:I:920:VAL:HA	2:I:921:PRO:HD3	1.92	0.40
3:J:401:VAL:HA	3:J:408:VAL:HG11	2.02	0.40
3:J:511:TYR:HE1	3:J:724:MET:CG	2.33	0.40
3:J:511:TYR:CE1	3:J:724:MET:HG2	2.53	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.40
5:L:568:ASN:ND2	5:L:568:ASN:H	2.19	0.40
1:B:19:VAL:O	1:B:23:HIS:HB3	2.21	0.40
2:C:10:ARG:HD3	2:C:1181:PRO:CG	2.46	0.40
2:C:838:CYS:HB2	2:C:918:LEU:HB3	2.03	0.40
3:D:1372:ARG:HE	3:D:1372:ARG:HB2	1.73	0.40
3:D:45:ASN:O	3:D:46:TYR:CB	2.70	0.40
5:F:316:PHE:CE1	5:F:337:VAL:HB	2.57	0.40
5:F:426:LYS:HE2	5:F:428:SER:OG	2.22	0.40
5:F:551:LEU:HD11	5:F:598:LEU:HD21	2.02	0.40
1:G:74:VAL:HG21	1:G:81:ILE:HD11	2.04	0.40
1:H:88:LEU:HD21	1:H:115:ILE:CD1	2.51	0.40
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.84	0.40
2:I:964:LEU:HD21	2:I:1022:LYS:HD2	2.03	0.40
2:I:197:ARG:HH22	2:I:203:LYS:HE2	1.86	0.40
2:I:337:PHE:CE2	2:I:343:HIS:HD2	2.40	0.40
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.85	0.40
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	2.04	0.40
3:J:268:LEU:HD22	3:J:306:LEU:HA	2.03	0.40
3:J:452:LEU:HD23	3:J:452:LEU:HA	1.81	0.40
3:J:41:PRO:HA	3:J:56:LEU:HD11	2.02	0.40
3:J:722:ILE:HG21	3:J:722:ILE:HD13	1.79	0.40
4:K:22:VAL:HG13	4:K:64:LEU:CD1	2.51	0.40
5:L:431:ALA:O	5:L:434:TRP:N	2.55	0.40
1:A:34:GLY:C	1:A:36:GLY:N	2.75	0.40
1:A:67:GLU:HG2	1:A:67:GLU:H	1.46	0.40
2:C:107:ARG:HA	2:C:108:GLU:HA	1.52	0.40
2:C:161:LYS:HA	2:C:170:VAL:HA	2.04	0.40
2:C:133:ASN:ND2	2:C:713:GLY:HA3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:723:VAL:HG12	2:C:724:VAL:N	2.37	0.40
2:C:901:LEU:HD12	2:C:901:LEU:O	2.21	0.40
3:D:34:SER:OG	3:D:103:GLY:HA2	2.21	0.40
3:D:121:PRO:HD2	3:D:123:ARG:HH21	1.86	0.40
3:D:647:PRO:HD3	3:D:697:MET:HB3	2.04	0.40
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.66	0.40
5:F:437:GLN:HG3	5:F:438:ALA:N	2.35	0.40
5:F:547:VAL:HG13	5:F:598:LEU:CD2	2.46	0.40
1:G:155:ALA:HA	1:G:158:ARG:HG3	2.03	0.40
1:G:219:ARG:HB2	1:G:219:ARG:HE	1.68	0.40
1:G:224:LEU:HD23	1:G:224:LEU:O	2.22	0.40
1:H:155:ALA:HB2	1:H:174:ASP:N	2.36	0.40
2:I:810:TYR:HB3	2:I:817:LEU:HD23	2.03	0.40
2:I:979:LEU:HD23	2:I:989:LEU:CD2	2.52	0.40
2:I:989:LEU:HD13	2:I:1000:LEU:HD13	2.04	0.40
3:J:1262:ARG:HH11	3:J:1262:ARG:HD3	1.73	0.40
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.87	0.40
3:J:804:ALA:O	3:J:806:ASP:N	2.54	0.40
5:L:219:GLU:O	5:L:222:ALA:HB3	2.21	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	
1	A	317/329 (96%)	243 (77%)	48 (15%)	26 (8%)	1	10
1	B	213/329 (65%)	193 (91%)	15 (7%)	5 (2%)	6	38
1	G	225/329 (68%)	195 (87%)	21 (9%)	9 (4%)	3	26
1	H	212/329 (64%)	193 (91%)	15 (7%)	4 (2%)	8	42
2	C	1338/1342 (100%)	1210 (90%)	111 (8%)	17 (1%)	12	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	1338/1342 (100%)	1207 (90%)	112 (8%)	19 (1%)	11	48
3	D	1157/1407 (82%)	1031 (89%)	101 (9%)	25 (2%)	6	39
3	J	1146/1407 (81%)	1032 (90%)	92 (8%)	22 (2%)	8	42
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	6	38
4	K	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	12	49
5	F	462/613 (75%)	424 (92%)	30 (6%)	8 (2%)	9	44
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	44
All	All	7035/8222 (86%)	6307 (90%)	582 (8%)	146 (2%)	7	40

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	107	ILE
1	A	114	ASP
1	A	136	GLU
1	A	195	ARG
1	A	217	ILE
1	A	232	VAL
1	A	320	ASN
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1159	VAL
3	D	339	ARG
3	D	341	ASN
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	566	ASP
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO

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Mol	Chain	Res	Type
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	426	ALA
3	J	710	ASP
3	J	850	LYS
3	J	1169	THR
3	J	1294	ALA
5	L	490	PRO
5	L	569	THR
5	L	584	ARG
1	A	14	VAL
1	A	104	LYS
1	A	162	GLU
1	A	167	PRO
1	A	177	TYR
1	A	179	PRO
1	A	242	VAL
1	A	319	GLU
2	C	121	GLU
2	C	747	GLY
2	C	897	PRO
2	C	1059	ARG
2	C	1153	ALA
2	C	1165	SER
3	D	10	ALA
3	D	13	LYS
3	D	49	PHE
3	D	417	ARG
3	D	745	GLY
3	D	805	GLN
3	D	850	LYS
5	F	569	THR
1	G	9	LEU

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Mol	Chain	Res	Type
1	G	14	VAL
1	G	196	THR
1	H	138	ALA
2	I	44	GLU
3	J	334	LYS
3	J	335	GLN
3	J	342	LEU
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
4	K	33	GLY
5	L	395	THR
5	L	475	GLY
5	L	566	ASP
1	A	52	PRO
1	A	196	THR
1	A	216	ALA
2	C	983	GLY
2	C	1154	ASP
3	D	46	TYR
3	D	806	ASP
3	D	1274	PHE
5	F	602	SER
1	G	62	ASP
1	H	193	GLU
2	I	983	GLY
2	I	1059	ARG
2	I	1165	SER
3	J	49	PHE
3	J	417	ARG
1	A	164	ASP
1	A	324	ALA
1	B	13	LEU
1	B	14	VAL
1	B	20	SER
2	C	63	SER
3	D	1297	LYS
3	D	1344	LEU
1	H	134	THR
2	I	201	ARG
3	J	46	TYR
5	L	96	ASP

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Mol	Chain	Res	Type
1	A	124	VAL
1	A	275	ILE
2	C	1151	LEU
3	D	454	CYS
5	F	96	ASP
5	F	395	THR
1	G	22	THR
1	H	20	SER
2	I	160	ASP
3	J	1180	VAL
3	J	1297	LYS
1	A	115	ILE
1	A	315	GLY
1	B	136	GLU
3	D	1180	VAL
1	G	232	VAL
2	I	892	GLU
3	J	314	ARG
3	J	712	GLN
3	D	89	GLY
3	D	831	VAL
5	F	475	GLY
2	C	1317	PRO
3	D	357	VAL
3	J	826	ILE
1	A	293	PRO
2	I	1186	VAL
3	J	89	GLY
5	L	97	PRO
3	D	828	GLY
4	E	86	ILE
2	I	1202	GLY
3	J	357	VAL
3	J	586	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	231 (83%)	47 (17%)	2	13
1	B	186/286 (65%)	172 (92%)	14 (8%)	13	45
1	G	193/286 (68%)	170 (88%)	23 (12%)	5	27
1	H	183/286 (64%)	170 (93%)	13 (7%)	14	48
2	C	1155/1157 (100%)	1048 (91%)	107 (9%)	9	38
2	I	1154/1157 (100%)	1055 (91%)	99 (9%)	10	41
3	D	964/1168 (82%)	867 (90%)	97 (10%)	7	35
3	J	962/1168 (82%)	869 (90%)	93 (10%)	8	36
4	E	72/75 (96%)	67 (93%)	5 (7%)	15	49
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	54
5	F	417/540 (77%)	376 (90%)	41 (10%)	8	36
5	L	418/540 (77%)	378 (90%)	40 (10%)	8	37
All	All	6049/7024 (86%)	5466 (90%)	583 (10%)	8	37

All (583) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	9	LEU
1	A	19	VAL
1	A	23	HIS
1	A	29	GLU
1	A	64	VAL
1	A	67	GLU
1	A	70	THR
1	A	74	VAL
1	A	77	ASP
1	A	79	LEU
1	A	83	LEU
1	A	98	VAL
1	A	102	LEU
1	A	104	LYS
1	A	110	VAL
1	A	137	ASN
1	A	140	ILE
1	A	145	LYS
1	A	156	SER
1	A	164	ASP

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	172	LEU
1	A	180	VAL
1	A	182	ARG
1	A	186	ASN
1	A	192	VAL
1	A	231	PHE
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	259	ASP
1	A	262	LEU
1	A	269	CYS
1	A	276	HIS
1	A	282	VAL
1	A	284	ARG
1	A	295	LEU
1	A	297	LYS
1	A	306	VAL
1	A	307	LEU
1	A	310	ARG
1	A	316	MET
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	B	16	ILE
1	B	18	GLN
1	B	27	THR
1	B	58	GLU
1	B	60	GLU
1	B	62	ASP
1	B	65	LEU
1	B	79	LEU
1	B	124	VAL
1	B	133	LEU
1	B	139	SER
1	B	183	ILE
1	B	191	ARG
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS

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Mol	Chain	Res	Type
2	C	23	ASP
2	C	46	GLN
2	C	55	SER
2	C	81	ASP
2	C	91	THR
2	C	107	ARG
2	C	108	GLU
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	131	THR
2	C	201	ARG
2	C	208	ILE
2	C	219	GLN
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	369	MET
2	C	419	ILE
2	C	423	ASP
2	C	451	ARG
2	C	456	VAL
2	C	484	LEU
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	521	LEU
2	C	539	THR
2	C	540	ARG
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	563	THR
2	C	604	HIS
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU

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Mol	Chain	Res	Type
2	C	635	THR
2	C	637	ARG
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	680	LEU
2	C	697	LYS
2	C	699	LEU
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	757	THR
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	782	VAL
2	C	791	LEU
2	C	800	MET
2	C	814	ASP
2	C	890	LYS
2	C	892	GLU
2	C	918	LEU
2	C	919	ARG
2	C	951	MET
2	C	979	LEU
2	C	984	VAL
2	C	992	LEU
2	C	1037	THR
2	C	1073	LYS
2	C	1076	ILE
2	C	1082	ILE
2	C	1090	ASN
2	C	1098	LEU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL

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Mol	Chain	Res	Type
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1206	THR
2	C	1233	LEU
2	C	1238	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1255	THR
2	C	1265	PHE
2	C	1269	ARG
2	C	1281	TYR
2	C	1287	LEU
2	C	1289	GLU
2	C	1299	ASN
2	C	1313	HIS
2	C	1327	LEU
2	C	1331	ARG
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	70	CYS
3	D	79	LYS
3	D	80	HIS
3	D	83	VAL
3	D	92	VAL
3	D	97	VAL
3	D	98	ARG
3	D	154	LEU
3	D	159	ILE
3	D	162	GLU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	218	THR
3	D	248	ASP

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Mol	Chain	Res	Type
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	269	TYR
3	D	324	LEU
3	D	330	MET
3	D	343	LEU
3	D	346	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	413	ASP
3	D	416	ILE
3	D	429	LEU
3	D	490	ILE
3	D	513	MET
3	D	532	GLU
3	D	536	LEU
3	D	544	LEU
3	D	545	HIS
3	D	563	LEU
3	D	568	SER
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	576	ARG
3	D	639	VAL
3	D	641	ILE
3	D	661	VAL
3	D	678	ARG
3	D	685	ILE
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	764	ARG
3	D	770	LEU
3	D	772	TYR
3	D	788	LEU

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Mol	Chain	Res	Type
3	D	797	THR
3	D	799	ARG
3	D	801	VAL
3	D	847	ASP
3	D	849	LEU
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	867	GLN
3	D	890	THR
3	D	897	HIS
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	913	GLU
3	D	918	ILE
3	D	1146	GLU
3	D	1155	ILE
3	D	1163	VAL
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1221	LEU
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1280	VAL
3	D	1283	SER
3	D	1332	LEU
3	D	1343	GLU
3	D	1361	THR
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	36	ASP
4	E	58	LEU
5	F	96	ASP
5	F	98	VAL
5	F	100	MET
5	F	102	MET

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Mol	Chain	Res	Type
5	F	114	GLU
5	F	154	GLU
5	F	230	VAL
5	F	261	LEU
5	F	267	ASP
5	F	277	MET
5	F	306	PHE
5	F	335	GLU
5	F	338	HIS
5	F	364	ARG
5	F	400	GLN
5	F	421	TYR
5	F	449	THR
5	F	450	ILE
5	F	469	GLN
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	529	GLU
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	559	LEU
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	573	LEU
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG

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Mol	Chain	Res	Type
1	G	50	SER
1	G	70	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	139	SER
1	G	145	LYS
1	G	158	ARG
1	G	163	GLU
1	G	166	ARG
1	G	168	ILE
1	G	171	LEU
1	G	178	SER
1	G	183	ILE
1	G	192	VAL
1	G	211	ILE
1	G	218	ARG
1	G	219	ARG
1	H	16	ILE
1	H	27	THR
1	H	38	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	124	VAL
1	H	133	LEU
1	H	176	CYS
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	17	LYS
2	I	23	ASP
2	I	46	GLN
2	I	60	GLN
2	I	91	THR
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE

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Mol	Chain	Res	Type
2	I	119	GLU
2	I	121	GLU
2	I	131	THR
2	I	156	PHE
2	I	179	TYR
2	I	201	ARG
2	I	208	ILE
2	I	219	GLN
2	I	285	ILE
2	I	306	THR
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	369	MET
2	I	419	ILE
2	I	423	ASP
2	I	445	ILE
2	I	451	ARG
2	I	456	VAL
2	I	484	LEU
2	I	490	GLN
2	I	492	MET
2	I	493	ILE
2	I	516	ASP
2	I	518	ASN
2	I	521	LEU
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	553	THR
2	I	558	VAL
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	635	THR
2	I	637	ARG
2	I	660	VAL
2	I	663	VAL

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Mol	Chain	Res	Type
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	724	VAL
2	I	739	ASP
2	I	742	TYR
2	I	748	ILE
2	I	757	THR
2	I	765	ILE
2	I	773	LEU
2	I	782	VAL
2	I	800	MET
2	I	814	ASP
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	967	LEU
2	I	979	LEU
2	I	992	LEU
2	I	1037	THR
2	I	1082	ILE
2	I	1114	GLU
2	I	1117	LEU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1206	THR
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1265	PHE
2	I	1287	LEU
2	I	1291	LEU
2	I	1299	ASN
2	I	1313	HIS
2	I	1326	LEU

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Mol	Chain	Res	Type
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	78	LEU
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	154	LEU
3	J	162	GLU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	218	THR
3	J	248	ASP
3	J	255	LEU
3	J	259	ARG
3	J	324	LEU
3	J	330	MET
3	J	342	LEU
3	J	343	LEU
3	J	345	LYS
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	429	LEU
3	J	490	ILE
3	J	510	LEU
3	J	513	MET
3	J	532	GLU
3	J	536	LEU
3	J	544	LEU
3	J	545	HIS

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Mol	Chain	Res	Type
3	J	563	LEU
3	J	568	SER
3	J	569	LEU
3	J	573	THR
3	J	605	LEU
3	J	641	ILE
3	J	661	VAL
3	J	678	ARG
3	J	698	MET
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	717	VAL
3	J	764	ARG
3	J	772	TYR
3	J	788	LEU
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	847	ASP
3	J	849	LEU
3	J	857	LEU
3	J	858	VAL
3	J	885	VAL
3	J	897	HIS
3	J	898	CYS
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1146	GLU
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1221	LEU
3	J	1251	LYS
3	J	1255	VAL
3	J	1261	LEU

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Mol	Chain	Res	Type
3	J	1266	ILE
3	J	1274	PHE
3	J	1284	ARG
3	J	1289	ASN
3	J	1290	ARG
3	J	1292	LEU
3	J	1293	GLU
3	J	1319	PHE
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
3	J	1355	ARG
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	28	ARG
4	K	39	VAL
5	L	98	VAL
5	L	102	MET
5	L	154	GLU
5	L	230	VAL
5	L	261	LEU
5	L	266	PHE
5	L	277	MET
5	L	297	MET
5	L	306	PHE
5	L	335	GLU
5	L	364	ARG
5	L	395	THR
5	L	421	TYR
5	L	445	ASP
5	L	449	THR
5	L	469	GLN
5	L	471	LEU
5	L	472	GLN
5	L	476	ARG
5	L	482	GLU
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	492	ASP
5	L	516	ASP

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Mol	Chain	Res	Type
5	L	527	THR
5	L	559	LEU
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	575	GLU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	268	ASN
1	B	84	ASN
1	B	117	HIS
2	C	120	GLN
2	C	139	ASN
2	C	150	HIS
2	C	343	HIS
2	C	604	HIS
2	C	1116	HIS
2	C	1136	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	424	ASN
3	D	450	HIS
3	D	690	ASN
3	D	702	GLN
3	D	716	GLN
3	D	861	ASN
5	F	129	GLN
5	F	301	ASN

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Mol	Chain	Res	Type
5	F	362	ASN
5	F	446	GLN
5	F	518	HIS
5	F	579	GLN
5	F	600	HIS
1	G	84	ASN
1	H	132	HIS
2	I	139	ASN
2	I	343	HIS
2	I	510	GLN
2	I	658	GLN
2	I	688	GLN
2	I	1010	GLN
2	I	1038	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1220	GLN
2	I	1237	HIS
2	I	1299	ASN
2	I	1314	GLN
3	J	157	GLN
3	J	200	GLN
3	J	206	ASN
3	J	320	ASN
3	J	450	HIS
3	J	465	GLN
3	J	477	GLN
3	J	702	GLN
3	J	716	GLN
3	J	771	GLN
3	J	817	HIS
3	J	861	ASN
3	J	910	ASN
3	J	1259	GLN
3	J	1366	HIS
4	K	7	GLN
5	L	131	GLN
5	L	406	GLN
5	L	446	GLN
5	L	469	GLN

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Mol	Chain	Res	Type
5	L	568	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	4C6	D	2004	-	32,34,34	1.23	3 (9%)	41,51,51	0.97	1 (2%)
8	4C6	J	2004	-	32,34,34	0.83	1 (3%)	41,51,51	1.32	6 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	4C6	D	2004	-	-	0/7/45/45	0/4/4/4
8	4C6	J	2004	-	-	0/7/45/45	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C6	C2-S	-5.01	1.71	1.79
8	D	2004	4C6	C4-C3	-2.16	1.46	1.48
8	D	2004	4C6	S-N	-2.05	1.60	1.64
8	J	2004	4C6	C2-S	-2.02	1.75	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C6	C4-C3-C2	4.75	134.41	129.47
8	D	2004	4C6	C4-C3-C2	4.24	133.87	129.47
8	J	2004	4C6	C7-C21-C	-2.81	85.26	88.04
8	J	2004	4C6	O3-S-C2	2.66	112.70	108.74
8	J	2004	4C6	C7-C1-N	2.40	135.43	129.93
8	J	2004	4C6	C3-C2-C5	-2.14	104.58	106.15
8	J	2004	4C6	C1-C-C21	2.05	89.98	88.37

There are no chirality outliers.

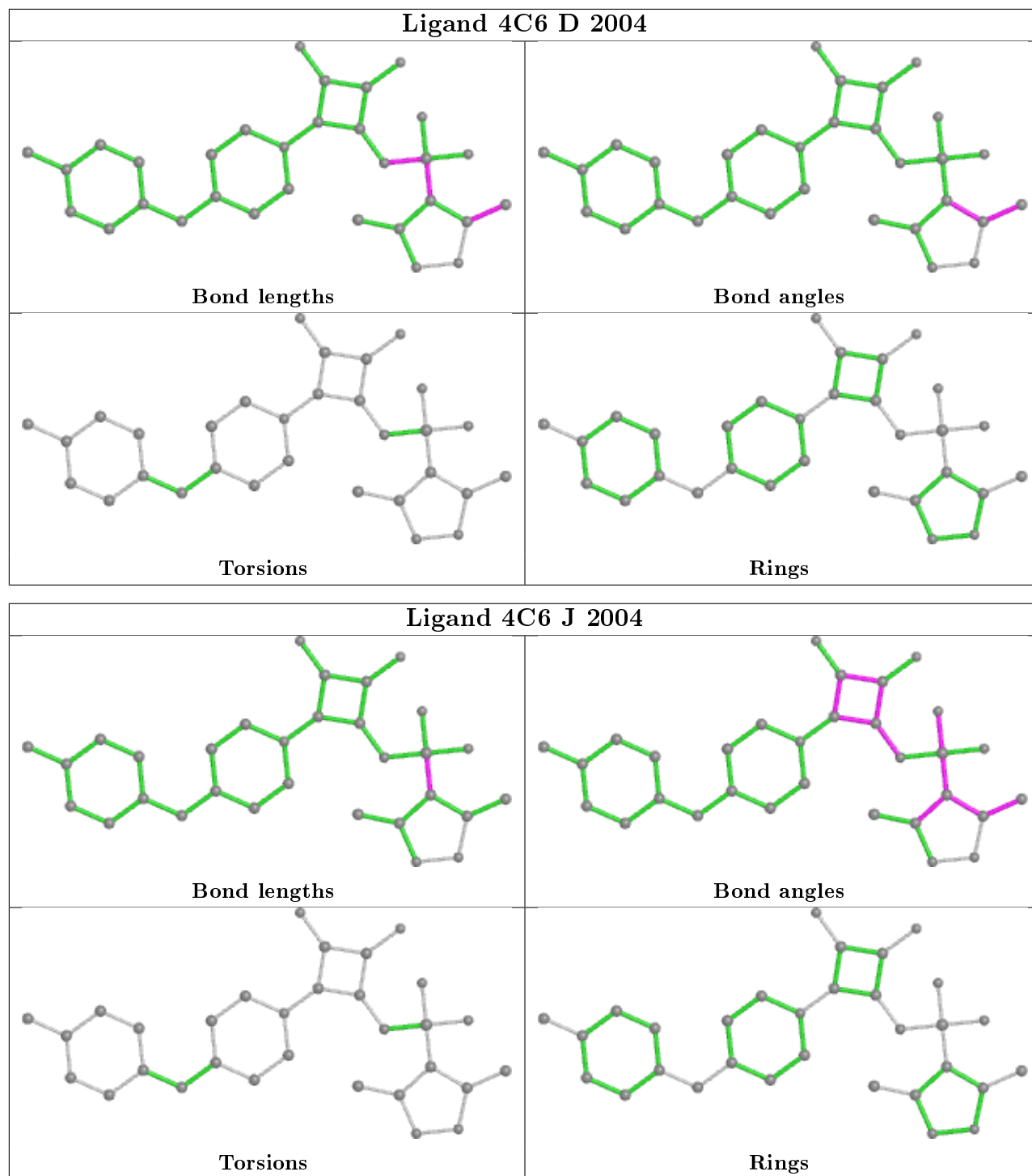
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C6	1	0
8	J	2004	4C6	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.33	5 (1%) 72 55	105, 138, 176, 185	0
1	B	217/329 (65%)	-0.16	4 (1%) 68 51	114, 172, 192, 198	0
1	G	227/329 (68%)	-0.38	0 100 100	138, 159, 175, 192	0
1	H	216/329 (65%)	-0.06	6 (2%) 53 35	130, 174, 192, 201	0
2	C	1340/1342 (99%)	-0.37	14 (1%) 82 69	88, 126, 202, 228	0
2	I	1340/1342 (99%)	-0.19	34 (2%) 57 39	108, 154, 212, 314	0
3	D	1163/1407 (82%)	-0.36	3 (0%) 94 88	90, 119, 164, 197	0
3	J	1152/1407 (81%)	-0.26	12 (1%) 82 69	103, 137, 181, 211	0
4	E	89/91 (97%)	-0.23	0 100 100	129, 159, 178, 184	0
4	K	79/91 (86%)	0.63	9 (11%) 5 3	186, 221, 249, 254	0
5	F	468/613 (76%)	-0.24	15 (3%) 47 31	113, 159, 233, 249	0
5	L	469/613 (76%)	-0.21	11 (2%) 60 42	127, 168, 244, 260	0
All	All	7079/8222 (86%)	-0.27	113 (1%) 72 55	88, 143, 205, 314	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.3
2	I	1003	THR	7.0
5	F	167	ASP	5.6
2	I	1002	LEU	5.1
2	I	979	LEU	4.9
2	I	1004	ASP	4.8
2	I	1006	GLU	4.6
2	I	983	GLY	4.6
5	L	167	ASP	4.6
2	C	231	GLU	4.1
3	J	208	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	I	1005	GLU	4.0
4	K	36	ASP	4.0
5	F	318	ALA	3.9
2	I	999	GLU	3.9
5	L	315	TRP	3.9
2	C	332	ARG	3.8
5	L	111	LEU	3.8
5	L	318	ALA	3.7
3	J	830	ASP	3.5
5	F	319	ALA	3.5
2	C	251	ALA	3.5
2	I	985	GLU	3.5
3	J	212	THR	3.4
5	F	305	LEU	3.4
2	C	333	ILE	3.4
2	I	1011	LEU	3.3
5	L	490	PRO	3.3
1	H	107	ILE	3.2
5	F	307	THR	3.2
2	I	981	ALA	3.1
5	F	337	VAL	3.1
2	C	1003	THR	3.0
2	C	241	LEU	3.0
2	I	984	VAL	3.0
2	C	230	PHE	3.0
4	K	37	PRO	3.0
5	L	321	ALA	2.9
5	F	315	TRP	2.9
1	H	13	LEU	2.9
4	K	58	LEU	2.9
2	I	105	TYR	2.9
1	A	294	ASN	2.8
5	L	319	ALA	2.8
2	I	970	GLY	2.8
5	L	314	THR	2.8
3	J	1198	VAL	2.8
2	I	725	GLN	2.7
2	I	1008	GLN	2.7
3	J	542	ALA	2.7
2	I	111	GLU	2.7
2	I	1010	GLN	2.7
1	H	28	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	250	THR	2.6
1	H	96	ASP	2.6
2	I	234	ASP	2.6
2	C	282	VAL	2.5
1	B	160	HIS	2.5
2	I	1007	LYS	2.5
2	I	1017	GLN	2.5
1	A	241	GLU	2.5
4	K	56	GLU	2.5
2	C	1002	LEU	2.5
5	L	489	MET	2.5
1	A	160	HIS	2.5
5	F	323	ASN	2.5
2	C	317	LEU	2.5
4	K	57	GLY	2.5
5	F	314	THR	2.5
2	I	978	VAL	2.5
2	I	980	VAL	2.4
3	J	930	LEU	2.4
2	I	987	GLU	2.4
1	B	97	GLU	2.4
5	F	321	ALA	2.4
1	B	172	LEU	2.4
2	I	998	LEU	2.4
1	A	245	GLU	2.4
3	J	207	GLU	2.3
2	I	414	ILE	2.3
5	F	333	VAL	2.3
2	C	165	HIS	2.3
2	I	720	ARG	2.3
2	I	322	LEU	2.3
3	D	212	THR	2.3
2	I	988	LYS	2.3
3	J	1297	LYS	2.3
5	L	305	LEU	2.2
1	H	12	ARG	2.2
4	K	70	GLN	2.2
1	H	106	GLY	2.2
3	J	712	GLN	2.2
5	F	312	SER	2.2
5	F	293	GLU	2.2
3	D	208	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	2.2
4	K	26	ARG	2.1
2	C	893	THR	2.1
5	F	283	GLN	2.1
2	I	734	ILE	2.1
1	A	25	LYS	2.1
3	J	149	GLY	2.1
3	D	930	LEU	2.1
3	J	521	LYS	2.1
2	I	1025	PHE	2.1
5	F	306	PHE	2.1
4	K	80	LEU	2.0
5	L	317	ASN	2.0
2	I	231	GLU	2.0
2	C	331	LYS	2.0
3	J	1203	ARG	2.0
4	K	30	MET	2.0
2	I	375	PRO	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	I	1401	1/1	0.85	0.37	127,127,127,127	0
6	MG	C	1401	1/1	0.86	0.35	127,127,127,127	0
6	MG	D	2001	1/1	0.93	0.27	127,127,127,127	0
6	MG	J	2001	1/1	0.95	0.23	127,127,127,127	0
8	4C6	J	2004	31/31	0.95	0.32	127,127,128,141	0

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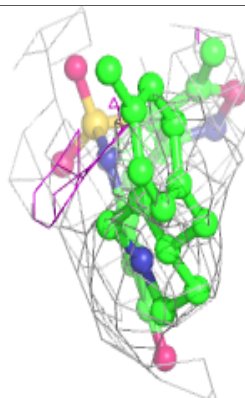
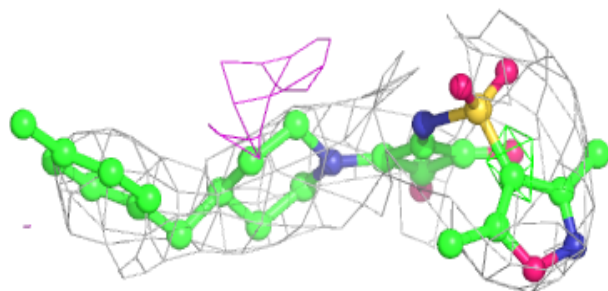
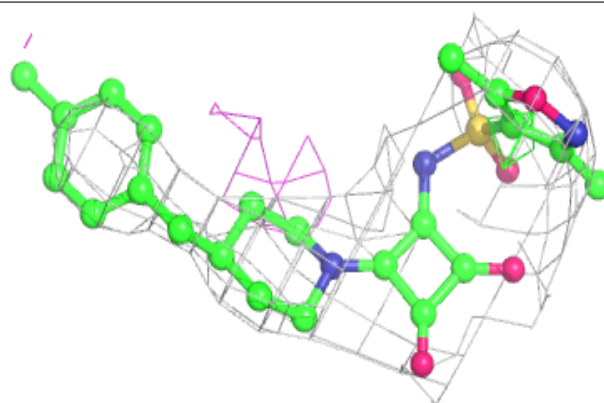
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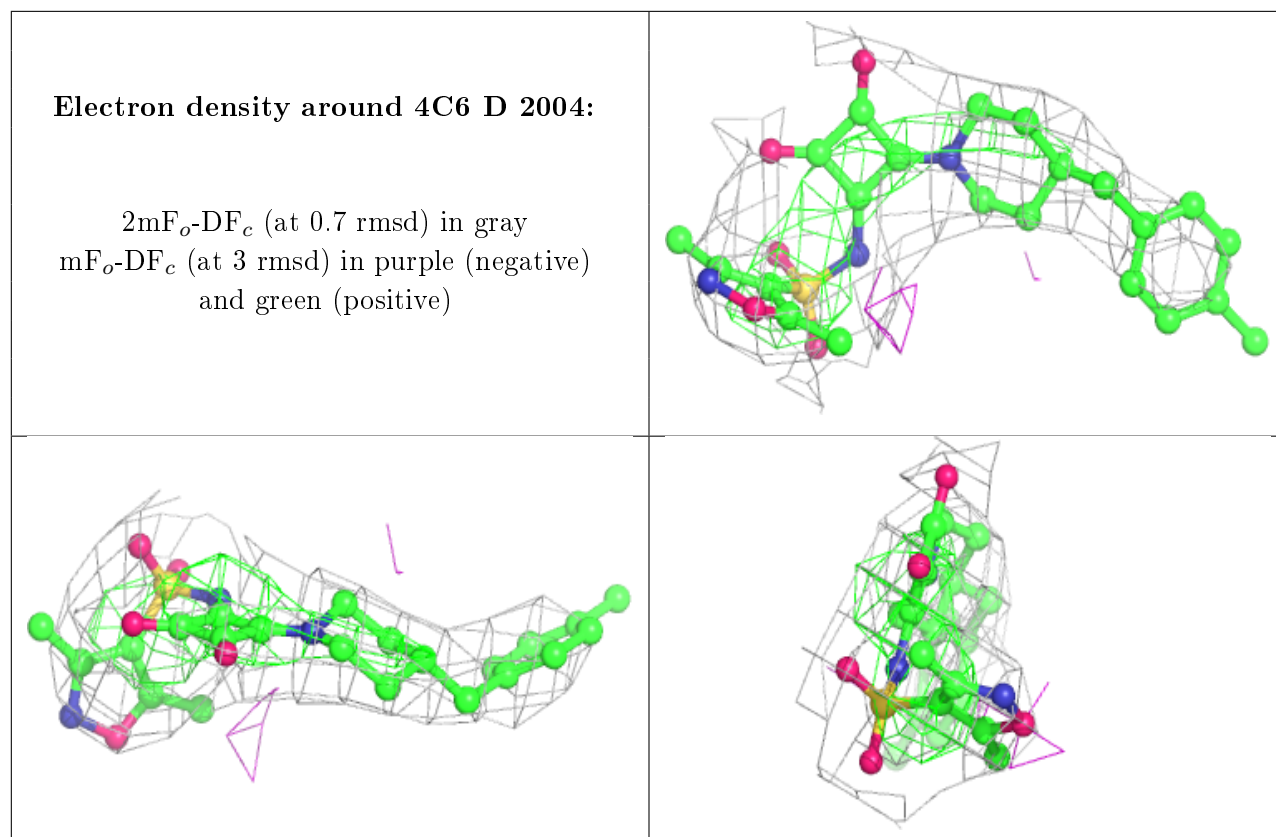
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	J	2003	1/1	0.96	0.20	127,127,127,127	0
7	ZN	J	2002	1/1	0.96	0.12	190,190,190,190	0
8	4C6	D	2004	31/31	0.97	0.34	127,127,127,127	0
7	ZN	D	2002	1/1	0.98	0.18	164,164,164,164	0
7	ZN	D	2003	1/1	0.99	0.22	127,127,127,127	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4C6 J 2004:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.