



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 AM UTC

PDB ID : 4YG2 / pdb_00004yg2
Title : X-ray crystal structur of Escherichia coli RNA polymerase sigma70 holoenzyme
Authors : Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

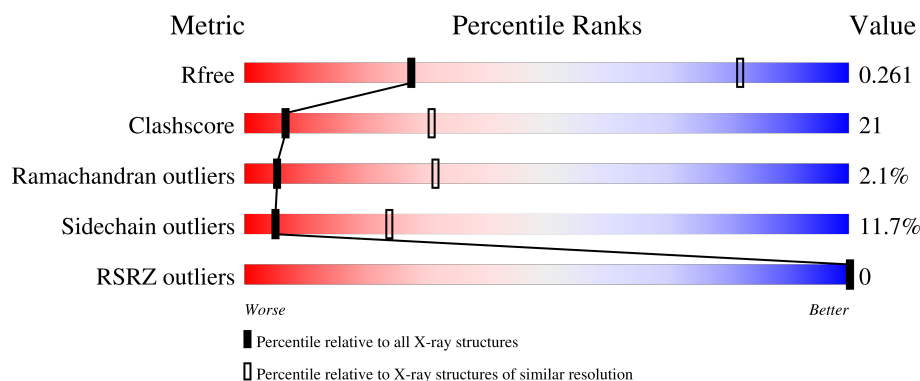
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



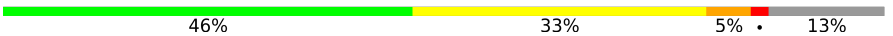
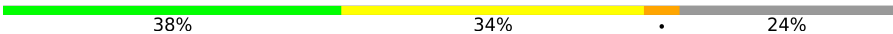
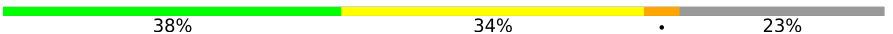
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	329	43% 41% 11% • •
1	B	329	34% 27% 5% 34%
1	G	329	32% 29% 6% • 31%
1	H	329	33% 29% • 34%
2	C	1342	51% 41% 8%

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Mol	Chain	Length	Quality of chain
2	I	1342	 56% 38% 5% •
3	D	1407	 40% 35% 8% 17%
3	J	1407	 42% 33% 7% 18%
4	E	91	 57% 31% 10% •
4	K	91	 46% 33% 5% • 13%
5	F	613	 38% 34% • 24%
5	L	613	 38% 34% • 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55741 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	1166	Total	C	N	O	S	0	0	0
			9060	5697	1621	1696	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	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 (CCD ID: MG) (formula: Mg).

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

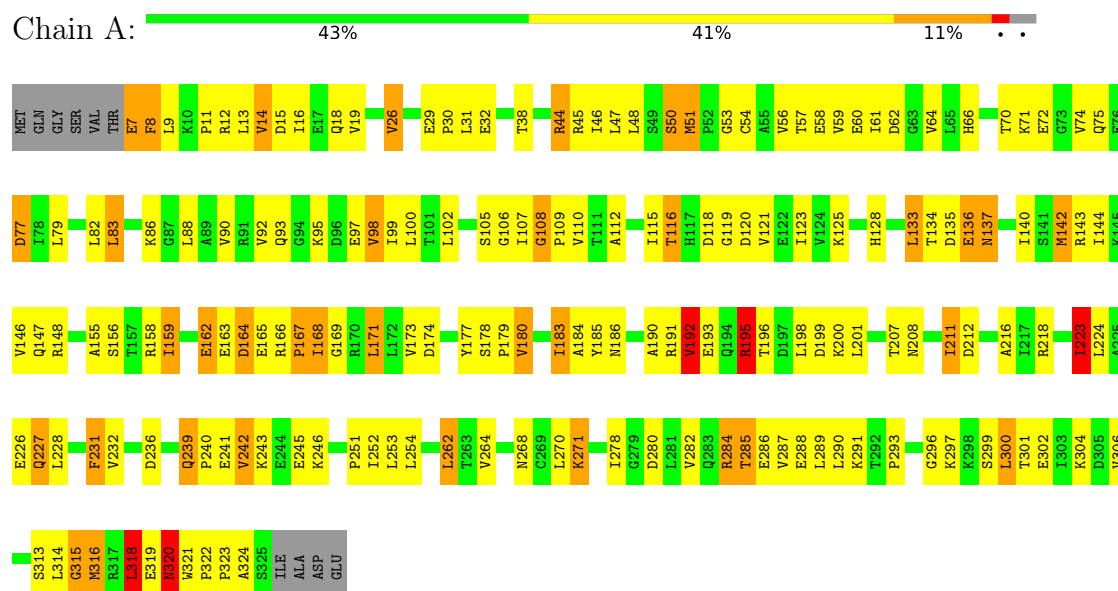
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

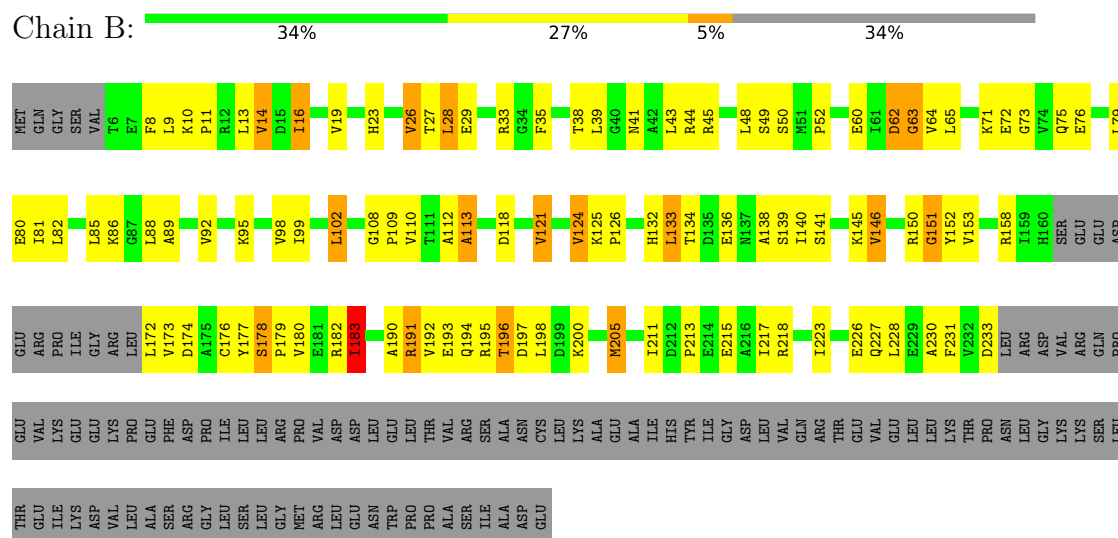
3 Residue-property plots

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

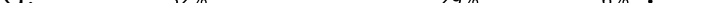
• Molecule 1: DNA-directed RNA polymerase subunit alpha

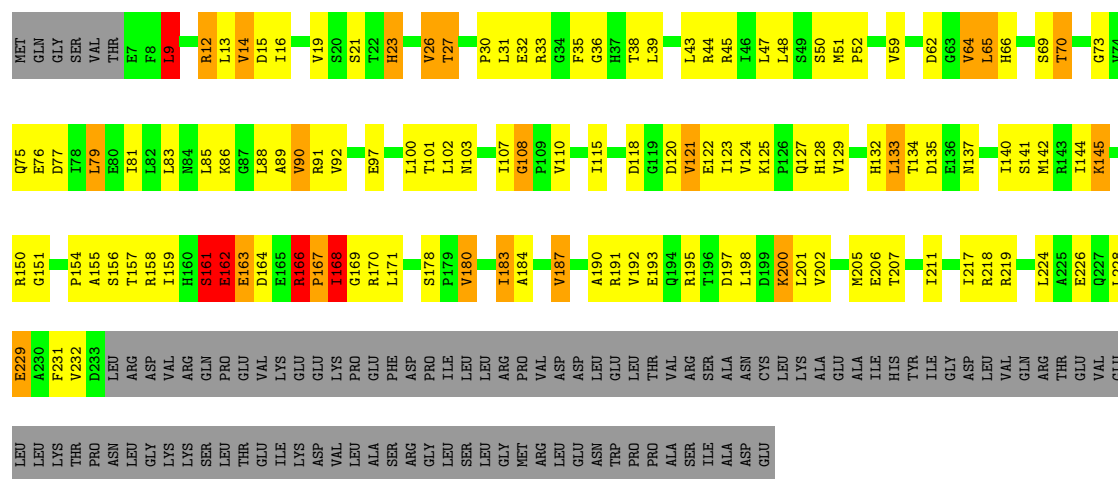


• Molecule 1: DNA-directed RNA polymerase subunit alpha

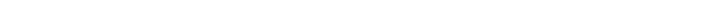


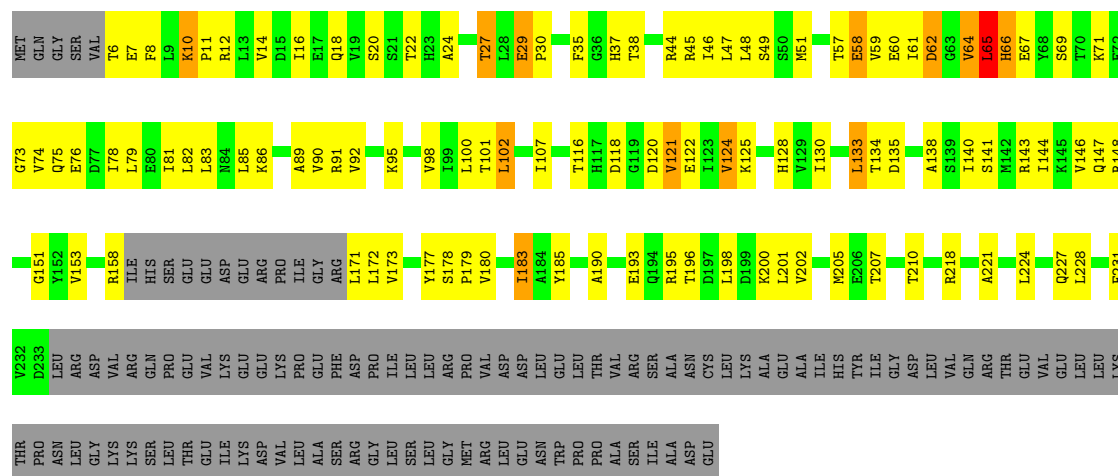
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:  32% 29% 6% • 31%



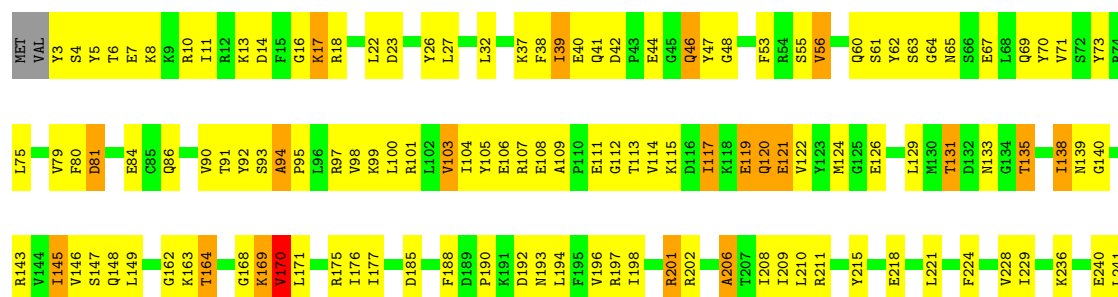
- Molecule 1: DNA-directed RNA polymerase subunit alpha

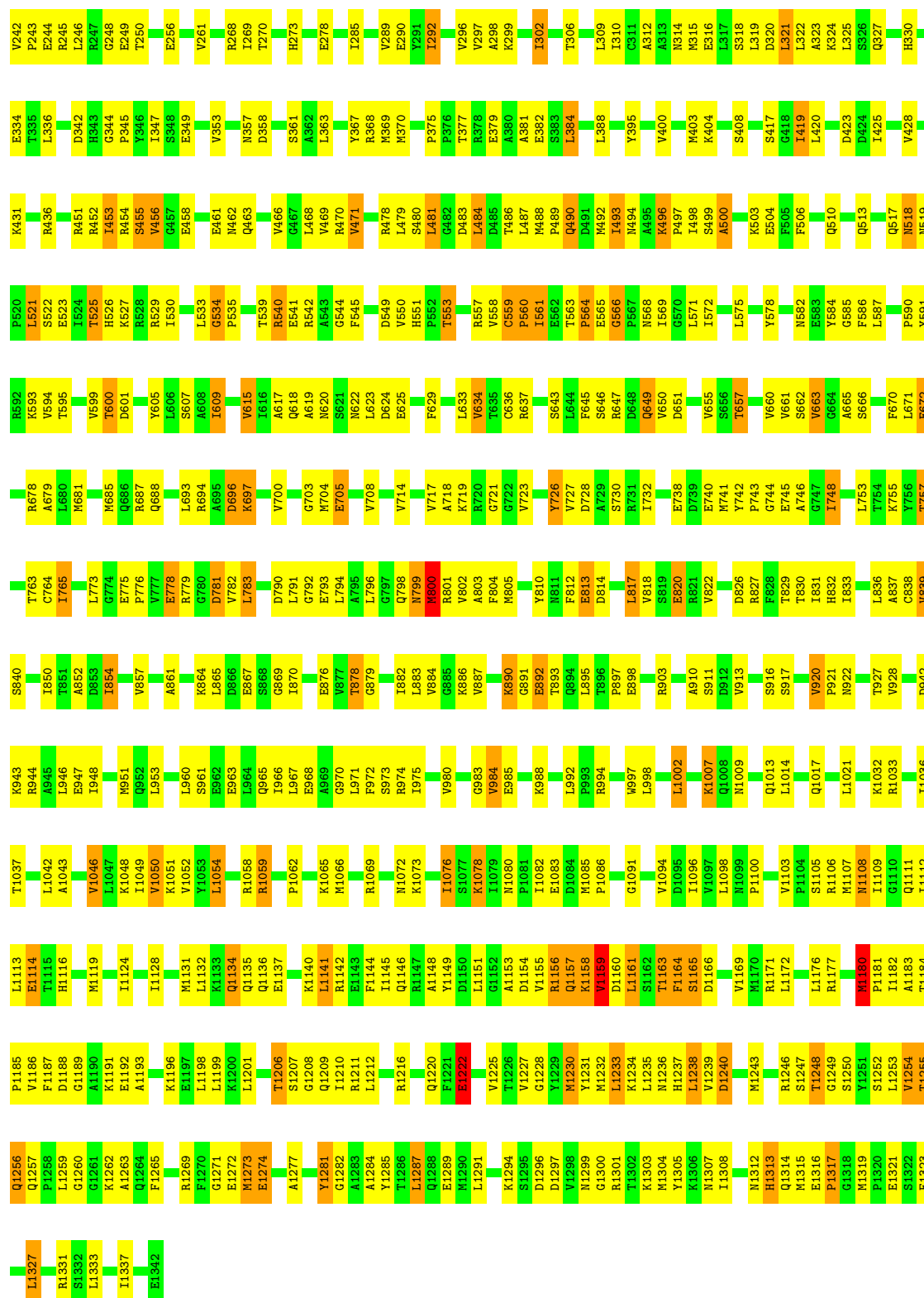
Chain H:  33% 29% . 34%



- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  51% 41% 8%





• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 56% 38% 5% •

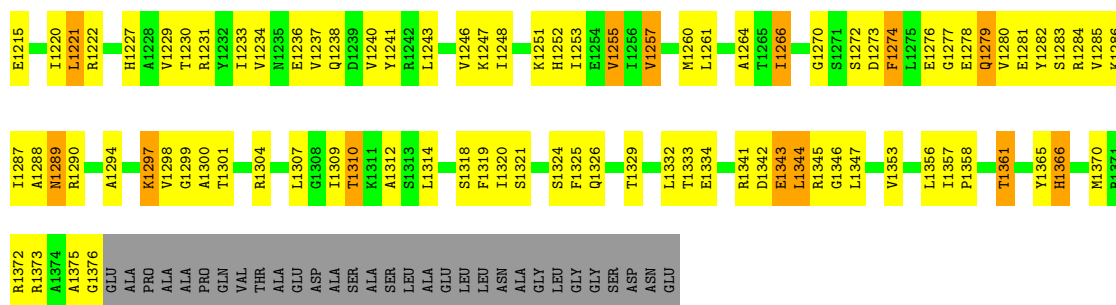
W1276	G1202	M1131	L1054	E963	I1850	P7433	S662	F586	V502	S398	L284	S167	V90	MET
A1280	D1203	Q1134	L1204	I966	T851	G744	V663	L587	K503	G401	I285	G168	T91	VAL
G1282	P1205	Q1135	P1205	L967	A852	E745	F670	P590	F506	R402	I292	V170	S93	Y3
A1283	T1206	Q1136	R1059	L971	N856	G747	E672	R592	F506	M403	A298	Y172	A94	S4
A1284	L1210	K1140	P1062	F972	L862	L763	R878	K593	S512	G416	I302	R175	P95	T6
Y1285	R1211	L1141	G1063	S973	G869	T754	R678	V594	Q513	L420	I310	I176	R97	E7
T1286	G1215	R1142	P1064	R974	T870	T755	M681	T595	F514	S421	I177	V98	K9	K8
L1287	R1216	K1145	K1065	R976	V871	K756	M685	D596	M515	K422	N310	I110	K99	R10
Q1288	R1217	R1146	M1066	R976	T757	T757	M686	G597	D516	D423	N314	W183	L100	I11
E1289	Q1220	R1147	A1067	L979	G874	I765	M686	T600	Q517	D423	N315	L184	R101	R12
M1290	F1221	A1148	N1072	L979	T878	I765	R687	D601	M519	V428	E316	D185	L102	K13
D1296	E1222	Y1149	K1073	G983	T878	P769	Q688	H604	P520	F186	F186	F186	V21	V21
D1297	R1223	D1150	G1074	V984	T878	E775	Q689	V605	L521	K431	D320	R107	R107	L22
V1298	P1224	L1151	V1075	E985	V884	E775	T692	L606	E522	L432	L322	E108	E108	Y26
N1299	V1225	G1152	I1076	A986	C885	E775	L693	S607	F524	L194	A323	A109	P110	L27
G1300	T1226	A1153	S1077	K987	K886	E778	R694	A608	T525	F195	K324	E111	E111	L28
R1301	V1227	R1156	K1078	K988	V887	E778	R694	L609	H526	L445	L325	V196	S29	S29
T1302	G1228	Q1157	N1080	D990	P889	D781	D696	E610	K527	L448	S326	R197	K115	I30
K1303	Y1229	K1158	P1081	K991	K890	V782	D696	E610	K527	L448	S326	R197	D116	Q31
M1304	M1230	V1159	P1081	K991	K890	V782	D696	E610	K527	L448	S326	R197	I117	L32
Y1305	Y1231	D1160	E1083	P993	C891	L783	P698	V615	R529	R452	F337	R201	K118	K37
I1308	Y1232	L1161	E1083	P993	C891	L783	P698	V615	R529	R452	F337	R201	E119	F39
H1313	L1233	S1162	D1084	R994	L895	D790	E704	A617	G534	S455	T338	R202	Q120	F39
K1314	K1234	T1163	P1086	R995	T896	L791	E705	Q618	P535	V456	D342	A206	E121	I39
P1317	L1238	F1164	Y1087	W997	T896	G792	M704	Q618	P535	V456	D342	A206	Q120	F39
G1316	V1239	S1165	Y1087	W997	T896	G792	M704	Q618	P535	V456	D342	A206	Q120	F39
M1319	Y1240	D1166	G1091	E999	R903	L796	S712	R540	R540	R465	Y346	I209	M124	D42
P1320	D1241	R1171	T1092	L1000	R903	L796	S712	R540	R540	R465	Y346	I209	M124	D42
L1326	K1242	L1172	P1093	G1001	E908	Q798	G713	R540	R540	R465	Y346	I209	M124	D42
L1327	M1243	L1172	Y1094	L1002	E908	Q798	G713	R540	R540	R465	Y346	I209	M124	D42
R1331	R1246	R1176	L1098	Q1013	A910	M800	A716	T635	V550	R470	L363	D222	M130	Q46
S1332	S1247	R1177	N1099	L1014	A910	M800	A716	T635	V550	R470	L363	D222	M130	Q46
L1333	G1249	M1180	P1100	Q1017	V913	R802	W177	C636	F552	Y471	V364	L223	D132	E50
G1334	L1253	I1182	S1105	Y1018	K914	A803	R720	R637	T553	E472	E365	K227	T135	S55
I1335	V1254	T1184	N1107	L1021	S916	H811	G721	R637	T553	E472	E365	K227	T135	S55
E1340	T1255	P1185	N1108	K1022	S917	H811	G721	R637	T553	E472	E365	K227	T135	S55
D1341	Q1256	V1186	I1109	H1023	N922	E813	G725	E641	G556	A474	M369	V228	F136	V56
E1342	Q1257	F1187	G1110	E1024	G923	D814	G725	E641	G556	A474	M369	V228	F136	V56
	P1258	D1188	Q1111	K1028	V924	L817	G727	F645	P560	L484	A381	L237	I138	I59
	L1259	G1189	L1113	K1028	V924	L817	G727	F645	P560	L484	A381	L237	I138	I59
	G1260	A1190	E1114	K1032	V931	S819	S730	Q649	G566	L487	L384	M239	N139	Q60
	G1261	K1191	T1115	K1035	V931	S819	S730	Q649	G566	L487	L384	M239	N139	Q60
	K1262	E1192	H1116	K1035	V931	S819	S730	Q649	G566	L487	L384	M239	N139	Q60
	A1263	A1193	L1117	K1036	K941	R827	W732	M653	S576	P489	F385	L241	R143	Y62
	Q1264	E1194	G1118	T1037	D942	F828	W734	D654	S576	P489	F385	L241	R143	Y62
	F1265	I1195	M1119	K943	R943	K735	W735	V655	S576	P489	F385	L241	R143	Y62
	G1266	K1196	P1044	A1043	R944	V839	W736	S656	Q550	I493	F389	L246	S159	C85
		E1197	P1044	A1043	R944	V839	W736	S656	Q550	I493	F389	L246	S159	C85
		L1198	I1124	P1044	R944	V839	W736	S656	Q550	I493	F389	L246	S159	C85
		L1199	I1128	K1048	E949	L845	E738	Q658	M522	P497	Y395	T250	D160	Q86
		K1200	I1048	K1048	E949	L845	E738	Q658	M522	P497	Y395	T250	D160	Q86
		L1201	I1049	K1049	E950	E848	D739	Q659	M522	P497	Y395	T250	D160	Q86
				V1050	N951	E849	Y742	V661	G585	S499	L397	R268	T164	R88

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

Chain D:

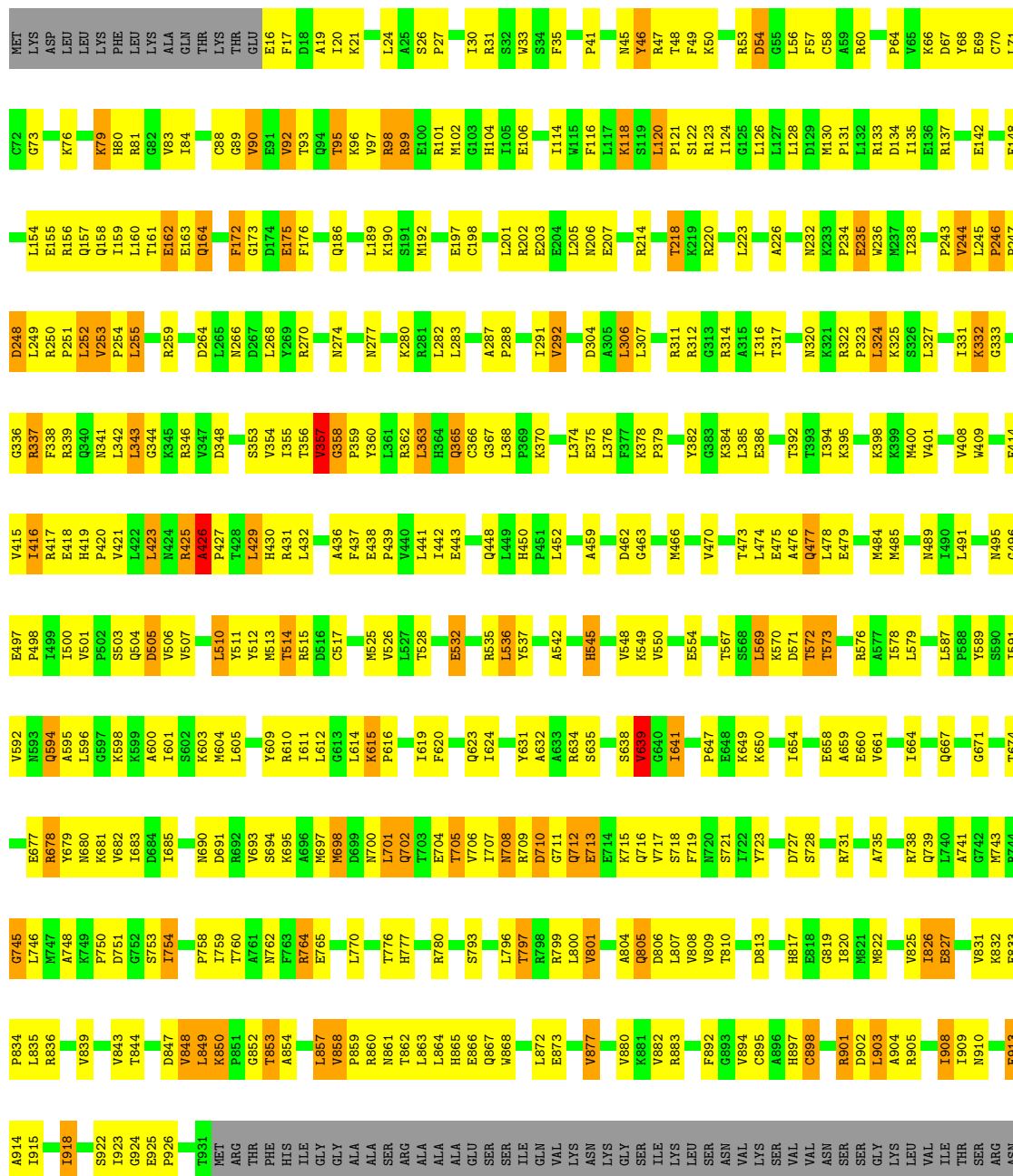


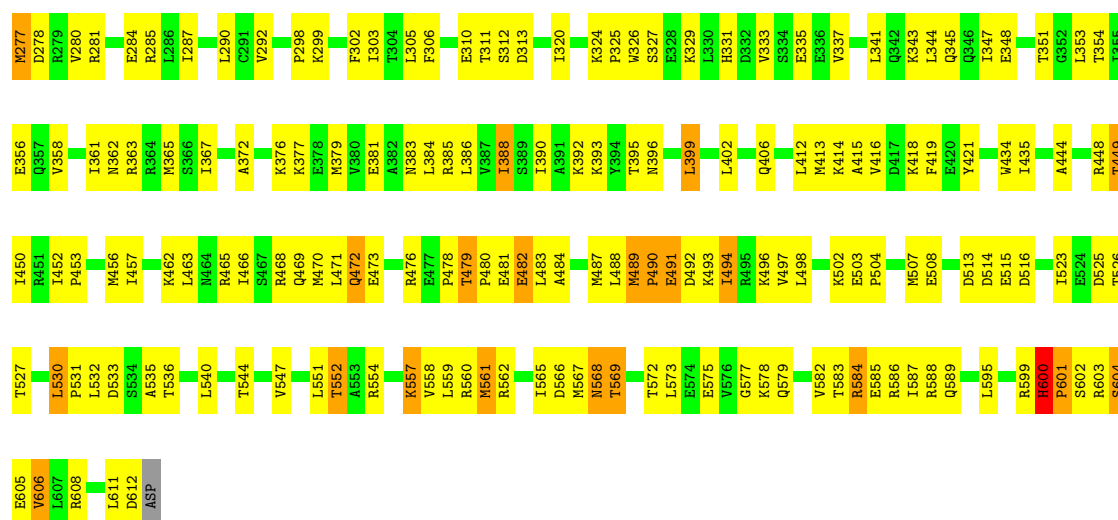
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GLN	THR	LYS	V885	D812	F719	R551	V470	R314	F227	G149	K79
GLY	MET	SER	V886	D813	N720	I552	P471	T393	S230	H80	R81
ASN	PRO	VAL			S721	E548	T472	T317	G231	L154	G82
ASP	VAL	VAL	T890	H817	I722	K649	T473	G318	N232	E155	R91
VAL	ILE	ASN			Y723	K557	L474	S319	V83	R156	V93
LEU	THR	SER	G893	T820	M724	D558	E475	K398	E235	Q157	I94
ILE	GLU	SER	V894	M821	M725	I654	A476	K321	L239	T161	C98
PRO	VAL	GLY		M822	T654	A559	A477	K322	E235	K9	L8
GLY	SER	LYS	R901	T823	R731	E562	L478	R323	L239	E162	G89
THR	GLY	LEU	D902	R824	G732	A859	E479	L324	E162	A10	A10
ASP	PHE	VAL	L903	V825	S733	K566		K325	L242	Q164	T12
MET	VAL	ILE	A904	I826	A734	V861	M484	D410	P243	Y165	E92
PRO	ARG	THR	R905	E827	A735	S568		I411	V244	T93	E15
ALA	PHE	SER	G906	G828	G736	L569	N489	I412	L245	Q94	E16
THR	ARG	ARG	H907	G829	I737	K570	T490	D413	P246	E170	T95
GLN	THR	ASN	H908	D830	R738	D571	L491	E414	P247	E171	K36
PHE	MET	THR	I909	V831	Q739	T572		K334	D248	F172	A25
ILE	ILE	GLU		R832	L740	T573	M495	Q335	L249	R97	S26
F1165	F1165	PRO	I918	E833	A741	L672	G496	R417		D174	R99
K1167	K1167	GLY		R834	G742	L579	E497	R416	L252	E175	P27
E1168	E1168	LYS	S922	L835	V673	M580	P498	E418	V253	R101	E100
T1163	T1163	THR	I923	R836	T674		M499	H419	F176	G103	R31
K1170	K1170	ALA	G924	D837	G745	G876	I500	P420	P254	M102	T30
G1171	G1171	VAL	E925	R838	L746	P988	V501	L422	L255	K179	S32
K1172	K1172	GLN	P926	V839	G747	E877	P502	K346	G257	M180	L107
R1173	R1173	LEU				Y589	S503	R346	G258	A184	S34
R1174	R1174	GLU	I930	R842	K749	I591	O504	V347	R259	S109	F35
L1175	L1175	ASP	T931	V843	D751	K681	D505	D348	P110	E110	K40
V1176	V1176	GLY	MET	T844	G752	V882	V606	P427	T262	L111	
I1177	I1177	VAL	ARG		S753	A595	V507	T428	S263	A112	
D1181	D1181	GLN	THR	D847	I754	L596	L508	L429	G353	L189	T43
G1182	G1182	ILE	GLY	V848	D684	G597	G509	H430	V354	K190	H13
S1183	S1183	SER	HIS	R849	N762	K598	L510	I355	N266	I144	N45
D1183	D1183	SER	VAL	ILE	F763	K599		L432	D267	N45	Y46
P1185	P1185	GLY	PRO	GLY	R764	A800	M513	G433	Y857	E197	R47
Y1186	Y1186	LEU	GLY	G852	I601	I601	T514	I434	R270	T48	P121
E1187	E1187	THR	VAL	T853	L770	S602	R515	Q435	L201	S122	F49
E1188	E1188	LEU	ALA	A854		S694	D516	A436	I273	R202	K50
		ALA	LEU	ARG	H777	K695	G517	P437	E203	R123	
		ASP	SER	L857		A896	V518	F438	R278	E204	R53
K1192	K1192	ILE	ALA	V858	A787	M697		L362	L279		D54
N1193	N1193	PRO	ALA	P859		M698	V526	H364	L279	E207	D54
R1194	R1194	GLY	ALA	R860	T790	I611	L527	Q365	I290	L56	G55
		GLU	GLU	N861		N700		C366	I291	L56	
N1197	N1197	GLY	THR	T862	S793	G613	E532	G367	V292	P131	
V1198	V1198	ALA	GLY	L863	G794	L614	A533	K445	E211	L132	R133
F1199	F1199	ILE	THR	L864	Y795	K615	E534	K446	T212	R133	R133
		GLN	GLN		L796	P616	R535	I447	R214	I135	I61
E1202	E1202	LYS	VAL	C869	T797	I706	E536	L448	K213	R136	P62
R1203	R1203	ASP	GLY	V875	R798	V707	Y537	L449	R297	G63	G83
V1204	V1204	ILE	LEU	ASN	R709	R709		H450	L299	K216	R137
E1205	E1205	ARG	GLY	LYS	I800	R709	L541	F377	Q300	L217	V138
R1206	R1206	THR	GLY	GLY	V801	I624	A542	K378	K219	T218	L139
G1207	G1207	ALA	SER	H875	D710	R634	A543	P379	R220	Y140	
D1208	D1208	LEU	ILE	Q805	Q712	R834	S943	D462	F141	E142	G72
V1209	V1209	LYS	ASN	V877	D806	E713	H545	D464	I221	E142	G73
I1210	I1210	ILE	TRP	LEU	L807	S638	H545	Y382	K222	S143	R74
S1211	S1211	VAL	ASP	R832	T810	G640	V548	D465	G310	Y75	Y144
		ASN	ASN	V832		T641	V548	R386	R311	K76	R77
		ASP	PRO					E385	P342	E225	



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

Chain J: 42% 33% 7% 18%





- Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.31Å 205.90Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.70 29.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.98-3.70) 92.3 (29.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.260 0.197 , 0.261	Depositor DCC
R_{free} test set	6183 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55741	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: MG, ZN

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	0.77	0/2524	1.16	16/3421 (0.5%)
1	B	0.76	0/1697	1.31	17/2300 (0.7%)
1	G	0.72	0/1777	1.12	7/2408 (0.3%)
1	H	0.72	1/1681 (0.1%)	1.21	7/2278 (0.3%)
2	C	0.88	7/10739 (0.1%)	1.25	63/14489 (0.4%)
2	I	0.73	0/10735	1.14	36/14484 (0.2%)
3	D	0.92	3/9200 (0.0%)	1.27	60/12423 (0.5%)
3	J	0.83	3/9140 (0.0%)	1.22	47/12341 (0.4%)
4	E	0.84	0/693	1.20	3/935 (0.3%)
4	K	0.77	0/629	1.15	4/847 (0.5%)
5	F	0.76	2/3864 (0.1%)	1.19	16/5194 (0.3%)
5	L	0.70	0/3872	1.07	8/5205 (0.2%)
All	All	0.81	16/56551 (0.0%)	1.20	284/76325 (0.4%)

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	2
2	I	0	2
3	D	0	2
3	J	0	3
5	F	0	2
All	All	0	11

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	221	ILE	CA-CB	7.37	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	ILE	CA-CB	-6.83	1.45	1.54
3	D	242	LEU	CA-C	-6.78	1.47	1.52
3	J	831	VAL	CA-CB	5.98	1.62	1.54
2	C	1163	THR	CA-CB	5.96	1.63	1.53
5	F	476	ARG	CA-C	5.69	1.55	1.52
2	C	1186	VAL	CA-CB	-5.50	1.47	1.54
2	C	700	VAL	CA-CB	-5.47	1.47	1.53
3	J	331	ILE	CA-CB	-5.44	1.48	1.54
2	C	564	PRO	CA-C	-5.29	1.46	1.52
2	C	1108	ASN	CA-C	-5.23	1.46	1.53
3	D	923	ILE	CA-CB	-5.23	1.47	1.54
1	H	14	VAL	CA-CB	5.23	1.60	1.54
3	J	705	THR	CA-CB	5.21	1.59	1.52
5	F	523	ILE	CA-C	-5.09	1.47	1.53
2	C	854	ILE	CA-CB	-5.01	1.49	1.54

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	GLY	CA-C-N	13.27	133.43	119.90
1	B	108	GLY	C-N-CA	13.27	133.43	119.90
5	F	600	HIS	CA-C-N	-12.33	107.79	120.98
5	F	600	HIS	C-N-CA	-12.33	107.79	120.98
3	D	833	GLU	CA-C-N	11.62	131.53	120.03
3	D	833	GLU	C-N-CA	11.62	131.53	120.03
2	C	920	VAL	CA-C-N	11.29	131.38	119.76
2	C	920	VAL	C-N-CA	11.29	131.38	119.76
2	C	94	ALA	CA-C-N	9.50	129.88	119.90
2	C	94	ALA	C-N-CA	9.50	129.88	119.90
1	H	10	LYS	CA-C-N	9.49	131.70	119.84
1	H	10	LYS	C-N-CA	9.49	131.70	119.84
2	C	1180	MET	CA-C-N	9.48	130.98	119.98
2	C	1180	MET	C-N-CA	9.48	130.98	119.98
3	J	1298	VAL	N-CA-C	-9.44	103.51	111.91
3	J	426	ALA	CA-C-N	-9.31	108.69	120.79
3	J	426	ALA	C-N-CA	-9.31	108.69	120.79
5	L	96	ASP	CA-C-N	9.27	130.22	119.47
5	L	96	ASP	C-N-CA	9.27	130.22	119.47
2	I	1262	LYS	N-CA-C	-9.15	100.18	112.26
5	F	137	TYR	CA-C-N	8.99	128.32	118.97
5	F	137	TYR	C-N-CA	8.99	128.32	118.97
1	B	8	PHE	N-CA-C	8.94	121.87	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	649	GLN	N-CA-C	-8.91	103.25	114.56
3	D	426	ALA	CA-C-N	-8.74	108.91	119.84
3	D	426	ALA	C-N-CA	-8.74	108.91	119.84
3	J	130	MET	CA-C-N	8.42	128.93	119.92
3	J	130	MET	C-N-CA	8.42	128.93	119.92
4	E	15	ASN	N-CA-C	8.30	121.37	111.33
2	C	566	GLY	CA-C-N	8.16	127.88	119.56
2	C	566	GLY	C-N-CA	8.16	127.88	119.56
2	C	1208	GLY	N-CA-C	-8.02	104.81	115.40
2	C	177	ILE	CA-C-N	8.00	128.15	120.31
2	C	177	ILE	C-N-CA	8.00	128.15	120.31
3	D	1152	GLU	CA-C-N	7.91	127.86	120.03
3	D	1152	GLU	C-N-CA	7.91	127.86	120.03
3	D	515	ARG	N-CA-C	-7.79	97.47	109.24
5	F	489	MET	CA-C-N	7.59	129.32	119.84
5	F	489	MET	C-N-CA	7.59	129.32	119.84
1	G	21	SER	N-CA-C	-7.46	103.16	111.82
2	C	1103	VAL	CA-C-N	-7.45	110.73	118.85
2	C	1103	VAL	C-N-CA	-7.45	110.73	118.85
1	A	51	MET	CA-C-N	7.43	127.44	119.78
1	A	51	MET	C-N-CA	7.43	127.44	119.78
1	B	151	GLY	N-CA-C	7.31	121.28	110.60
2	I	1180	MET	CA-C-N	7.15	127.55	119.83
2	I	1180	MET	C-N-CA	7.15	127.55	119.83
2	C	1316	GLU	CA-C-N	7.11	128.73	119.84
2	C	1316	GLU	C-N-CA	7.11	128.73	119.84
2	C	1157	GLN	N-CA-C	7.08	118.89	111.03
3	D	311	ARG	N-CA-C	-7.06	105.02	112.93
3	D	45	ASN	N-CA-C	7.06	120.00	111.82
2	C	1319	MET	N-CA-C	6.93	120.45	109.64
3	J	120	LEU	CA-C-N	-6.87	111.25	119.84
3	J	120	LEU	C-N-CA	-6.87	111.25	119.84
3	D	1211	SER	N-CA-C	-6.87	99.11	108.38
1	B	65	LEU	N-CA-C	6.82	119.74	111.82
2	I	1099	ASN	CA-C-N	6.72	126.34	119.56
2	I	1099	ASN	C-N-CA	6.72	126.34	119.56
3	D	149	GLY	N-CA-C	6.71	121.85	114.40
3	J	358	GLY	CA-C-N	6.70	126.33	119.56
3	J	358	GLY	C-N-CA	6.70	126.33	119.56
2	C	6	THR	N-CA-C	-6.68	104.75	113.17
2	C	206	ALA	N-CA-C	6.67	119.39	111.33
2	C	865	LEU	N-CA-C	6.66	120.31	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	831	ILE	N-CA-C	6.63	117.68	107.99
2	I	1241	ASP	N-CA-C	-6.55	105.82	113.88
2	I	1265	PHE	N-CA-C	6.55	119.39	110.55
2	I	566	GLY	CA-C-N	6.53	126.11	119.19
2	I	566	GLY	C-N-CA	6.53	126.11	119.19
3	D	262	THR	N-CA-C	6.52	118.99	109.07
3	D	470	VAL	N-CA-C	6.52	115.07	107.77
3	D	1197	ASN	N-CA-C	-6.51	105.91	114.31
2	C	893	THR	N-CA-C	6.51	118.45	111.36
2	I	1022	LYS	N-CA-C	6.50	118.16	111.14
1	G	108	GLY	CA-C-N	6.49	126.84	119.83
1	G	108	GLY	C-N-CA	6.49	126.84	119.83
2	C	804	PHE	N-CA-C	6.46	118.80	108.41
2	I	1257	GLN	CA-C-N	6.46	127.91	119.84
2	I	1257	GLN	C-N-CA	6.46	127.91	119.84
3	J	365	GLN	N-CA-C	6.45	118.75	109.14
3	J	1168	GLU	N-CA-C	6.45	118.96	108.76
3	D	469	HIS	CA-C-N	-6.44	116.32	123.02
3	D	469	HIS	C-N-CA	-6.44	116.32	123.02
1	B	205	MET	N-CA-C	6.41	119.95	109.06
2	C	812	PHE	N-CA-C	6.36	118.09	111.03
3	J	501	VAL	CA-C-N	6.36	126.73	119.93
3	J	501	VAL	C-N-CA	6.36	126.73	119.93
2	I	167	SER	N-CA-C	-6.35	105.84	113.97
1	A	323	PRO	CA-C-O	-6.33	114.34	122.13
3	D	1290	ARG	N-CA-C	-6.31	106.80	114.75
3	J	659	ALA	N-CA-C	-6.31	104.28	112.23
5	L	600	HIS	CA-C-N	-6.27	114.27	120.98
5	L	600	HIS	C-N-CA	-6.27	114.27	120.98
3	D	273	ILE	N-CA-C	6.26	116.43	110.42
3	D	365	GLN	N-CA-C	6.22	117.64	108.86
2	I	1157	GLN	N-CA-C	6.22	117.94	111.03
1	H	172	LEU	N-CA-C	6.22	119.29	109.96
1	A	212	ASP	CA-C-N	6.20	127.59	119.84
1	A	212	ASP	C-N-CA	6.20	127.59	119.84
3	J	765	GLU	N-CA-C	-6.19	102.55	110.53
2	I	1326	LEU	N-CA-C	-6.17	104.56	111.28
2	I	223	LEU	N-CA-C	6.16	117.80	111.14
2	C	560	PRO	CA-C-N	-6.16	114.88	121.84
2	C	560	PRO	C-N-CA	-6.16	114.88	121.84
3	J	1276	GLU	N-CA-C	6.16	118.72	110.35
2	I	98	VAL	N-CA-C	6.15	116.73	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LYS	N-CA-C	-6.14	104.50	111.07
3	D	239	LEU	N-CA-C	6.12	118.62	109.25
5	L	137	TYR	CA-C-N	6.12	125.61	119.24
5	L	137	TYR	C-N-CA	6.12	125.61	119.24
1	B	113	ALA	N-CA-C	-6.12	105.78	113.18
4	E	14	GLY	N-CA-C	6.12	120.60	112.77
1	H	29	GLU	C-N-CD	-6.11	107.17	120.60
2	I	1266	GLY	N-CA-C	-6.09	104.92	111.93
3	D	852	GLY	N-CA-C	-6.08	103.35	113.02
2	C	717	VAL	N-CA-C	6.08	116.68	108.17
3	D	587	LEU	CA-C-N	6.05	126.55	120.14
3	D	587	LEU	C-N-CA	6.05	126.55	120.14
2	I	708	VAL	N-CA-C	6.04	117.58	111.00
3	D	837	ASP	N-CA-C	6.04	117.86	111.28
3	D	101	ARG	N-CA-C	6.03	119.35	109.76
3	J	611	ILE	CB-CA-C	-6.02	105.69	111.05
2	I	94	ALA	CA-C-N	5.99	125.75	119.76
2	I	94	ALA	C-N-CA	5.99	125.75	119.76
2	C	544	GLY	N-CA-C	-5.96	96.01	113.30
3	D	1273	ASP	N-CA-C	5.96	120.07	113.21
3	D	358	GLY	CA-C-N	5.95	126.06	119.87
3	D	358	GLY	C-N-CA	5.95	126.06	119.87
3	J	702	GLN	N-CA-C	5.94	117.56	111.14
2	C	559	CYS	CA-C-N	5.93	127.25	119.84
2	C	559	CYS	C-N-CA	5.93	127.25	119.84
2	I	929	ILE	N-CA-C	5.90	118.82	113.10
1	G	151	GLY	N-CA-C	5.88	122.46	112.22
1	B	28	LEU	N-CA-C	5.87	117.04	107.23
2	C	534	GLY	CA-C-N	5.87	127.17	119.84
2	C	534	GLY	C-N-CA	5.87	127.17	119.84
3	J	1273	ASP	N-CA-C	5.85	117.45	110.19
2	C	375	PRO	N-CA-C	5.84	117.82	110.70
2	C	839	VAL	N-CA-C	5.83	116.28	108.11
3	D	750	PRO	CA-C-N	5.81	129.54	120.82
3	D	750	PRO	C-N-CA	5.81	129.54	120.82
3	J	1248	ILE	CB-CA-C	-5.80	103.82	110.73
1	H	29	GLU	CA-C-N	5.80	140.93	127.00
1	H	29	GLU	C-N-CA	5.80	140.93	127.00
3	D	1176	VAL	N-CA-C	5.80	116.50	107.28
5	F	604	SER	N-CA-C	5.79	117.60	111.28
3	J	253	VAL	CA-C-N	5.77	125.96	120.31
3	J	253	VAL	C-N-CA	5.77	125.96	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	MET	N-CA-C	5.74	118.01	108.99
2	I	131	THR	N-CA-C	5.73	118.26	110.35
2	C	518	ASN	N-CA-C	-5.72	104.97	112.41
3	J	611	ILE	N-CA-C	5.72	116.14	111.62
1	A	195	ARG	N-CA-C	-5.72	98.62	110.80
1	A	192	VAL	N-CA-C	-5.70	101.42	109.63
3	J	572	THR	N-CA-C	5.70	115.54	108.19
2	I	1335	ILE	N-CA-C	5.65	116.43	108.36
2	I	484	LEU	CA-CB-CG	5.64	136.06	116.30
3	D	109	SER	CA-C-N	5.63	125.63	119.89
3	D	109	SER	C-N-CA	5.63	125.63	119.89
3	J	99	ARG	N-CA-C	-5.62	106.41	113.72
4	K	15	ASN	N-CA-C	5.62	122.78	110.80
3	J	807	LEU	N-CA-C	5.62	117.84	109.25
3	J	164	GLN	N-CA-C	5.62	117.21	111.14
3	D	368	LEU	CA-C-N	5.60	125.61	119.90
3	D	368	LEU	C-N-CA	5.60	125.61	119.90
3	D	257	GLY	N-CA-C	-5.57	107.28	115.30
3	D	1365	TYR	N-CA-C	5.57	117.16	111.14
2	C	820	GLU	N-CA-C	-5.57	105.31	111.71
3	D	719	PHE	N-CA-C	-5.54	105.73	112.88
3	D	1162	ILE	N-CA-C	5.52	116.72	109.21
3	J	368	LEU	CA-C-N	5.52	125.53	119.90
3	J	368	LEU	C-N-CA	5.52	125.53	119.90
2	C	64	GLY	N-CA-C	-5.51	106.96	115.73
1	G	161	SER	N-CA-C	-5.51	104.66	111.33
3	J	1278	GLU	N-CA-C	5.51	117.17	108.96
3	D	653	ILE	CB-CA-C	-5.50	104.83	112.04
5	F	600	HIS	N-CA-C	5.47	121.91	109.81
5	F	600	HIS	CA-CB-CG	-5.46	108.33	113.80
1	H	65	LEU	N-CA-C	-5.46	106.66	113.38
3	D	752	GLY	N-CA-C	-5.46	107.49	114.37
1	G	180	VAL	N-CA-C	5.45	116.24	107.73
1	A	223	ILE	CB-CA-C	-5.45	104.90	111.88
1	B	178	SER	CA-C-N	5.45	125.54	119.87
1	B	178	SER	C-N-CA	5.45	125.54	119.87
5	F	514	ASP	CA-C-N	5.45	130.07	120.87
5	F	514	ASP	C-N-CA	5.45	130.07	120.87
3	D	1240	VAL	N-CA-C	5.44	116.21	110.72
5	F	244	THR	N-CA-C	-5.43	106.65	113.28
2	I	1320	PRO	CA-C-O	-5.43	115.15	121.34
2	C	818	VAL	N-CA-C	5.42	116.28	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	519	ASN	CA-C-N	5.41	125.23	119.28
2	C	519	ASN	C-N-CA	5.41	125.23	119.28
5	F	452	ILE	CA-C-N	5.40	125.34	119.78
5	F	452	ILE	C-N-CA	5.40	125.34	119.78
3	J	1233	ILE	N-CA-C	-5.40	105.06	110.30
1	B	183	ILE	CB-CA-C	-5.40	101.75	110.28
2	C	800	MET	N-CA-C	5.39	116.99	108.96
2	I	109	ALA	CA-C-N	-5.38	113.11	119.84
2	I	109	ALA	C-N-CA	-5.38	113.11	119.84
2	C	763	THR	N-CA-C	-5.38	103.59	110.53
3	J	1247	LYS	N-CA-C	5.37	117.38	108.20
2	I	746	ALA	CB-CA-C	-5.37	110.37	116.54
3	D	1161	GLY	CA-C-O	-5.34	118.47	122.37
2	I	374	GLU	CA-C-N	5.34	125.88	120.38
2	I	374	GLU	C-N-CA	5.34	125.88	120.38
3	J	477	GLN	N-CA-C	-5.34	105.37	111.14
2	C	1042	LEU	N-CA-C	5.34	117.98	109.65
2	I	534	GLY	CA-C-N	5.34	125.64	119.93
2	I	534	GLY	C-N-CA	5.34	125.64	119.93
2	C	1281	TYR	N-CA-C	-5.33	103.58	110.19
3	J	1151	LYS	N-CA-C	5.33	116.78	111.07
1	B	153	VAL	CA-C-N	5.33	125.30	120.03
1	B	153	VAL	C-N-CA	5.33	125.30	120.03
2	I	717	VAL	N-CA-C	5.32	115.62	108.17
2	I	518	ASN	N-CA-C	-5.32	106.02	112.88
3	J	337	ARG	N-CA-C	5.32	122.12	110.80
3	J	1161	GLY	N-CA-C	5.32	118.23	111.85
3	D	464	ASP	N-CA-C	-5.31	103.01	110.50
1	B	63	GLY	CA-C-N	-5.28	115.10	122.71
1	B	63	GLY	C-N-CA	-5.28	115.10	122.71
3	J	592	VAL	CB-CA-C	-5.28	105.14	111.85
3	D	344	GLY	N-CA-C	-5.27	98.01	113.30
3	J	587	LEU	CA-C-N	5.27	125.72	120.14
3	J	587	LEU	C-N-CA	5.27	125.72	120.14
2	C	496	LYS	CA-C-N	5.26	124.89	119.05
2	C	496	LYS	C-N-CA	5.26	124.89	119.05
5	F	557	LYS	N-CA-C	-5.25	105.68	111.71
3	J	118	LYS	N-CA-C	5.23	120.32	112.94
1	B	110	VAL	N-CA-C	5.23	115.15	107.15
3	D	40	LYS	CA-C-N	5.22	126.37	119.84
3	D	40	LYS	C-N-CA	5.22	126.37	119.84
3	J	90	VAL	CB-CA-C	-5.22	105.29	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1210	ILE	N-CA-C	-5.22	106.79	112.80
4	E	17	PHE	N-CA-C	-5.22	104.61	111.96
1	B	11	PRO	N-CA-C	5.20	118.88	111.13
3	J	246	PRO	CA-C-N	5.19	124.82	119.05
3	J	246	PRO	C-N-CA	5.19	124.82	119.05
5	L	489	MET	CA-C-N	5.19	126.33	119.84
5	L	489	MET	C-N-CA	5.19	126.33	119.84
2	C	911	SER	N-CA-C	5.17	117.36	110.53
2	C	1007	LYS	N-CA-C	-5.17	105.82	111.82
3	D	490	ILE	N-CA-C	-5.17	107.79	113.43
1	A	108	GLY	CA-C-N	5.17	126.30	119.84
1	A	108	GLY	C-N-CA	5.17	126.30	119.84
2	C	1161	LEU	CA-CB-CG	-5.17	98.22	116.30
2	I	4	SER	N-CA-C	5.16	116.64	109.31
1	A	177	TYR	CB-CA-C	-5.15	103.60	111.83
2	C	1230	MET	N-CA-C	5.14	116.79	108.41
1	G	64	VAL	N-CA-C	5.14	115.52	108.12
3	D	333	GLY	N-CA-C	5.14	125.36	113.18
2	C	1273	MET	N-CA-C	5.13	116.88	111.28
3	D	1169	THR	N-CA-C	5.13	121.74	110.80
2	C	344	GLY	CA-C-N	5.13	126.26	119.84
2	C	344	GLY	C-N-CA	5.13	126.26	119.84
2	C	1046	VAL	N-CA-C	5.13	115.69	108.36
3	D	253	VAL	CA-C-N	5.11	125.09	120.03
3	D	253	VAL	C-N-CA	5.11	125.09	120.03
2	C	726	TYR	N-CA-C	5.11	117.74	108.69
2	C	671	LEU	N-CA-C	-5.11	105.71	111.28
1	A	177	TYR	CA-CB-CG	5.10	123.08	113.90
2	C	500	ALA	CA-C-N	5.10	127.62	120.28
2	C	500	ALA	C-N-CA	5.10	127.62	120.28
4	K	39	VAL	CA-C-N	5.09	125.38	119.93
4	K	39	VAL	C-N-CA	5.09	125.38	119.93
2	C	510	GLN	N-CA-C	-5.09	106.17	112.38
2	C	1222	GLU	N-CA-C	-5.09	103.62	110.24
4	K	43	ASN	N-CA-C	-5.09	107.02	113.23
3	D	123	ARG	CG-CD-NE	-5.08	100.83	112.00
3	D	708	ASN	N-CA-C	5.08	117.77	109.59
3	J	1248	ILE	N-CA-C	5.08	115.77	107.24
3	D	331	ILE	N-CA-C	-5.07	106.85	111.67
2	C	1274	GLU	N-CA-C	-5.06	106.37	112.54
3	D	419	HIS	CA-C-N	5.05	124.98	119.78
3	D	419	HIS	C-N-CA	5.05	124.98	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	PRO	CA-C-N	5.04	130.77	121.70
1	A	323	PRO	C-N-CA	5.04	130.77	121.70
5	F	388	ILE	N-CA-C	5.04	115.25	110.42
3	J	67	ASP	N-CA-C	5.03	117.63	110.24
2	C	813	GLU	N-CA-C	-5.03	100.09	110.80
3	D	497	GLU	CA-C-N	5.03	125.26	119.83
3	D	497	GLU	C-N-CA	5.03	125.26	119.83
3	D	817	HIS	N-CA-C	-5.00	106.96	113.16
3	J	470	VAL	N-CA-C	5.00	113.37	107.77

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	853	THR	Peptide
3	J	901	ARG	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	135	0
1	B	1677	0	1703	79	0
1	G	1755	0	1773	103	0
1	H	1662	0	1687	81	0
2	C	10570	0	10582	479	0
2	I	10566	0	10576	426	1
3	D	9060	0	9209	473	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	9001	0	9168	431	0
4	E	691	0	695	27	0
4	K	627	0	634	28	0
5	F	3813	0	3880	161	0
5	L	3821	0	3884	176	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
All	All	55741	0	56333	2396	1

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 21.

All (2396) 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	1.42	1.01
1:A:296:GLY:H	1:A:299:SER:HB2	1.26	1.00
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.41	0.99
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.47	0.97
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.29	0.96
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.32	0.95
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.29	0.94
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.31	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.49	0.94
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.33	0.93
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.52	0.92
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.50	0.92
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.36	0.90
5:L:134:VAL:HA	5:L:273:MET:HE1	1.51	0.90
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.55	0.89
1:G:12:ARG:H	1:G:30:PRO:HD2	1.38	0.88
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.55	0.87
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.56	0.87
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.56	0.87
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.10	0.87
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.56	0.87
2:I:148:GLN:NE2	2:I:535:PRO:O	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.54	0.86
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.23	0.86
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.09	0.86
1:A:45:ARG:HG2	1:B:38:THR:HB	1.55	0.85
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.57	0.85
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.58	0.85
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.56	0.85
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	1.59	0.84
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.59	0.84
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.43	0.84
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.83
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.59	0.83
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.14	0.83
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.44	0.82
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.60	0.82
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.10	0.82
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.61	0.82
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.43	0.82
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.60	0.81
1:B:35:PHE:HA	1:B:38:THR:HG22	1.59	0.81
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.61	0.81
1:G:45:ARG:HG2	1:H:38:THR:HB	1.63	0.81
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.61	0.81
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.62	0.80
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.29	0.80
3:J:48:THR:O	3:J:50:LYS:N	2.13	0.80
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.17	0.79
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.79
1:A:47:LEU:HD23	1:A:51:MET:HE2	1.65	0.79
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.17	0.79
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.65	0.79
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.65	0.79
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.17	0.78
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.66	0.78
5:F:134:VAL:HA	5:F:273:MET:HE1	1.63	0.78
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.65	0.78
3:D:48:THR:O	3:D:50:LYS:N	2.16	0.78
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.65	0.78
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.66	0.78
3:D:722:ILE:HA	3:D:725:MET:HE3	1.66	0.78
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.49	0.78
3:D:156:ARG:NH2	3:D:191:SER:OG	2.16	0.77
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.19	0.77
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.46	0.77
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.66	0.77
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.66	0.77
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.18	0.77
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.16	0.77
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.66	0.77
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.66	0.77
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.66	0.77
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.15	0.77
4:K:32:VAL:O	4:K:34:GLY:N	2.17	0.77
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.77
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.66	0.76
2:I:5:TYR:HD1	2:I:8:LYS:HD3	1.51	0.76
3:D:490:ILE:H	3:D:490:ILE:HD13	1.50	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.65	0.76
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.66	0.76
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.67	0.76
1:H:35:PHE:HA	1:H:38:THR:HG22	1.66	0.76
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.18	0.76
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.67	0.76
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.50	0.76
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.66	0.75
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.51	0.75
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.19	0.75
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.51	0.75
5:F:487:MET:HA	5:F:487:MET:HE2	1.67	0.75
1:H:134:THR:HG23	1:H:135:ASP:H	1.50	0.75
3:D:418:GLU:HG3	4:E:45:LYS:H	1.52	0.75
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.69	0.75
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.68	0.75
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.67	0.75
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.50	0.74
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.70	0.74
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.21	0.74
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.70	0.74
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.68	0.74
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.87	0.74
2:I:30:ILE:HD12	2:I:30:ILE:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:170:VAL:HG21	2:I:172:TYR:CZ	2.23	0.74
3:D:252:LEU:HD23	3:D:262:THR:HB	1.70	0.74
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.69	0.74
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.69	0.73
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.70	0.73
2:C:890:LYS:NZ	2:C:891:GLY:O	2.17	0.73
2:I:560:PRO:O	3:J:780:ARG:NH2	2.21	0.73
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.69	0.73
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.69	0.73
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.70	0.73
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.70	0.73
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.68	0.73
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.70	0.73
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.52	0.73
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.88	0.73
2:I:1066:MET:HE1	2:I:1076:ILE:HD12	1.71	0.73
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.70	0.73
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.68	0.73
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.71	0.73
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.02	0.73
4:E:32:VAL:O	4:E:34:GLY:N	2.22	0.73
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.70	0.72
3:J:700:ASN:O	3:J:704:GLU:HB2	1.88	0.72
3:J:797:THR:O	3:J:801:VAL:HG12	1.89	0.72
1:A:191:ARG:NH1	1:A:198:LEU:O	2.22	0.72
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.71	0.72
3:D:495:ASN:O	3:D:497:GLU:N	2.21	0.72
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.71	0.72
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.71	0.72
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.22	0.72
5:L:244:THR:O	5:L:247:GLU:HG2	1.89	0.72
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.18	0.72
2:I:4:SER:OG	2:I:5:TYR:N	2.20	0.72
3:J:1290:ARG:HD2	3:J:1295:ASN:HD22	1.53	0.72
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.69	0.72
2:C:703:GLY:N	2:C:705:GLU:OE2	2.17	0.72
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.69	0.72
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.71	0.72
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.22	0.72
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.72	0.72
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.72	0.72
1:A:14:VAL:HG22	1:A:15:ASP:H	1.55	0.72
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.55	0.72
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.04	0.71
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.21	0.71
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.72	0.71
1:B:52:PRO:HG3	1:B:150:ARG:HG2	1.71	0.71
2:C:582:ASN:HB3	2:C:586:PHE:H	1.56	0.71
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.71	0.71
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.70	0.71
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.23	0.71
3:D:849:LEU:H	3:D:849:LEU:HD22	1.56	0.71
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.54	0.71
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.73	0.71
1:A:77:ASP:OD1	1:A:77:ASP:N	2.23	0.71
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.72	0.71
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.56	0.71
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.25	0.71
2:I:324:LYS:O	2:I:327:GLN:NE2	2.24	0.71
3:D:317:THR:HG22	3:D:322:ARG:O	1.91	0.70
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.73	0.70
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.71	0.70
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.06	0.70
3:D:694:SER:OG	3:D:738:ARG:NE	2.23	0.70
2:I:1013:GLN:O	2:I:1017:GLN:HG2	1.91	0.70
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.72	0.70
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	2.05	0.70
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.74	0.70
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.74	0.70
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.74	0.69
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.23	0.69
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.75	0.69
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.74	0.69
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.73	0.69
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.22	0.69
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.74	0.69
2:C:566:GLY:O	2:C:569:ILE:HG13	1.92	0.69
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.72	0.69
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.06	0.69
2:I:1124:ILE:O	2:I:1128:ILE:HG13	1.92	0.69
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.74	0.69
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.75	0.69
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.73	0.69
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.74	0.69
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.74	0.69
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.75	0.68
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.75	0.68
1:G:167:PRO:O	1:G:169:GLY:N	2.25	0.68
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.28	0.68
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.73	0.68
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.09	0.68
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.75	0.68
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.28	0.68
2:I:620:ASN:O	2:I:620:ASN:ND2	2.27	0.68
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.75	0.68
3:J:495:ASN:O	3:J:497:GLU:N	2.25	0.68
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.75	0.68
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.75	0.68
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.75	0.68
2:I:892:GLU:OE1	3:J:66:LYS:NZ	2.27	0.68
3:J:1260:MET:HE3	3:J:1306:LEU:HD21	1.74	0.68
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.23	0.68
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.57	0.68
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.28	0.68
3:D:425:ARG:HG2	3:D:426:ALA:H	1.58	0.68
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.74	0.68
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.76	0.68
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.74	0.68
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.56	0.68
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.73	0.68
2:I:138:ILE:O	2:I:139:ASN:ND2	2.27	0.68
2:I:347:ILE:HD11	2:I:433:ILE:HD11	1.74	0.68
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.25	0.67
3:D:43:THR:OG1	5:F:449:THR:O	2.12	0.67
3:J:709:ARG:O	3:J:711:GLY:N	2.26	0.67
1:B:102:LEU:O	1:B:141:SER:HA	1.93	0.67
2:C:201:ARG:NH2	2:C:370:MET:O	2.27	0.67
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.28	0.67
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.74	0.67
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.27	0.67
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.60	0.67
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.74	0.67
2:C:744:GLY:C	2:C:746:ALA:H	2.02	0.67
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.75	0.67
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.28	0.67
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.77	0.67
2:C:705:GLU:HB2	2:C:794:LEU:H	1.59	0.67
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.09	0.67
3:D:797:THR:O	3:D:801:VAL:HG12	1.95	0.67
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.67
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.59	0.67
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.77	0.67
5:L:487:MET:HE2	5:L:487:MET:HA	1.77	0.66
2:I:963:GLU:O	2:I:967:LEU:HB2	1.95	0.66
3:D:708:ASN:OD1	3:D:708:ASN:N	2.23	0.66
5:F:532:LEU:O	5:F:536:THR:HG23	1.96	0.66
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.27	0.66
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.60	0.66
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.76	0.66
1:G:166:ARG:HH11	1:G:168:ILE:HG12	1.61	0.66
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.66
3:D:638:SER:OG	3:D:639:VAL:N	2.28	0.66
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.76	0.66
3:D:48:THR:C	3:D:50:LYS:H	2.03	0.66
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.78	0.66
3:D:425:ARG:HG2	3:D:426:ALA:N	2.10	0.66
5:F:281:ARG:O	5:F:285:ARG:HG3	1.95	0.66
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.60	0.66
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.60	0.66
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.59	0.66
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.30	0.66
3:D:647:PRO:HD3	3:D:697:MET:HB3	1.78	0.66
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.77	0.66
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.75	0.66
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.29	0.66
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.77	0.66
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.77	0.66
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.96	0.65
5:L:573:LEU:HD23	5:L:573:LEU:H	1.59	0.65
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.76	0.65
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.78	0.65
4:K:14:GLY:O	4:K:16:ARG:N	2.29	0.65
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.29	0.65
2:C:624:ASP:OD1	2:C:625:GLU:N	2.27	0.65
1:A:38:THR:HG1	1:B:45:ARG:NH1	1.95	0.65
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.77	0.65
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.78	0.65
3:D:363:LEU:HG	3:D:363:LEU:O	1.96	0.65
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.32	0.65
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.20	0.65
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.79	0.65
3:D:515:ARG:O	3:D:545:HIS:HB3	1.97	0.65
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.17	0.65
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.78	0.65
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.29	0.65
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.31	0.65
3:D:56:LEU:H	3:D:56:LEU:HD12	1.60	0.65
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.65
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.79	0.65
2:C:617:ALA:HA	2:C:636:CYS:SG	2.37	0.65
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.61	0.65
2:I:705:GLU:HB2	2:I:794:LEU:H	1.62	0.65
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.76	0.65
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.28	0.65
3:D:504:GLN:HG3	3:D:505:ASP:H	1.61	0.65
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.78	0.65
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.77	0.65
1:G:9:LEU:O	1:H:227:GLN:NE2	2.30	0.65
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.79	0.64
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.79	0.64
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.78	0.64
1:A:92:VAL:O	1:A:148:ARG:NH1	2.22	0.64
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.79	0.64
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.79	0.64
4:K:40:PRO:O	4:K:52:ARG:NH2	2.30	0.64
3:D:88:CYS:O	3:D:90:VAL:N	2.30	0.64
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.80	0.64
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.79	0.64
2:C:726:TYR:HE2	2:C:728:ASP:HB2	1.63	0.64
3:D:1183:SER:CA	3:J:206:ASN:HD21	2.07	0.64
2:I:1247:SER:HB3	3:J:375:GLU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:600:ALA:O	3:J:603:LYS:HG2	1.98	0.64
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.62	0.64
2:C:1243:MET:HA	3:D:353:SER:HB3	1.80	0.64
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.64
3:D:262:THR:OG1	3:D:263:SER:N	2.30	0.64
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.80	0.64
5:L:316:PHE:HZ	5:L:334:SER:HA	1.63	0.64
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.62	0.63
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.16	0.63
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.80	0.63
2:I:201:ARG:NH2	2:I:370:MET:O	2.30	0.63
2:I:596:ASP:CG	2:I:597:GLY:H	2.06	0.63
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.63	0.63
1:G:97:GLU:OE2	1:G:145:LYS:HE2	1.99	0.63
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.63
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.79	0.63
1:B:35:PHE:HA	1:B:38:THR:CG2	2.28	0.63
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.81	0.63
2:I:655:VAL:N	2:I:659:GLN:OE1	2.32	0.63
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.80	0.63
2:C:197:ARG:NH1	2:C:201:ARG:O	2.32	0.63
2:C:250:THR:HA	2:C:268:ARG:HA	1.80	0.63
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.81	0.63
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.80	0.63
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.62	0.63
2:C:168:GLY:O	2:C:170:VAL:N	2.26	0.63
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.80	0.63
1:G:27:THR:HG23	1:G:202:VAL:HG22	1.81	0.63
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.80	0.63
2:I:250:THR:HA	2:I:268:ARG:HA	1.80	0.63
1:A:297:LYS:O	1:A:301:THR:OG1	2.14	0.63
3:D:392:THR:HG21	5:F:606:VAL:HA	1.81	0.63
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.81	0.63
1:A:12:ARG:H	1:A:30:PRO:HD2	1.64	0.62
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.80	0.62
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.24	0.62
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.27	0.62
5:L:561:MET:HA	5:L:567:MET:HE1	1.82	0.62
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.34	0.62
1:A:241:GLU:HG3	1:A:242:VAL:H	1.65	0.62
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.13	0.62
1:G:229:GLU:HA	1:G:231:PHE:CZ	2.34	0.62
3:D:1281:GLU:O	3:D:1285:VAL:HG13	1.99	0.62
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.82	0.62
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.81	0.62
1:H:49:SER:O	1:H:151:GLY:HA2	1.99	0.62
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.33	0.62
2:I:169:LYS:O	2:I:170:VAL:HG22	2.00	0.62
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.81	0.62
5:F:354:THR:O	5:F:358:VAL:HG23	1.99	0.62
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.80	0.62
2:C:1032:LYS:O	2:C:1036:ILE:HG13	1.99	0.62
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.30	0.62
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.82	0.62
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.81	0.62
3:D:598:LYS:O	3:D:601:ILE:HG22	1.99	0.62
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.81	0.62
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.81	0.61
2:C:1066:MET:HE2	2:C:1076:ILE:HG22	1.80	0.61
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.30	0.61
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.15	0.61
2:C:886:LYS:H	2:C:917:SER:HB3	1.65	0.61
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.82	0.61
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.65	0.61
4:E:62:GLN:O	4:E:66:VAL:HG23	2.00	0.61
2:I:975:ILE:O	2:I:979:LEU:HB2	2.01	0.61
2:C:521:LEU:O	2:C:525:THR:HB	2.01	0.61
3:D:395:LYS:HG2	5:F:536:THR:HG21	1.83	0.61
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.82	0.61
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.36	0.61
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.36	0.61
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.00	0.61
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.36	0.61
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.83	0.61
2:C:147:SER:OG	2:C:455:SER:HB3	2.01	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.40	0.61
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.83	0.61
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.82	0.61
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.35	0.61
1:A:59:VAL:HG22	1:A:144:ILE:HA	1.83	0.61
1:A:95:LYS:O	1:A:148:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.82	0.61
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.81	0.61
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.34	0.61
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.35	0.61
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.82	0.61
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.82	0.61
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.16	0.61
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.83	0.61
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.25	0.61
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.81	0.61
1:A:166:ARG:O	1:A:168:ILE:N	2.34	0.60
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.82	0.60
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.83	0.60
3:J:425:ARG:HG2	3:J:426:ALA:H	1.65	0.60
2:C:1164:PHE:O	2:C:1166:ASP:N	2.33	0.60
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.60
3:D:848:VAL:HG13	3:D:857:LEU:HB2	1.81	0.60
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.83	0.60
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.66	0.60
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.66	0.60
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.83	0.60
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.34	0.60
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.81	0.60
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.35	0.60
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.82	0.60
3:D:103:GLY:C	3:D:244:VAL:HG22	2.27	0.60
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.83	0.60
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.84	0.60
2:I:998:LEU:H	2:I:998:LEU:HD12	1.67	0.60
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.83	0.60
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.36	0.60
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.64	0.60
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.60
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.34	0.60
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.83	0.60
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.84	0.60
5:L:469:GLN:O	5:L:473:GLU:HB2	2.02	0.60
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.32	0.60
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.82	0.60
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.84	0.60
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HA	3:D:192:MET:HE1	1.83	0.60
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.84	0.60
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.82	0.60
2:I:168:GLY:C	2:I:170:VAL:H	2.10	0.60
2:I:582:ASN:HB3	2:I:586:PHE:H	1.66	0.60
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.66	0.60
3:J:632:ALA:O	3:J:635:SER:OG	2.15	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.35	0.60
1:B:48:LEU:HA	1:B:180:VAL:HG21	1.84	0.60
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.17	0.60
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.35	0.60
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.84	0.60
1:H:62:ASP:OD1	1:H:62:ASP:N	2.27	0.60
2:I:168:GLY:O	2:I:170:VAL:N	2.34	0.60
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.84	0.59
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.83	0.59
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.84	0.59
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.66	0.59
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.82	0.59
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.35	0.59
1:B:99:ILE:HD12	1:B:145:LYS:HB2	1.85	0.59
2:C:41:GLN:NE2	2:C:73:TYR:O	2.35	0.59
3:D:27:PRO:O	3:D:31:ARG:HG3	2.01	0.59
5:F:600:HIS:CG	5:F:601:PRO:HD3	2.37	0.59
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.12	0.59
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.84	0.59
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.59
5:L:474:MET:HE2	5:L:478:PRO:HA	1.84	0.59
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.84	0.59
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.17	0.59
5:L:474:MET:C	5:L:476:ARG:H	2.11	0.59
3:D:81:ARG:C	3:D:83:VAL:H	2.09	0.59
3:D:203:GLU:O	3:D:207:GLU:HG2	2.01	0.59
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.83	0.59
3:J:598:LYS:O	3:J:601:ILE:HG22	2.03	0.59
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.84	0.59
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.84	0.59
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.37	0.59
3:J:418:GLU:HG3	4:K:45:LYS:H	1.67	0.59
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.84	0.59
1:A:54:CYS:HA	1:A:148:ARG:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.18	0.59
3:J:801:VAL:O	3:J:805:GLN:HB2	2.02	0.59
1:A:290:LEU:HB3	1:A:291:LYS:HE2	1.85	0.59
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.02	0.59
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.37	0.59
3:D:491:LEU:HD22	3:D:496:GLY:O	2.02	0.59
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.37	0.59
3:J:362:ARG:H	3:J:365:GLN:HE21	1.51	0.59
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.84	0.59
3:J:1290:ARG:HD2	3:J:1295:ASN:ND2	2.17	0.59
3:D:355:ILE:HG12	3:D:464:ASP:O	2.03	0.59
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.16	0.59
5:L:281:ARG:O	5:L:285:ARG:HG3	2.02	0.59
5:L:312:SER:OG	5:L:313:ASP:N	2.34	0.59
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.84	0.58
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.84	0.58
1:A:169:GLY:O	1:A:171:LEU:HD22	2.03	0.58
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.85	0.58
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.03	0.58
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.85	0.58
5:F:462:LYS:HD2	5:F:487:MET:SD	2.43	0.58
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.85	0.58
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.30	0.58
2:I:1119:MET:HE3	2:I:1204:LEU:HD22	1.84	0.58
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.37	0.58
3:D:709:ARG:HD2	3:D:710:ASP:H	1.68	0.58
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.84	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.03	0.58
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.85	0.58
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.03	0.58
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.85	0.58
3:J:683:ILE:HD11	3:J:754:ILE:HD13	1.84	0.58
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.03	0.58
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	1.85	0.58
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.83	0.58
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.85	0.58
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.85	0.58
2:C:746:ALA:CB	2:C:974:ARG:HE	2.16	0.58
3:D:647:PRO:HG3	3:D:697:MET:CA	2.34	0.58
2:I:206:ALA:O	2:I:209:ILE:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.85	0.58
1:B:62:ASP:OD1	1:B:62:ASP:N	2.34	0.58
3:D:836:ARG:HD2	3:D:873:GLU:OE1	2.04	0.58
2:I:494:ASN:HB3	2:I:497:PRO:HG2	1.85	0.58
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.84	0.58
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.36	0.58
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.04	0.58
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.86	0.58
1:A:218:ARG:HG3	1:B:231:PHE:O	2.04	0.58
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.38	0.58
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.04	0.58
1:H:35:PHE:HA	1:H:38:THR:CG2	2.33	0.58
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.85	0.58
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.86	0.58
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.87	0.58
2:C:796:LEU:H	2:C:796:LEU:HD12	1.67	0.58
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.01	0.58
3:D:510:LEU:O	3:D:514:THR:HG22	2.04	0.58
5:F:311:THR:HB	5:F:345:GLN:HG2	1.85	0.58
5:F:584:ARG:O	5:F:588:ARG:HG3	2.04	0.58
3:D:473:THR:HG23	3:D:476:ALA:H	1.69	0.58
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.03	0.58
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.04	0.58
5:L:296:LYS:HB2	5:L:329:LYS:HD3	1.86	0.58
1:A:7:GLU:HB3	1:B:150:ARG:HH12	1.69	0.57
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.86	0.57
3:D:854:ALA:HB1	3:J:1372:ARG:CZ	2.34	0.57
4:E:49:ILE:O	4:E:53:GLU:HG3	2.04	0.57
5:F:222:ALA:O	5:F:226:ALA:N	2.35	0.57
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.86	0.57
3:J:1168:GLU:OE2	3:J:1169:THR:OG1	2.21	0.57
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.37	0.57
1:G:92:VAL:HA	1:G:120:ASP:O	2.03	0.57
1:H:101:THR:H	1:H:116:THR:HG22	1.69	0.57
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.38	0.57
3:J:825:VAL:C	3:J:826:ILE:HG13	2.28	0.57
5:F:267:ASP:O	5:F:271:ASN:N	2.32	0.57
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.85	0.57
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.86	0.57
3:J:197:GLU:O	3:J:201:LEU:HG	2.05	0.57
3:J:473:THR:HG23	3:J:476:ALA:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.86	0.57
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.85	0.57
2:I:1063:GLY:O	3:J:354:VAL:HG11	2.03	0.57
3:J:809:VAL:HA	3:J:894:VAL:O	2.04	0.57
1:A:118:ASP:H	1:A:121:VAL:HB	1.68	0.57
2:I:1106:ARG:O	2:I:1108:ASN:N	2.36	0.57
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.05	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.34	0.57
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.21	0.57
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.19	0.57
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.39	0.57
3:J:69:GLU:HG3	3:J:76:LYS:HG2	1.85	0.57
3:J:902:ASP:OD1	3:J:903:LEU:N	2.38	0.57
3:D:227:PHE:O	3:D:230:SER:HB3	2.03	0.57
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.86	0.57
2:I:170:VAL:HG21	2:I:172:TYR:OH	2.04	0.57
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.04	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
2:C:953:LEU:HD13	2:C:1036:ILE:HD12	1.87	0.57
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.40	0.57
5:F:612:ASP:OD1	5:F:612:ASP:N	2.36	0.57
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.86	0.57
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.40	0.57
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.39	0.57
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.86	0.57
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.04	0.57
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.85	0.57
5:F:343:LYS:H	5:F:343:LYS:HD2	1.70	0.57
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.86	0.57
2:I:1075:VAL:HG21	3:J:463:GLY:HA2	1.87	0.57
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.85	0.57
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.05	0.57
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.57
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.87	0.57
3:D:678:ARG:O	3:D:682:VAL:HG23	2.04	0.57
3:D:825:VAL:C	3:D:826:ILE:HG13	2.30	0.57
5:F:261:LEU:H	5:F:261:LEU:HD12	1.70	0.57
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.86	0.57
2:I:1263:ALA:O	2:I:1265:PHE:HD1	1.88	0.57
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.87	0.57
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:908:ILE:HG12	3:J:909:ILE:N	2.20	0.57
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.19	0.57
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.87	0.56
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.87	0.56
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.05	0.56
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.70	0.56
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.86	0.56
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.87	0.56
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.35	0.56
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.87	0.56
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.35	0.56
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.24	0.56
1:G:75:GLN:HA	2:I:729:ALA:N	2.19	0.56
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.96	0.56
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.37	0.56
3:J:16:GLU:HG3	3:J:17:PHE:H	1.69	0.56
5:L:465:ARG:HB3	5:L:468:ARG:HH12	1.70	0.56
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.20	0.56
2:C:246:LEU:HB2	2:C:269:ILE:HG21	1.86	0.56
2:C:1274:GLU:O	2:C:1277:ALA:HB3	2.06	0.56
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.88	0.56
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.41	0.56
3:D:549:LYS:HD3	3:D:569:LEU:HD23	1.87	0.56
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.88	0.56
3:D:1285:VAL:HG23	3:D:1286:LYS:HG3	1.85	0.56
5:F:226:ALA:O	5:F:229:VAL:HG22	2.06	0.56
1:G:13:LEU:HD23	1:G:13:LEU:H	1.69	0.56
1:G:76:GLU:OE1	1:G:132:HIS:N	2.32	0.56
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.86	0.56
2:I:1131:MET:HB3	2:I:1141:LEU:HD11	1.88	0.56
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.05	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.88	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.40	0.56
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.87	0.56
5:L:470:MET:O	5:L:478:PRO:HD3	2.05	0.56
5:L:612:ASP:N	5:L:612:ASP:OD1	2.33	0.56
2:C:1160:ASP:HB2	2:C:1161:LEU:HD12	1.87	0.56
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.40	0.56
2:I:601:ASP:OD1	2:I:601:ASP:N	2.37	0.56
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.88	0.56
3:J:70:CYS:SG	3:J:90:VAL:HB	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.20	0.56
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.06	0.56
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.88	0.56
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.39	0.56
5:L:245:ALA:O	5:L:249:ILE:HG13	2.05	0.56
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.88	0.56
2:C:325:LEU:O	2:C:330:HIS:HB2	2.05	0.56
2:C:738:GLU:HA	2:C:741:MET:HE2	1.87	0.56
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.86	0.56
5:F:311:THR:HG21	5:F:348:GLU:CD	2.30	0.56
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.88	0.56
2:I:1017:GLN:O	2:I:1021:LEU:HG	2.05	0.56
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.06	0.56
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.36	0.56
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.87	0.56
5:F:127:ILE:O	5:F:130:VAL:HG22	2.05	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
2:I:499:SER:O	2:I:503:LYS:HB2	2.06	0.56
2:I:672:GLU:HB3	2:I:1187:PHE:HD2	1.70	0.56
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.88	0.56
3:J:277:ASN:HA	3:J:280:LYS:HG3	1.88	0.56
5:L:455:HIS:O	5:L:459:THR:OG1	2.16	0.56
1:A:137:ASN:N	1:A:137:ASN:OD1	2.39	0.56
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.71	0.56
2:C:499:SER:O	2:C:503:LYS:HB2	2.06	0.56
3:D:770:LEU:H	3:D:770:LEU:HD22	1.70	0.56
3:D:825:VAL:HG22	3:D:833:GLU:H	1.71	0.56
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.87	0.56
5:F:513:ASP:C	5:F:515:GLU:H	2.14	0.56
2:I:1253:LEU:HD11	3:J:253:VAL:HG11	1.87	0.56
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.87	0.56
3:J:903:LEU:HD21	3:J:913:GLU:OE1	2.06	0.56
3:J:1168:GLU:OE1	3:J:1173:ARG:HG3	2.06	0.56
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.20	0.56
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.38	0.56
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.87	0.56
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.88	0.56
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.86	0.56
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.88	0.56
5:L:515:GLU:HG2	5:L:516:ASP:N	2.21	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ILE:O	2:C:139:ASN:ND2	2.39	0.56
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.71	0.56
3:D:709:ARG:HD2	3:D:710:ASP:N	2.21	0.56
1:A:268:ASN:O	1:A:271:LYS:HB3	2.05	0.55
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.21	0.55
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.88	0.55
2:I:941:LYS:HD3	2:I:949:GLU:OE1	2.06	0.55
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.87	0.55
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.21	0.55
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.22	0.55
3:J:770:LEU:H	3:J:770:LEU:HD22	1.71	0.55
3:J:1174:ARG:HH21	3:J:1189:MET:HE1	1.72	0.55
5:F:147:GLN:O	5:F:151:VAL:HG23	2.07	0.55
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.88	0.55
2:I:499:SER:HA	2:I:502:VAL:HG12	1.88	0.55
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.41	0.55
4:K:15:ASN:C	4:K:17:PHE:H	2.15	0.55
1:A:159:ILE:HG13	1:A:162:GLU:HG3	1.88	0.55
2:C:778:GLU:O	2:C:781:ASP:HB2	2.06	0.55
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.41	0.55
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.71	0.55
3:J:245:LEU:O	3:J:250:ARG:NE	2.37	0.55
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.07	0.55
5:L:262:VAL:HG11	5:L:264:LYS:HZ2	1.72	0.55
1:A:115:ILE:HG22	1:A:116:THR:H	1.70	0.55
2:C:61:SER:O	2:C:63:SER:N	2.38	0.55
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.88	0.55
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.42	0.55
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.22	0.55
5:L:476:ARG:HB3	5:L:476:ARG:HH11	1.71	0.55
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.89	0.55
2:C:149:LEU:HD12	2:C:452:ARG:O	2.07	0.55
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.87	0.55
2:C:452:ARG:HH12	2:C:585:GLY:HA3	1.71	0.55
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.37	0.55
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.88	0.55
5:F:575:GLU:O	5:F:579:GLN:HG2	2.07	0.55
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.88	0.55
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.87	0.55
2:C:541:GLU:OE1	2:C:541:GLU:N	2.39	0.55
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.89	0.55
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.07	0.55
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.40	0.55
1:A:14:VAL:HG22	1:A:15:ASP:N	2.23	0.55
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.87	0.55
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.88	0.55
1:G:159:ILE:HG13	1:G:162:GLU:HG3	1.89	0.55
2:I:1148:ALA:HB1	2:I:1180:MET:HE1	1.88	0.55
3:J:56:LEU:HD12	3:J:56:LEU:H	1.71	0.55
3:J:251:PRO:HB2	3:J:253:VAL:HG13	1.89	0.55
3:J:515:ARG:NH2	3:J:718:SER:O	2.27	0.55
3:J:793:SER:O	3:J:797:THR:HG23	2.07	0.55
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.89	0.54
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.88	0.54
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.72	0.54
4:E:58:LEU:HD12	4:E:58:LEU:H	1.71	0.54
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.88	0.54
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.12	0.54
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.88	0.54
5:L:347:ILE:HB	5:L:355:ILE:HD11	1.88	0.54
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.88	0.54
2:C:1255:THR:O	2:C:1257:GLN:N	2.40	0.54
3:D:325:LYS:HG2	3:D:330:MET:HE3	1.89	0.54
5:F:245:ALA:O	5:F:249:ILE:HG13	2.07	0.54
1:H:27:THR:HB	1:H:202:VAL:HG22	1.87	0.54
1:H:101:THR:H	1:H:116:THR:CG2	2.21	0.54
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.89	0.54
1:A:112:ALA:O	1:A:115:ILE:HG13	2.07	0.54
1:B:192:VAL:O	1:B:194:GLN:N	2.41	0.54
2:C:1066:MET:HG2	2:C:1234:LYS:HA	1.90	0.54
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.54
3:J:436:ALA:HB3	3:J:485:MET:HA	1.89	0.54
5:L:601:PRO:HA	5:L:604:SER:HB3	1.88	0.54
2:C:417:SER:OG	2:C:419:ILE:O	2.23	0.54
3:D:1344:LEU:O	3:D:1346:GLY:N	2.36	0.54
2:I:637:ARG:HA	2:I:642:SER:HA	1.88	0.54
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.54
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.89	0.54
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.07	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.71	0.54
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.73	0.54
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.07	0.54
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.90	0.54
2:C:607:SER:OG	2:C:609:ILE:HG13	2.06	0.54
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.07	0.54
5:F:392:LYS:O	5:F:395:THR:HG23	2.06	0.54
2:C:211:ARG:NH1	2:C:357:ASN:O	2.41	0.54
2:C:980:VAL:O	2:C:984:VAL:HB	2.08	0.54
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.90	0.54
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.90	0.54
2:C:730:SER:O	2:C:753:LEU:HB2	2.08	0.54
2:C:1207:SER:HB2	2:C:1209:GLN:H	1.72	0.54
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.89	0.54
3:D:1372:ARG:O	3:D:1375:ALA:HB3	2.08	0.54
3:D:1376:GLY:O	3:J:852:GLY:HA2	2.08	0.54
1:H:59:VAL:HG23	1:H:173:VAL:HG21	1.89	0.54
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.73	0.54
2:I:149:LEU:HD12	2:I:452:ARG:O	2.08	0.54
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.90	0.54
3:J:514:THR:O	3:J:514:THR:OG1	2.17	0.54
3:J:844:THR:OG1	3:J:860:ARG:O	2.21	0.54
2:C:466:VAL:O	2:C:470:ARG:HG2	2.06	0.54
3:D:1170:LYS:C	3:D:1172:LYS:H	2.15	0.54
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.89	0.54
1:G:107:ILE:HG12	1:G:135:ASP:O	2.08	0.54
2:I:124:MET:HE2	2:I:493:ILE:HD11	1.90	0.54
2:C:367:TYR:HA	2:C:384:LEU:HD22	1.90	0.54
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.89	0.54
2:C:998:LEU:H	2:C:998:LEU:HD12	1.73	0.54
3:D:197:GLU:O	3:D:201:LEU:HG	2.07	0.54
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.88	0.54
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.90	0.54
2:C:297:VAL:HG12	2:C:315:MET:O	2.09	0.53
2:C:1066:MET:HE2	2:C:1076:ILE:CG2	2.38	0.53
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.16	0.53
3:J:478:LEU:HG	4:K:47:THR:HG23	1.89	0.53
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.23	0.53
5:L:476:ARG:HD2	5:L:477:GLU:HG2	1.89	0.53
1:A:115:ILE:HG22	1:A:116:THR:N	2.23	0.53
2:C:242:VAL:HG12	2:C:244:GLU:H	1.74	0.53
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.43	0.53
5:F:377:LYS:O	5:F:381:GLU:HG3	2.08	0.53
2:I:577:VAL:HG23	2:I:661:VAL:O	2.08	0.53
5:L:127:ILE:O	5:L:130:VAL:HG22	2.08	0.53
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.39	0.53
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.53
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.90	0.53
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.91	0.53
3:D:336:GLY:HA3	3:D:1324:SER:O	2.08	0.53
4:E:15:ASN:HB3	4:E:18:ASP:H	1.72	0.53
2:C:882:ILE:HD12	2:C:882:ILE:H	1.73	0.53
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.89	0.53
3:D:1280:VAL:CG2	3:D:1304:ARG:HH21	2.11	0.53
5:F:469:GLN:O	5:F:473:GLU:HB2	2.08	0.53
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.43	0.53
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.91	0.53
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.43	0.53
1:A:7:GLU:HB3	1:B:150:ARG:NH1	2.22	0.53
1:A:92:VAL:HG11	1:A:98:VAL:HG11	1.91	0.53
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.73	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.73	0.53
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.74	0.53
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.44	0.53
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.89	0.53
3:J:370:LYS:HZ3	3:J:409:TRP:CG	2.27	0.53
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.34	0.53
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.74	0.53
3:D:1266:ILE:HD11	3:D:1276:GLU:HB3	1.91	0.53
5:F:557:LYS:O	5:F:561:MET:HE3	2.09	0.53
1:H:102:LEU:O	1:H:141:SER:HA	2.09	0.53
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.90	0.53
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.09	0.53
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.74	0.53
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.53
1:B:81:ILE:O	1:B:85:LEU:HG	2.09	0.53
2:C:198:ILE:O	2:C:201:ARG:HB2	2.09	0.53
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.89	0.53
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.90	0.53
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.72	0.53
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.74	0.53
5:F:225:ARG:O	5:F:229:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:228:TYR:CE2	5:F:232:ARG:HD3	2.44	0.53
3:J:358:GLY:N	3:J:359:PRO:HD3	2.24	0.53
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.90	0.53
2:C:202:ARG:HH12	2:C:368:ARG:HH22	1.56	0.53
3:D:266:ASN:O	3:D:270:ARG:HB2	2.09	0.53
3:D:647:PRO:CG	3:D:697:MET:HB3	2.38	0.53
2:I:724:VAL:HG23	2:I:775:GLU:H	1.74	0.53
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.91	0.53
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.74	0.53
3:J:48:THR:C	3:J:50:LYS:H	2.12	0.53
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.39	0.53
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.91	0.53
1:A:296:GLY:N	1:A:299:SER:HB2	2.10	0.53
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.09	0.53
5:F:312:SER:OG	5:F:313:ASP:N	2.42	0.53
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.89	0.53
2:I:310:ILE:HD13	2:I:325:LEU:HB3	1.91	0.53
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.74	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.74	0.53
3:J:425:ARG:HG2	3:J:426:ALA:N	2.24	0.53
3:J:697:MET:SD	3:J:741:ALA:HB3	2.49	0.53
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.28	0.53
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.91	0.52
3:D:398:LYS:HE2	5:F:532:LEU:CD2	2.39	0.52
3:D:787:ALA:O	3:D:790:THR:HB	2.09	0.52
1:G:12:ARG:H	1:G:30:PRO:CD	2.14	0.52
1:G:14:VAL:HG13	1:G:15:ASP:H	1.74	0.52
3:J:128:LEU:HA	3:J:192:MET:HE1	1.91	0.52
4:K:50:ALA:O	4:K:54:ILE:HG12	2.09	0.52
1:B:76:GLU:OE2	1:B:132:HIS:N	2.40	0.52
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.73	0.52
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.74	0.52
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.91	0.52
3:J:525:MET:O	3:J:548:VAL:HG13	2.09	0.52
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.73	0.52
2:C:746:ALA:HB2	2:C:974:ARG:HE	1.72	0.52
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.40	0.52
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.90	0.52
2:C:42:ASP:C	2:C:44:GLU:H	2.17	0.52
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.40	0.52
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.41	0.52
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.42	0.52
3:D:79:LYS:HB2	5:F:568:ASN:OD1	2.09	0.52
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.44	0.52
3:J:697:MET:HG3	3:J:698:MET:N	2.24	0.52
5:L:395:THR:OG1	5:L:396:ASN:N	2.42	0.52
1:A:47:LEU:O	1:A:180:VAL:HG21	2.10	0.52
1:A:190:ALA:H	1:A:199:ASP:HA	1.74	0.52
1:B:205:MET:HE1	1:B:217:ILE:HG13	1.91	0.52
2:C:169:LYS:O	2:C:170:VAL:HG22	2.09	0.52
2:C:620:ASN:ND2	2:C:620:ASN:O	2.43	0.52
3:D:81:ARG:HG3	3:D:82:GLY:H	1.74	0.52
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.92	0.52
1:H:65:LEU:HD13	1:H:171:LEU:HD21	1.92	0.52
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.91	0.52
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.09	0.52
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.45	0.52
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.91	0.52
2:I:607:SER:N	2:I:610:GLU:HB2	2.25	0.52
2:I:617:ALA:HA	2:I:636:CYS:SG	2.50	0.52
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.45	0.52
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.24	0.52
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.10	0.52
3:D:356:THR:OG1	3:D:357:VAL:N	2.43	0.52
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.45	0.52
2:I:96:LEU:HD23	2:I:124:MET:HG3	1.92	0.52
2:I:384:LEU:O	2:I:388:LEU:HG	2.10	0.52
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.44	0.52
5:L:343:LYS:O	5:L:347:ILE:HG13	2.10	0.52
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.92	0.52
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.91	0.52
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.92	0.52
5:F:267:ASP:HA	5:F:270:VAL:HB	1.92	0.52
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.52
5:F:117:ILE:HA	5:F:120:ALA:HB3	1.92	0.52
5:F:299:LYS:O	5:F:303:ILE:HG12	2.10	0.52
3:J:220:ARG:O	3:J:223:LEU:HB3	2.10	0.52
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.45	0.52
1:A:31:LEU:HB2	1:A:199:ASP:O	2.10	0.51
2:C:345:PRO:O	2:C:349:GLU:HG2	2.10	0.51
3:D:707:ILE:HD12	3:D:707:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.92	0.51
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.10	0.51
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.38	0.51
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.46	0.51
2:I:896:THR:HB	2:I:897:PRO:HD2	1.92	0.51
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.75	0.51
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.92	0.51
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.75	0.51
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.93	0.51
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.75	0.51
3:J:311:ARG:O	3:J:312:ARG:HD3	2.09	0.51
3:J:432:LEU:HD21	3:J:489:ASN:HB3	1.92	0.51
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.93	0.51
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.40	0.51
1:B:228:LEU:C	1:B:230:ALA:H	2.18	0.51
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.93	0.51
2:C:198:ILE:HD13	2:C:388:LEU:HD13	1.91	0.51
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.40	0.51
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.92	0.51
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.91	0.51
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.75	0.51
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.75	0.51
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.91	0.51
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.93	0.51
5:L:226:ALA:O	5:L:229:VAL:HG22	2.10	0.51
1:B:76:GLU:CD	1:B:132:HIS:H	2.19	0.51
2:C:105:TYR:HD1	2:C:112:GLY:H	1.58	0.51
2:C:1211:ARG:HE	2:C:1220:GLN:HE21	1.59	0.51
5:F:453:PRO:O	5:F:456:MET:HB2	2.10	0.51
2:I:151:ARG:NH2	2:I:177:ILE:HD11	2.26	0.51
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.10	0.51
4:K:3:ARG:NE	4:K:3:ARG:HA	2.25	0.51
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.92	0.51
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.92	0.51
3:D:1177:ILE:HG13	3:D:1186:TYR:HB3	1.93	0.51
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.92	0.51
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.93	0.51
3:J:363:LEU:HG	3:J:363:LEU:O	2.11	0.51
3:J:594:GLN:HG3	3:J:596:LEU:HD22	1.92	0.51
3:J:903:LEU:HB3	3:J:905:ARG:H	1.74	0.51
3:D:252:LEU:CD2	3:D:262:THR:HB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.40	0.51
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.44	0.51
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.76	0.51
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.73	0.51
2:I:739:ASP:OD1	2:I:739:ASP:N	2.40	0.51
2:I:1131:MET:HB3	2:I:1141:LEU:CD1	2.40	0.51
3:J:850:LYS:HB2	3:J:852:GLY:O	2.11	0.51
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.91	0.51
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.26	0.51
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.93	0.51
2:C:800:MET:HE1	2:C:822:VAL:HG13	1.93	0.51
2:C:1148:ALA:HB1	2:C:1180:MET:HE1	1.92	0.51
3:D:80:HIS:CB	3:D:83:VAL:HG11	2.38	0.51
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.93	0.51
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.76	0.51
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.41	0.51
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.51	0.51
1:A:285:THR:OG1	1:A:287:VAL:HG23	2.10	0.51
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.92	0.51
3:D:54:ASP:OD1	3:D:54:ASP:N	2.43	0.51
3:D:500:ILE:HG22	3:D:500:ILE:O	2.11	0.51
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.51
2:I:5:TYR:O	2:I:8:LYS:HG2	2.10	0.51
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.93	0.51
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.93	0.51
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.92	0.51
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.93	0.51
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.93	0.51
2:C:1207:SER:C	2:C:1209:GLN:H	2.18	0.51
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.92	0.51
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.93	0.51
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.76	0.51
3:J:1167:LYS:CE	3:J:1174:ARG:HD2	2.39	0.51
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.50
2:C:169:LYS:HE2	2:C:190:PRO:O	2.11	0.50
2:C:961:SER:O	2:C:965:GLN:HG3	2.10	0.50
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.46	0.50
3:D:72:CYS:SG	3:D:73:GLY:N	2.84	0.50
3:D:647:PRO:CD	3:D:697:MET:HB3	2.40	0.50
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.92	0.50
2:I:125:GLY:CA	2:I:499:SER:HB2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:226:ALA:O	3:D:230:SER:N	2.42	0.50
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.93	0.50
2:I:1210:ILE:HD11	2:I:1227:VAL:HG21	1.91	0.50
1:A:156:SER:HB3	2:C:1059:ARG:NH2	2.26	0.50
2:C:1164:PHE:C	2:C:1166:ASP:H	2.19	0.50
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.93	0.50
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.93	0.50
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.25	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.93	0.50
1:G:91:ARG:HB3	1:G:122:GLU:HB3	1.93	0.50
1:H:64:VAL:HG12	1:H:66:HIS:H	1.77	0.50
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.92	0.50
3:J:223:LEU:O	3:J:226:ALA:HB3	2.11	0.50
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.26	0.50
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.27	0.50
4:K:15:ASN:HB3	4:K:18:ASP:H	1.76	0.50
5:L:141:ILE:HD13	5:L:256:PHE:CD1	2.46	0.50
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.94	0.50
2:C:719:LYS:O	2:C:779:ARG:HG3	2.12	0.50
2:C:1106:ARG:O	2:C:1108:ASN:N	2.42	0.50
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.77	0.50
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.58	0.50
5:F:354:THR:OG1	5:F:356:GLU:HB3	2.11	0.50
1:G:125:LYS:HG3	1:G:128:HIS:HB2	1.94	0.50
2:C:1124:ILE:HG21	2:C:1180:MET:CE	2.41	0.50
2:C:1282:GLY:O	2:C:1284:ALA:N	2.44	0.50
3:D:75:TYR:HB3	3:D:80:HIS:HD2	1.76	0.50
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.77	0.50
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.93	0.50
2:I:1286:THR:O	2:I:1290:MET:HB2	2.11	0.50
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.10	0.50
3:J:515:ARG:O	3:J:545:HIS:HB3	2.12	0.50
5:L:483:LEU:HD12	5:L:483:LEU:H	1.76	0.50
1:B:76:GLU:HB3	1:B:80:GLU:HG2	1.93	0.50
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.41	0.50
1:G:103:ASN:OD1	1:G:141:SER:HB2	2.12	0.50
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.94	0.50
3:J:647:PRO:HG3	3:J:697:MET:CA	2.42	0.50
5:L:414:LYS:HD3	5:L:434:TRP:HZ3	1.76	0.50
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.93	0.50
2:C:408:SER:O	2:C:431:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:ASN:O	2:C:498:ILE:HD13	2.12	0.50
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.50
5:F:320:ILE:HG23	5:F:327:SER:O	2.11	0.50
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.92	0.50
2:I:757:THR:O	2:I:765:ILE:HG23	2.12	0.50
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.94	0.50
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.94	0.50
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.47	0.50
2:C:796:LEU:HD12	2:C:796:LEU:N	2.25	0.50
2:C:799:ASN:HB3	2:C:1231:TYR:HA	1.93	0.50
2:C:876:GLU:HG2	2:C:927:THR:OG1	2.12	0.50
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.47	0.50
2:C:1269:ARG:HD3	3:D:343:LEU:HD23	1.94	0.50
3:D:224:LEU:O	3:D:227:PHE:N	2.45	0.50
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.94	0.50
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.93	0.50
1:G:45:ARG:NH2	1:H:37:HIS:HB3	2.26	0.50
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.94	0.50
2:I:553:THR:O	2:I:557:ARG:HD2	2.12	0.50
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.46	0.50
3:J:849:LEU:H	3:J:849:LEU:HD22	1.77	0.50
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.94	0.49
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.94	0.49
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.39	0.49
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.77	0.49
5:F:487:MET:HA	5:F:487:MET:CE	2.41	0.49
1:H:51:MET:HB3	1:H:178:SER:HB2	1.94	0.49
2:I:465:ARG:O	2:I:469:VAL:HG13	2.12	0.49
2:I:466:VAL:O	2:I:469:VAL:HG22	2.12	0.49
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.93	0.49
3:J:266:ASN:O	3:J:270:ARG:HB2	2.12	0.49
5:L:287:ILE:HD13	5:L:315:TRP:CH2	2.47	0.49
2:C:5:TYR:O	2:C:8:LYS:HG2	2.11	0.49
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.94	0.49
2:C:131:THR:HB	2:C:133:ASN:H	1.77	0.49
2:C:540:ARG:HB2	2:C:540:ARG:HH11	1.77	0.49
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.27	0.49
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.27	0.49
3:D:60:ARG:HA	3:D:89:GLY:O	2.12	0.49
3:D:144:TYR:HE2	3:D:162:GLU:HG2	1.77	0.49
3:D:347:VAL:HG12	3:D:348:ASP:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:8:ASP:HB2	4:E:55:GLU:OE2	2.13	0.49
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.49
3:J:81:ARG:C	3:J:83:VAL:H	2.18	0.49
1:A:195:ARG:HE	1:A:198:LEU:HD21	1.76	0.49
1:B:33:ARG:NH2	2:C:820:GLU:OE2	2.45	0.49
2:C:4:SER:OG	2:C:5:TYR:N	2.45	0.49
2:C:600:THR:HG22	2:C:601:ASP:H	1.77	0.49
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.41	0.49
1:H:11:PRO:O	1:H:12:ARG:HG3	2.13	0.49
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.27	0.49
5:L:165:PHE:HD1	5:L:259:PHE:HA	1.77	0.49
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.94	0.49
3:D:749:LYS:HB2	3:D:750:PRO:CD	2.42	0.49
5:F:456:MET:HE1	5:F:497:VAL:HG13	1.94	0.49
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.42	0.49
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.94	0.49
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.34	0.49
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	1.94	0.49
5:L:515:GLU:HG2	5:L:516:ASP:H	1.77	0.49
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.95	0.49
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.46	0.49
2:I:9:LYS:HD2	2:I:791:LEU:HD21	1.93	0.49
2:I:32:LEU:HD23	2:I:130:MET:SD	2.52	0.49
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.95	0.49
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.95	0.49
3:J:647:PRO:HG3	3:J:697:MET:N	2.27	0.49
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.93	0.49
3:D:218:THR:HA	3:D:221:ILE:HG22	1.94	0.49
3:D:825:VAL:HG22	3:D:833:GLU:N	2.26	0.49
4:E:15:ASN:C	4:E:17:PHE:H	2.20	0.49
2:I:117:ILE:HD12	2:I:488:MET:CG	2.43	0.49
2:I:143:ARG:NH2	2:I:512:SER:O	2.46	0.49
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.95	0.49
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.12	0.49
3:J:1170:LYS:C	3:J:1172:LYS:H	2.20	0.49
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.95	0.49
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.27	0.49
1:A:7:GLU:O	1:B:150:ARG:NH1	2.45	0.49
1:A:253:LEU:HA	1:A:278:ILE:HD11	1.93	0.49
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.48	0.49
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.95	0.49
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.48	0.49
3:J:423:LEU:HB3	3:J:466:MET:HE1	1.95	0.49
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.95	0.49
2:C:298:ALA:N	2:C:334:GLU:O	2.37	0.49
2:C:643:SER:HG	2:C:645:PHE:HE1	1.61	0.49
3:D:647:PRO:HG3	3:D:697:MET:CB	2.42	0.49
1:G:88:LEU:HD12	1:G:89:ALA:H	1.78	0.49
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.46	0.49
2:I:468:LEU:O	2:I:471:VAL:HG12	2.12	0.49
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.95	0.49
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.94	0.49
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.43	0.49
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.94	0.49
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.93	0.49
5:L:281:ARG:HG3	5:L:285:ARG:NH1	2.26	0.49
2:C:229:ILE:HB	2:C:240:GLU:CD	2.37	0.49
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.28	0.49
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.95	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.95	0.49
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.11	0.49
3:J:918:ILE:O	3:J:922:SER:OG	2.29	0.49
1:A:12:ARG:H	1:A:30:PRO:CD	2.25	0.49
2:C:79:VAL:HG23	2:C:80:PHE:H	1.78	0.49
2:C:93:SER:OG	2:C:126:GLU:OE1	2.19	0.49
2:C:619:ALA:HB1	2:C:657:THR:HA	1.95	0.49
2:C:836:LEU:HD12	2:C:836:LEU:N	2.27	0.49
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.94	0.49
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.47	0.49
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.27	0.49
5:F:363:ARG:O	5:F:367:ILE:HG13	2.12	0.49
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.94	0.49
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.95	0.49
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.77	0.49
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.95	0.49
5:L:148:TYR:OH	5:L:218:ARG:HA	2.13	0.49
1:A:224:LEU:O	1:A:228:LEU:HD12	2.12	0.48
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.93	0.48
2:C:323:ALA:O	2:C:327:GLN:HG3	2.12	0.48
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.94	0.48
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ARG:N	1:G:30:PRO:HD2	2.18	0.48
1:G:167:PRO:HG2	1:G:170:ARG:HD2	1.95	0.48
1:H:60:GLU:HG3	1:H:143:ARG:O	2.12	0.48
1:H:98:VAL:HG21	1:H:121:VAL:HG23	1.95	0.48
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.21	0.48
2:C:40:GLU:HG2	2:C:41:GLN:N	2.28	0.48
2:C:104:ILE:O	2:C:113:THR:HA	2.13	0.48
2:C:162:GLY:O	2:C:164:THR:N	2.45	0.48
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.78	0.48
1:H:18:GLN:HA	1:H:24:ALA:HA	1.95	0.48
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.26	0.48
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.13	0.48
3:J:79:LYS:HB2	5:L:569:THR:H	1.79	0.48
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.38	0.48
1:A:166:ARG:O	1:A:167:PRO:C	2.56	0.48
1:B:195:ARG:CB	1:B:198:LEU:HD21	2.43	0.48
3:D:81:ARG:O	3:D:83:VAL:N	2.46	0.48
3:D:317:THR:HA	3:D:324:LEU:HD23	1.94	0.48
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.95	0.48
3:J:98:ARG:O	3:J:248:ASP:HB2	2.13	0.48
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.28	0.48
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.96	0.48
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.94	0.48
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.44	0.48
3:D:140:TYR:HB3	5:F:100:MET:SD	2.53	0.48
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.29	0.48
1:H:98:VAL:O	1:H:146:VAL:HG22	2.12	0.48
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.96	0.48
2:I:580:GLN:HB2	2:I:605:TYR:HE1	1.78	0.48
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.95	0.48
3:J:650:LYS:HZ2	3:J:762:ASN:HD22	1.62	0.48
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.48	0.48
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.95	0.48
5:F:227:GLN:HE22	5:F:251:LYS:NZ	2.11	0.48
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.77	0.48
2:I:1239:VAL:C	2:I:1241:ASP:H	2.21	0.48
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.48	0.48
1:A:156:SER:HB3	2:C:1059:ARG:HH22	1.78	0.48
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.95	0.48
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.94	0.48
1:G:195:ARG:HG3	1:G:198:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.28	0.48
3:J:694:SER:O	3:J:698:MET:HB2	2.14	0.48
5:L:433:TRP:HE3	5:L:434:TRP:CD1	2.31	0.48
5:L:561:MET:HA	5:L:567:MET:CE	2.43	0.48
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.95	0.48
2:C:458:GLU:O	2:C:461:GLU:HB3	2.14	0.48
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.96	0.48
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.13	0.48
5:F:561:MET:HA	5:F:567:MET:HE1	1.96	0.48
1:G:75:GLN:HG3	1:G:76:GLU:OE2	2.14	0.48
1:H:44:ARG:HG2	1:H:183:ILE:HD13	1.95	0.48
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.48
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.96	0.48
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.95	0.48
3:D:708:ASN:HB3	3:D:712:GLN:O	2.12	0.48
1:H:92:VAL:HG13	1:H:120:ASP:O	2.14	0.48
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.48	0.48
2:I:715:THR:OG1	2:I:782:VAL:HG12	2.13	0.48
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.94	0.48
3:J:116:PHE:O	3:J:123:ARG:HB2	2.14	0.48
5:L:139:GLU:HG2	5:L:351:THR:HA	1.96	0.48
5:L:230:VAL:O	5:L:234:THR:HG23	2.13	0.48
5:L:476:ARG:HH11	5:L:477:GLU:H	1.62	0.48
1:A:284:ARG:HG3	1:A:288:GLU:HG3	1.96	0.48
2:C:721:GLY:N	2:C:740:GLU:OE1	2.41	0.48
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.96	0.48
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.44	0.48
3:D:1283:SER:O	3:D:1286:LYS:N	2.46	0.48
1:G:39:LEU:HD21	1:H:224:LEU:HD11	1.96	0.48
2:I:871:VAL:O	2:I:944:ARG:NH1	2.46	0.48
2:I:1269:ARG:HA	3:J:346:ARG:HA	1.96	0.48
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.14	0.48
3:J:691:ASP:O	3:J:695:LYS:HG2	2.14	0.48
1:A:321:TRP:CD2	1:A:322:PRO:HB3	2.49	0.48
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.48	0.48
2:C:462:ASN:O	2:C:466:VAL:HG23	2.14	0.48
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	1.95	0.48
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.96	0.48
1:H:81:ILE:HG23	1:H:130:ILE:O	2.14	0.48
2:I:646:SER:HB3	2:I:649:GLN:CD	2.39	0.48
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1284:ALA:N	3:J:479:GLU:OE1	2.47	0.48
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.78	0.48
5:L:470:MET:HA	5:L:473:GLU:HB3	1.96	0.48
1:A:118:ASP:O	1:A:120:ASP:N	2.47	0.47
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.95	0.47
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.49	0.47
2:C:1263:ALA:O	2:C:1265:PHE:HD1	1.97	0.47
3:D:244:VAL:HA	3:D:269:TYR:OH	2.13	0.47
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.46	0.47
3:D:744:ARG:HG3	3:D:744:ARG:O	2.14	0.47
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.47
1:H:67:GLU:O	1:H:78:ILE:HB	2.14	0.47
1:H:76:GLU:OE1	1:H:76:GLU:N	2.47	0.47
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.96	0.47
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.94	0.47
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.14	0.47
2:I:160:ASP:O	2:I:164:THR:OG1	2.30	0.47
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.96	0.47
2:C:149:LEU:HG	2:C:451:ARG:HH11	1.79	0.47
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.95	0.47
3:D:719:PHE:O	3:D:724:MET:HE2	2.14	0.47
5:F:277:MET:HE3	5:F:281:ARG:HH21	1.80	0.47
2:I:521:LEU:O	2:I:525:THR:HB	2.15	0.47
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.48	0.47
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.97	0.47
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.44	0.47
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.15	0.47
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.46	0.47
2:I:1273:MET:HG2	2:I:1276:TRP:CZ3	2.49	0.47
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.47
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.28	0.47
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.44	0.47
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.79	0.47
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.97	0.47
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.79	0.47
2:I:310:ILE:HG21	2:I:325:LEU:HD23	1.97	0.47
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.14	0.47
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.96	0.47
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.71	0.47
2:C:106:GLU:HG3	2:C:107:ARG:N	2.29	0.47
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:342:LEU:HA	3:D:343:LEU:HA	1.64	0.47
3:D:1282:TYR:HD2	3:D:1286:LYS:NZ	2.13	0.47
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.25	0.47
5:F:468:ARG:HH11	5:F:469:GLN:NE2	2.12	0.47
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.97	0.47
2:I:972:PHE:HB3	2:I:994:ARG:HH21	1.79	0.47
3:J:214:ARG:O	3:J:218:THR:HB	2.15	0.47
3:J:826:ILE:HD12	3:J:826:ILE:O	2.15	0.47
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.44	0.47
3:J:1219:ASP:O	3:J:1222:ARG:N	2.48	0.47
4:K:6:VAL:O	4:K:10:VAL:HG23	2.15	0.47
1:A:316:MET:HE3	1:A:316:MET:HB2	1.73	0.47
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.47	0.47
2:C:565:GLU:HG2	2:C:565:GLU:O	2.14	0.47
2:C:1285:TYR:CE2	3:D:1356:LEU:HD11	2.49	0.47
3:D:239:LEU:HD23	3:D:239:LEU:HA	1.55	0.47
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.95	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47
2:I:136:PHE:CE1	2:I:506:PHE:HE2	2.33	0.47
2:I:540:ARG:H	2:I:540:ARG:HD2	1.79	0.47
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.45	0.47
5:L:101:TYR:CE2	5:L:405:ILE:HD11	2.49	0.47
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.79	0.47
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.80	0.47
1:A:313:SER:OG	1:A:314:LEU:N	2.48	0.47
1:B:223:ILE:O	1:B:226:GLU:HB2	2.14	0.47
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.96	0.47
2:C:363:LEU:C	2:C:381:ALA:HB1	2.39	0.47
2:C:826:ASP:O	2:C:829:THR:HB	2.14	0.47
2:C:1247:SER:OG	2:C:1248:THR:N	2.47	0.47
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.23	0.47
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.15	0.47
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.97	0.47
3:D:292:VAL:O	3:D:296:LYS:HG3	2.14	0.47
3:D:298:MET:SD	5:F:402:LEU:HB3	2.55	0.47
3:D:705:THR:OG1	3:D:718:SER:HA	2.15	0.47
5:F:448:ARG:HE	5:F:448:ARG:HB3	1.54	0.47
1:H:57:THR:HG22	1:H:58:GLU:OE1	2.15	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.48	0.47
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.14	0.47
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.80	0.47
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.97	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.54	0.47
3:J:198:CYS:O	3:J:202:ARG:HG3	2.15	0.47
3:J:342:LEU:HA	3:J:343:LEU:HA	1.69	0.47
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.50	0.47
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.15	0.47
3:J:638:SER:OG	3:J:639:VAL:N	2.48	0.47
3:J:708:ASN:OD1	3:J:708:ASN:N	2.42	0.47
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.95	0.47
3:J:1270:GLY:HA2	3:J:1298:VAL:HG22	1.97	0.47
3:J:1270:GLY:HA3	3:J:1298:VAL:O	2.15	0.47
5:L:261:LEU:H	5:L:261:LEU:HD12	1.80	0.47
5:L:460:ILE:O	5:L:463:LEU:HB2	2.15	0.47
1:B:76:GLU:OE1	1:B:76:GLU:N	2.47	0.47
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.15	0.47
3:D:848:VAL:HG11	3:D:872:LEU:HD21	1.96	0.47
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.48	0.47
5:F:233:ASP:O	5:F:236:LYS:HE2	2.15	0.47
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.96	0.47
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.49	0.47
2:I:994:ARG:HD2	2:I:997:TRP:CZ2	2.50	0.47
3:J:817:HIS:CE1	3:J:860:ARG:NH1	2.83	0.47
3:J:835:LEU:O	3:J:839:VAL:HG23	2.14	0.47
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.14	0.47
3:J:1285:VAL:HG12	3:J:1286:LYS:HG2	1.96	0.47
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.50	0.47
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.78	0.47
1:A:118:ASP:O	1:A:121:VAL:N	2.42	0.47
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.35	0.47
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.97	0.47
2:C:666:SER:OG	2:C:704:MET:HG3	2.15	0.47
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.29	0.47
3:D:805:GLN:O	3:D:807:LEU:N	2.48	0.47
5:F:163:THR:O	5:F:260:ARG:NH2	2.48	0.47
2:I:1204:LEU:HB3	2:I:1205:PRO:HD2	1.97	0.47
3:J:432:LEU:HD21	3:J:489:ASN:CB	2.45	0.47
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.15	0.47
2:C:107:ARG:HA	2:C:108:GLU:HA	1.43	0.47
5:F:562:ARG:HH21	5:F:573:LEU:HD23	1.79	0.47
1:G:65:LEU:O	1:G:169:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.48	0.47
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.97	0.47
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.80	0.46
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.97	0.46
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.50	0.46
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.42	0.46
5:F:585:GLU:HA	5:F:588:ARG:CD	2.46	0.46
1:H:151:GLY:O	1:H:177:TYR:HB2	2.16	0.46
2:I:131:THR:HG22	2:I:132:ASP:OD1	2.15	0.46
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.80	0.46
5:L:322:MET:HE2	5:L:324:LYS:HZ3	1.79	0.46
2:C:883:LEU:HB3	2:C:1052:VAL:HG21	1.97	0.46
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.97	0.46
3:D:668:PHE:HE1	3:D:675:ALA:HB2	1.80	0.46
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.47	0.46
4:E:50:ALA:O	4:E:54:ILE:HG12	2.15	0.46
5:F:277:MET:HE3	5:F:281:ARG:NH2	2.31	0.46
1:G:38:THR:HG1	1:H:45:ARG:NH1	2.12	0.46
2:I:402:ARG:HG2	2:I:416:GLY:N	2.30	0.46
2:I:526:HIS:O	2:I:529:ARG:HB2	2.14	0.46
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.28	0.46
3:J:923:ILE:O	3:J:926:PRO:HD2	2.15	0.46
4:K:49:ILE:O	4:K:53:GLU:HG3	2.16	0.46
5:L:230:VAL:HG22	5:L:248:GLU:OE2	2.16	0.46
1:A:12:ARG:HG2	1:A:13:LEU:H	1.81	0.46
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.49	0.46
3:D:83:VAL:O	3:D:91:GLU:HA	2.15	0.46
3:D:128:LEU:HD23	3:D:192:MET:CE	2.45	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.15	0.46
3:D:826:ILE:HD12	3:D:826:ILE:O	2.16	0.46
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.58	0.46
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.24	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.40	0.46
5:L:311:THR:HG21	5:L:348:GLU:CD	2.41	0.46
5:L:482:GLU:O	5:L:486:ARG:NH2	2.49	0.46
2:C:854:ILE:O	2:C:857:VAL:HG22	2.16	0.46
3:D:518:VAL:N	3:D:716:GLN:HE22	2.13	0.46
3:D:741:ALA:O	3:D:762:ASN:ND2	2.47	0.46
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.97	0.46
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.50	0.46
2:I:810:TYR:CD1	2:I:1078:LYS:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1243:MET:HA	3:J:353:SER:HB3	1.97	0.46
3:J:620:PHE:CE2	3:J:624:ILE:HD11	2.50	0.46
3:J:667:GLN:O	3:J:671:GLY:N	2.49	0.46
5:L:225:ARG:O	5:L:229:VAL:HG13	2.16	0.46
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.50	0.46
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.29	0.46
2:C:705:GLU:CD	2:C:705:GLU:H	2.24	0.46
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.96	0.46
3:D:1158:GLU:HB2	3:D:1177:ILE:HD11	1.98	0.46
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.98	0.46
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.45	0.46
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.96	0.46
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.98	0.46
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.97	0.46
4:K:44:ASP:HB3	4:K:48:VAL:HB	1.97	0.46
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.30	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.96	0.46
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.97	0.46
3:D:793:SER:O	3:D:797:THR:HG23	2.16	0.46
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.98	0.46
2:I:402:ARG:HG2	2:I:416:GLY:H	1.81	0.46
2:I:462:ASN:O	2:I:466:VAL:HG23	2.14	0.46
2:I:975:ILE:HD13	2:I:998:LEU:HG	1.98	0.46
3:J:64:PRO:O	3:J:95:THR:OG1	2.29	0.46
5:L:253:SER:O	5:L:257:LYS:HG3	2.14	0.46
5:L:274:ARG:NH2	5:L:365:MET:HE3	2.31	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.46
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.45	0.46
3:D:53:ARG:HA	3:D:54:ASP:HA	1.65	0.46
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.82	0.46
3:D:171:GLU:HB3	3:D:172:PHE:CD2	2.51	0.46
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.98	0.46
5:F:494:ILE:O	5:F:498:LEU:HB2	2.16	0.46
5:F:551:LEU:HA	5:F:551:LEU:HD23	1.68	0.46
1:G:150:ARG:NH1	1:H:7:GLU:O	2.35	0.46
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.79	0.46
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.96	0.46
2:I:891:GLY:O	2:I:892:GLU:HG3	2.15	0.46
3:J:401:VAL:HG12	3:J:408:VAL:HG11	1.98	0.46
3:J:514:THR:HG21	3:J:596:LEU:HG	1.97	0.46
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.82	0.46
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.81	0.46
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.98	0.46
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.70	0.46
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.81	0.46
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.46
3:D:81:ARG:C	3:D:83:VAL:N	2.74	0.46
5:F:262:VAL:HG11	5:F:264:LYS:NZ	2.31	0.46
5:L:114:GLU:O	5:L:117:ILE:N	2.41	0.46
5:L:316:PHE:O	5:L:320:ILE:HG13	2.16	0.46
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.53	0.46
1:A:83:LEU:HB3	2:C:694:ARG:HH21	1.81	0.46
1:A:195:ARG:HD2	1:A:196:THR:H	1.80	0.46
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.16	0.46
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.60	0.46
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.46
2:C:744:GLY:C	2:C:746:ALA:N	2.70	0.46
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.97	0.46
3:D:850:LYS:HB2	3:D:852:GLY:O	2.16	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.96	0.46
4:E:15:ASN:CB	4:E:18:ASP:HB2	2.45	0.46
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.81	0.46
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.98	0.46
5:L:300:LYS:HE3	5:L:301:ASN:HD21	1.81	0.46
5:L:363:ARG:O	5:L:367:ILE:HG13	2.15	0.46
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.96	0.46
1:B:88:LEU:HD12	1:B:89:ALA:H	1.81	0.46
1:B:98:VAL:O	1:B:146:VAL:HG13	2.16	0.46
2:C:103:VAL:C	2:C:104:ILE:HD12	2.41	0.46
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.51	0.46
2:C:980:VAL:HA	2:C:984:VAL:HA	1.97	0.46
3:D:710:ASP:OD1	3:D:711:GLY:N	2.49	0.46
3:D:1345:ARG:HG2	3:D:1370:MET:HE1	1.98	0.46
1:G:197:ASP:O	1:G:198:LEU:HD23	2.15	0.46
1:H:22:THR:OG1	1:H:207:THR:O	2.34	0.46
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.78	0.46
2:I:596:ASP:CG	2:I:597:GLY:N	2.74	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.16	0.46
3:J:156:ARG:HH12	3:J:157:GLN:NE2	2.14	0.46
3:J:288:PRO:O	3:J:292:VAL:HG13	2.16	0.46
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.97	0.45
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.98	0.45
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.81	0.45
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.98	0.45
3:D:504:GLN:HG3	3:D:505:ASP:N	2.29	0.45
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.97	0.45
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.97	0.45
5:F:230:VAL:O	5:F:234:THR:HG23	2.16	0.45
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.97	0.45
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.98	0.45
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.82	0.45
3:J:500:ILE:HG22	3:J:500:ILE:O	2.16	0.45
3:J:548:VAL:CG1	3:J:550:VAL:HG13	2.46	0.45
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.98	0.45
3:J:796:LEU:HD12	3:J:796:LEU:HA	1.57	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
1:A:155:ALA:H	1:A:174:ASP:HA	1.81	0.45
1:B:118:ASP:HB2	1:B:121:VAL:HB	1.98	0.45
2:C:498:ILE:HD12	2:C:498:ILE:N	2.31	0.45
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.81	0.45
2:C:790:ASP:O	2:C:793:GLU:N	2.34	0.45
2:C:1131:MET:HE1	2:C:1140:LYS:C	2.41	0.45
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.23	0.45
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.98	0.45
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.24	0.45
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.98	0.45
3:J:322:ARG:HG3	3:J:323:PRO:HD2	1.99	0.45
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.98	0.45
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.98	0.45
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.63	0.45
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.31	0.45
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.97	0.45
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.46	0.45
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.50	0.45
3:D:400:MET:HB3	3:D:400:MET:HE2	1.77	0.45
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.98	0.45
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.17	0.45
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.99	0.45
1:G:140:ILE:HG13	1:G:140:ILE:O	2.15	0.45
1:G:154:PRO:HG2	1:G:157:THR:OG1	2.16	0.45
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.16	0.45
3:J:650:LYS:NZ	3:J:762:ASN:HD22	2.13	0.45
5:L:277:MET:SD	5:L:359:LYS:HG2	2.57	0.45
5:L:390:ILE:O	5:L:393:LYS:HB2	2.16	0.45
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.97	0.45
2:C:91:THR:HB	2:C:138:ILE:O	2.16	0.45
2:C:468:LEU:O	2:C:471:VAL:HG12	2.17	0.45
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.99	0.45
2:C:960:LEU:O	2:C:963:GLU:HB2	2.16	0.45
3:D:26:SER:O	3:D:29:MET:HB3	2.15	0.45
3:D:210:SER:HB2	3:D:213:LYS:CB	2.31	0.45
3:D:361:LEU:HD22	3:D:365:GLN:HG3	1.99	0.45
2:I:4:SER:OG	2:I:7:GLU:HG3	2.17	0.45
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.38	0.45
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.17	0.45
2:C:63:SER:C	2:C:65:ASN:H	2.25	0.45
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.51	0.45
3:D:165:TYR:CE2	3:D:169:LEU:HG	2.52	0.45
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.99	0.45
3:D:362:ARG:H	3:D:365:GLN:HE21	1.64	0.45
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.99	0.45
3:D:827:GLU:O	3:D:829:GLY:N	2.43	0.45
3:D:908:ILE:HD13	3:D:909:ILE:N	2.30	0.45
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.97	0.45
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.64	0.45
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.85	0.45
2:I:692:THR:OG1	2:I:827:ARG:O	2.34	0.45
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.32	0.45
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.78	0.45
3:J:649:LYS:HD3	3:J:649:LYS:HA	1.66	0.45
3:J:1265:THR:HG22	3:J:1277:GLY:CA	2.45	0.45
5:L:399:LEU:HG	5:L:403:ASP:HB3	1.98	0.45
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.48	0.45
3:D:566:LYS:HE2	3:D:570:LYS:HZ1	1.81	0.45
4:E:15:ASN:HB2	4:E:18:ASP:HB2	1.99	0.45
5:F:395:THR:OG1	5:F:396:ASN:N	2.49	0.45
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.71	0.45
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.35	0.45
2:I:730:SER:O	2:I:753:LEU:HB2	2.17	0.45
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.31	0.45
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1231:ARG:HA	3:J:1234:VAL:HG22	1.98	0.45
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.50	0.45
5:L:322:MET:HE2	5:L:324:LYS:NZ	2.32	0.45
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.82	0.45
2:C:1069:ARG:HH21	2:C:1114:GLU:CD	2.25	0.45
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.67	0.45
2:C:1236:ASN:HB2	2:C:1238:LEU:HD11	1.99	0.45
3:D:653:ILE:HG23	3:D:692:ARG:CZ	2.47	0.45
3:D:820:ILE:HD11	3:D:822:MET:HE2	1.98	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.46	0.45
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.31	0.45
2:I:819:SER:HB3	2:I:1085:MET:SD	2.56	0.45
3:J:400:MET:HB3	3:J:400:MET:HE2	1.53	0.45
2:C:800:MET:HE3	2:C:800:MET:HB3	1.60	0.45
3:D:537:TYR:CE2	3:D:544:LEU:HD13	2.52	0.45
3:D:649:LYS:HA	3:D:649:LYS:HD3	1.77	0.45
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.47	0.45
5:F:557:LYS:O	5:F:561:MET:HB2	2.17	0.45
1:G:75:GLN:HA	2:I:729:ALA:H	1.81	0.45
2:I:1180:MET:HA	2:I:1181:PRO:HD3	1.77	0.45
2:I:1340:GLU:OE2	3:J:21:LYS:HD3	2.17	0.45
3:J:601:ILE:O	3:J:604:MET:HB3	2.17	0.45
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.17	0.45
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.81	0.45
1:A:8:PHE:CZ	1:B:150:ARG:HD2	2.52	0.45
1:B:151:GLY:O	1:B:177:TYR:HB2	2.17	0.45
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.98	0.45
2:C:193:ASN:ND2	2:C:353:VAL:HG21	2.31	0.45
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.31	0.45
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.52	0.45
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.99	0.45
5:F:143:TYR:CE2	5:F:147:GLN:HG3	2.52	0.45
1:G:108:GLY:O	1:G:133:LEU:HB2	2.17	0.45
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.17	0.45
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.25	0.45
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.47	0.45
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.46	0.45
3:J:47:ARG:NE	3:J:47:ARG:HA	2.31	0.45
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.98	0.45
3:J:1167:LYS:HZ1	3:J:1170:LYS:HB2	1.82	0.45
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:744:GLY:O	2:C:746:ALA:N	2.47	0.45
3:D:501:VAL:HG22	3:D:502:PRO:O	2.17	0.45
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.98	0.45
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.98	0.45
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.45
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.17	0.44
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.98	0.44
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.25	0.44
1:A:180:VAL:HG12	1:A:183:ILE:HD13	1.99	0.44
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.32	0.44
2:C:487:LEU:HD23	2:C:487:LEU:H	1.82	0.44
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.46	0.44
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.99	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.17	0.44
3:D:1321:SER:O	3:D:1324:SER:HB2	2.16	0.44
2:I:672:GLU:HG2	2:I:1186:VAL:O	2.17	0.44
3:J:355:ILE:HG21	3:J:466:MET:HG3	2.00	0.44
3:J:694:SER:OG	3:J:738:ARG:NE	2.50	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.17	0.44
1:A:236:ASP:HA	1:B:14:VAL:O	2.17	0.44
1:B:62:ASP:OD2	1:B:140:ILE:HD12	2.17	0.44
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.52	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.54	0.44
2:C:970:GLY:O	2:C:973:SER:OG	2.35	0.44
2:C:1254:VAL:HG22	2:C:1255:THR:N	2.33	0.44
3:D:255:LEU:HD13	3:D:255:LEU:HA	1.62	0.44
3:D:918:ILE:O	3:D:922:SER:OG	2.25	0.44
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.31	0.44
2:I:151:ARG:HH12	2:I:175:ARG:HH11	1.64	0.44
2:I:360:LEU:O	2:I:364:VAL:HG23	2.17	0.44
3:J:619:ILE:O	3:J:623:GLN:HG2	2.16	0.44
5:L:137:TYR:CD2	5:L:273:MET:HE2	2.51	0.44
5:L:489:MET:HE2	5:L:493:LYS:CB	2.46	0.44
2:C:218:GLU:HG3	2:C:299:LYS:HA	2.00	0.44
2:C:745:GLU:O	2:C:746:ALA:C	2.61	0.44
2:C:960:LEU:HD13	2:C:960:LEU:HA	1.81	0.44
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.47	0.44
3:D:64:PRO:O	3:D:95:THR:OG1	2.36	0.44
3:D:412:LEU:HD23	3:D:416:ILE:HG12	1.99	0.44
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.98	0.44
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.47	0.44
4:E:30:MET:HE1	4:E:49:ILE:HB	1.98	0.44
5:F:390:ILE:O	5:F:393:LYS:HB2	2.17	0.44
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.99	0.44
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.17	0.44
3:J:513:MET:HE2	3:J:513:MET:HB3	1.76	0.44
1:B:228:LEU:C	1:B:230:ALA:N	2.75	0.44
2:C:16:GLY:H	2:C:17:LYS:NZ	2.15	0.44
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.99	0.44
3:D:310:GLY:C	3:D:312:ARG:H	2.24	0.44
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.17	0.44
1:G:65:LEU:HA	1:G:65:LEU:HD13	1.71	0.44
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.32	0.44
1:G:127:GLN:CD	1:G:127:GLN:H	2.25	0.44
1:G:134:THR:HG23	1:G:135:ASP:N	2.32	0.44
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.16	0.44
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.64	0.44
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.98	0.44
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.33	0.44
3:J:804:ALA:O	3:J:806:ASP:N	2.50	0.44
3:J:1345:ARG:NE	3:J:1370:MET:HE1	2.32	0.44
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.99	0.44
2:C:81:ASP:OD2	2:C:84:GLU:HG3	2.17	0.44
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.55	0.44
2:C:517:GLN:HG3	2:C:523:GLU:OE2	2.18	0.44
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.52	0.44
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.81	0.44
3:D:412:LEU:O	3:D:415:VAL:HG22	2.17	0.44
3:D:514:THR:HG21	3:D:596:LEU:HB2	2.00	0.44
3:D:541:LEU:HA	3:D:541:LEU:HD23	1.72	0.44
1:G:51:MET:HA	1:G:52:PRO:HD3	1.86	0.44
1:G:76:GLU:OE2	1:G:76:GLU:N	2.48	0.44
2:I:487:LEU:H	2:I:487:LEU:HD23	1.83	0.44
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.00	0.44
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.50	0.44
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.44
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.18	0.44
5:L:525:ASP:CG	5:L:528:LEU:HG	2.43	0.44
1:B:16:ILE:HB	1:B:26:VAL:HG13	1.99	0.44
2:C:757:THR:O	2:C:765:ILE:HG23	2.17	0.44
2:C:1131:MET:HE2	2:C:1131:MET:HB3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.32	0.44
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.82	0.44
5:F:343:LYS:O	5:F:347:ILE:HG13	2.18	0.44
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.42	0.44
5:F:530:LEU:HD11	5:F:533:ASP:OD2	2.17	0.44
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.99	0.44
1:G:187:VAL:HG13	1:G:201:LEU:HD13	2.00	0.44
1:H:134:THR:HG23	1:H:135:ASP:N	2.25	0.44
2:I:488:MET:O	2:I:490:GLN:N	2.48	0.44
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.53	0.44
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.52	0.44
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.50	0.44
3:J:1328:THR:O	3:J:1332:LEU:HD23	2.18	0.44
5:L:308:GLY:HA2	5:L:356:GLU:OE1	2.18	0.44
5:L:479:THR:HG23	5:L:481:GLU:H	1.83	0.44
5:L:489:MET:HE2	5:L:493:LYS:HB2	1.99	0.44
1:A:45:ARG:CG	1:B:38:THR:HB	2.38	0.44
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.99	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.74	0.44
2:C:94:ALA:HA	2:C:95:PRO:HD3	1.66	0.44
2:C:221:LEU:HD12	2:C:298:ALA:O	2.18	0.44
2:C:452:ARG:NH1	2:C:584:TYR:O	2.50	0.44
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.51	0.44
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.17	0.44
3:D:749:LYS:HG3	3:D:751:ASP:HB2	1.99	0.44
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.47	0.44
2:I:800:MET:O	2:I:1229:TYR:HA	2.18	0.44
3:J:19:ALA:HB2	3:J:1373:ARG:NH2	2.33	0.44
3:J:30:ILE:HD13	3:J:243:PRO:HG3	1.99	0.44
3:J:528:THR:HG22	3:J:532:GLU:CD	2.43	0.44
3:J:820:ILE:HD11	3:J:822:MET:HE2	2.00	0.44
5:L:137:TYR:CD1	5:L:138:PRO:HD2	2.52	0.44
5:L:346:GLN:HA	5:L:349:GLU:OE2	2.18	0.44
5:L:368:GLY:O	5:L:371:LYS:HB3	2.17	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
1:A:82:LEU:HD22	1:A:173:VAL:CG1	2.48	0.44
1:A:133:LEU:HD21	1:A:140:ILE:HG12	1.99	0.44
1:A:262:LEU:H	1:A:262:LEU:HD12	1.82	0.44
1:B:158:ARG:HB3	1:B:172:LEU:HD23	2.00	0.44
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.81	0.44
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:CD	2:C:1161:LEU:HD22	2.47	0.44
3:D:48:THR:HB	3:D:50:LYS:HG3	2.00	0.44
3:D:490:ILE:HD13	3:D:490:ILE:N	2.26	0.44
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.80	0.44
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.98	0.44
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.52	0.44
3:J:73:GLY:O	3:J:76:LYS:NZ	2.48	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.18	0.44
3:J:1287:ILE:HG22	3:J:1300:ALA:H	1.82	0.44
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.50	0.44
2:C:95:PRO:CA	2:C:126:GLU:HG2	2.48	0.44
2:C:480:SER:HB3	2:C:481:LEU:HD22	1.99	0.44
2:C:534:GLY:HA3	2:C:535:PRO:HD2	1.83	0.44
2:C:878:THR:OG1	2:C:879:GLY:N	2.48	0.44
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.44
3:D:1184:ASP:O	3:D:1186:TYR:N	2.51	0.44
5:F:484:ALA:O	5:F:491:GLU:HB2	2.18	0.44
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.99	0.44
1:H:153:VAL:HG11	1:H:158:ARG:NH1	2.33	0.44
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.33	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.52	0.44
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.82	0.44
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.99	0.44
3:J:658:GLU:O	3:J:661:VAL:HG22	2.18	0.44
3:J:1162:ILE:HA	3:J:1203:ARG:HA	2.00	0.44
4:K:15:ASN:CB	4:K:18:ASP:HB2	2.48	0.44
5:L:280:VAL:O	5:L:284:GLU:HG3	2.18	0.44
3:D:660:GLU:O	3:D:664:ILE:HG12	2.17	0.43
5:F:230:VAL:HG13	5:F:231:THR:H	1.82	0.43
1:G:127:GLN:CD	1:G:127:GLN:N	2.76	0.43
1:H:183:ILE:HG23	1:H:205:MET:HG3	1.99	0.43
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.52	0.43
2:I:672:GLU:HB3	2:I:1187:PHE:CD2	2.53	0.43
2:I:778:GLU:HB3	2:I:781:ASP:OD1	2.18	0.43
3:J:664:ILE:HG21	3:J:681:LYS:HB3	2.00	0.43
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.18	0.43
3:J:690:ASN:ND2	3:J:745:GLY:HA2	2.33	0.43
3:J:860:ARG:HB3	3:J:861:ASN:H	1.61	0.43
3:J:865:HIS:CE1	3:J:868:TRP:CD1	3.06	0.43
3:J:903:LEU:HD23	3:J:905:ARG:CG	2.48	0.43
4:K:42:GLU:O	4:K:43:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB3	1:A:208:ASN:HD21	1.84	0.43
2:C:70:TYR:HA	2:C:100:LEU:HD23	2.00	0.43
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.80	0.43
3:D:810:THR:HG21	3:D:893:GLY:HA3	2.00	0.43
5:F:310:GLU:O	5:F:344:LEU:HD21	2.18	0.43
1:H:62:ASP:HB3	1:H:141:SER:O	2.18	0.43
2:I:997:TRP:HA	2:I:1000:LEU:HD12	2.00	0.43
3:J:429:LEU:HA	3:J:429:LEU:HD13	1.76	0.43
3:J:442:ILE:HD13	3:J:442:ILE:HA	1.87	0.43
3:J:495:ASN:C	3:J:497:GLU:H	2.23	0.43
3:J:594:GLN:HB2	3:J:595:ALA:H	1.48	0.43
3:J:697:MET:O	3:J:701:LEU:N	2.32	0.43
3:J:1314:LEU:HA	3:J:1326:GLN:NE2	2.34	0.43
2:C:38:PHE:HE1	2:C:461:GLU:HA	1.82	0.43
2:C:833:ILE:HA	2:C:1054:LEU:O	2.17	0.43
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.18	0.43
3:D:418:GLU:O	3:D:420:PRO:HD3	2.18	0.43
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.80	0.43
3:D:1285:VAL:O	3:D:1288:ALA:HB3	2.18	0.43
5:F:372:ALA:O	5:F:376:LYS:HG3	2.18	0.43
5:F:413:MET:HE2	5:F:413:MET:HB3	1.87	0.43
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.53	0.43
1:G:166:ARG:N	1:G:167:PRO:HD2	2.32	0.43
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.33	0.43
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.43
2:I:1124:ILE:HG21	2:I:1180:MET:HE3	2.00	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.53	0.43
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.60	0.43
3:J:133:ARG:HD2	3:J:133:ARG:HA	1.85	0.43
3:J:609:TYR:CE2	3:J:614:LEU:HD12	2.51	0.43
3:J:872:LEU:O	3:J:877:VAL:HG12	2.19	0.43
3:J:1257:VAL:HA	3:J:1260:MET:HG3	2.00	0.43
4:K:71:GLU:HA	4:K:74:GLU:HG3	2.00	0.43
5:L:458:GLU:O	5:L:462:LYS:HG3	2.19	0.43
2:C:4:SER:HB3	2:C:7:GLU:CG	2.45	0.43
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.01	0.43
3:D:1142:ALA:O	3:D:1146:GLU:N	2.48	0.43
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	2.00	0.43
4:E:3:ARG:CZ	4:E:3:ARG:HA	2.48	0.43
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.18	0.43
1:G:43:LEU:HD23	1:G:43:LEU:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.43
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.32	0.43
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.58	0.43
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.79	0.43
3:J:615:LYS:HE2	3:J:616:PRO:HD3	2.01	0.43
5:L:306:PHE:CE2	5:L:310:GLU:HG3	2.53	0.43
1:A:195:ARG:HD2	1:A:196:THR:N	2.33	0.43
1:B:195:ARG:HB2	1:B:198:LEU:HD21	2.01	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.99	0.43
2:C:268:ARG:HD2	2:C:270:THR:CG2	2.48	0.43
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.84	0.43
2:C:805:MET:HB2	2:C:805:MET:HE3	1.83	0.43
3:D:421:VAL:HG13	3:D:439:PRO:HG3	2.00	0.43
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.47	0.43
3:D:461:PHE:C	3:D:463:GLY:H	2.26	0.43
2:I:519:ASN:ND2	2:I:689:ALA:O	2.48	0.43
3:J:484:MET:HE2	3:J:484:MET:HB3	1.74	0.43
2:C:256:GLU:OE2	2:C:261:VAL:HG22	2.19	0.43
2:C:861:ALA:HB1	2:C:882:ILE:HD13	2.00	0.43
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.52	0.43
3:D:45:ASN:O	3:D:46:TYR:HB3	2.19	0.43
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.43
3:D:69:GLU:OE2	3:D:76:LYS:HD3	2.19	0.43
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.31	0.43
3:D:1343:GLU:HG2	3:D:1373:ARG:NH1	2.34	0.43
5:F:111:LEU:HD13	5:F:116:GLU:HA	2.01	0.43
5:F:142:THR:O	5:F:146:GLU:HG3	2.19	0.43
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.00	0.43
2:I:102:LEU:HB2	2:I:489:PRO:HG3	2.00	0.43
2:I:498:ILE:HD12	2:I:498:ILE:N	2.32	0.43
2:I:528:ARG:NH2	2:I:576:SER:O	2.52	0.43
2:I:930:ASP:OD2	2:I:931:VAL:N	2.51	0.43
2:I:1081:PRO:HB3	2:I:1083:GLU:OE2	2.18	0.43
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.34	0.43
1:A:192:VAL:O	1:A:193:GLU:C	2.62	0.43
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.53	0.43
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.83	0.43
2:C:782:VAL:HG21	2:C:792:GLY:HA3	2.00	0.43
2:C:1273:MET:HE3	2:C:1273:MET:HB2	1.73	0.43
3:D:147:ILE:HG22	3:D:188:LEU:HG	2.01	0.43
5:F:130:VAL:HB	5:F:365:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:LEU:HG	1:H:221:ALA:HB1	2.00	0.43
2:I:55:SER:OG	2:I:56:VAL:N	2.51	0.43
2:I:1124:ILE:HG21	2:I:1180:MET:CE	2.49	0.43
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.43
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.00	0.43
5:L:453:PRO:O	5:L:456:MET:HB2	2.19	0.43
1:A:316:MET:SD	5:F:600:HIS:CE1	3.12	0.43
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.99	0.43
2:C:732:ILE:HG21	2:C:783:LEU:HD12	2.01	0.43
2:C:1009:ASN:O	2:C:1013:GLN:HG2	2.19	0.43
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.83	0.43
3:D:733:SER:C	3:D:735:ALA:N	2.73	0.43
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.19	0.43
1:H:83:LEU:HA	1:H:86:LYS:HE2	2.01	0.43
2:I:590:PRO:HA	2:I:604:HIS:O	2.19	0.43
2:I:1319:MET:HE2	2:I:1319:MET:HB3	1.69	0.43
3:J:45:ASN:HB3	3:J:48:THR:O	2.18	0.43
3:J:554:GLU:OE1	3:J:570:LYS:NZ	2.50	0.43
3:J:865:HIS:HE1	3:J:867:GLN:HB2	1.81	0.43
5:L:372:ALA:O	5:L:376:LYS:HG3	2.18	0.43
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.64	0.43
2:C:545:PHE:CZ	2:C:549:ASP:HB2	2.54	0.43
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	2.01	0.43
3:D:171:GLU:HB3	3:D:172:PHE:CE2	2.54	0.43
5:F:531:PRO:O	5:F:535:ALA:N	2.42	0.43
1:G:125:LYS:HE2	1:G:128:HIS:HB2	2.01	0.43
1:H:85:LEU:HD13	1:H:144:ILE:HD12	1.99	0.43
2:I:796:LEU:H	2:I:796:LEU:HD12	1.84	0.43
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.00	0.43
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.19	0.43
3:J:259:ARG:HD3	5:L:502:LYS:HD2	2.00	0.43
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.84	0.43
3:J:709:ARG:HD2	3:J:710:ASP:H	1.84	0.43
3:J:1184:ASP:O	3:J:1186:TYR:N	2.52	0.43
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.49	0.43
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.01	0.43
3:D:597:GLY:O	3:D:601:ILE:HB	2.17	0.43
3:D:646:ILE:H	3:D:646:ILE:HG12	1.63	0.43
3:D:674:THR:N	3:D:677:GLU:OE1	2.42	0.43
5:F:228:TYR:HA	5:F:252:LEU:HD13	2.00	0.43
5:F:276:MET:O	5:F:280:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:ALA:HA	1:G:158:ARG:HD3	2.01	0.43
1:H:59:VAL:HG22	1:H:144:ILE:HG13	2.01	0.43
2:I:41:GLN:NE2	2:I:73:TYR:O	2.51	0.43
2:I:42:ASP:C	2:I:44:GLU:H	2.27	0.43
2:I:685:MET:HE3	2:I:685:MET:HB2	1.77	0.43
2:I:1273:MET:HE3	2:I:1273:MET:HB2	1.76	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.67	0.43
3:J:572:THR:HG21	3:J:589:TYR:OH	2.19	0.43
3:J:596:LEU:HD11	3:J:604:MET:CE	2.49	0.43
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.87	0.43
1:A:92:VAL:HA	1:A:120:ASP:O	2.19	0.42
1:B:73:GLY:O	1:B:133:LEU:HA	2.18	0.42
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.33	0.42
2:C:968:GLU:O	2:C:971:LEU:N	2.52	0.42
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	2.01	0.42
3:D:1203:ARG:NH2	3:D:1205:GLU:OE2	2.52	0.42
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.65	0.42
5:F:384:LEU:HD23	5:F:384:LEU:HA	1.80	0.42
5:F:470:MET:O	5:F:478:PRO:HD3	2.18	0.42
5:F:531:PRO:O	5:F:532:LEU:C	2.62	0.42
1:H:107:ILE:HG23	1:H:134:THR:O	2.18	0.42
2:I:593:LYS:HG3	2:I:595:THR:HG23	2.01	0.42
2:I:799:ASN:HB3	2:I:1231:TYR:HD1	1.84	0.42
3:J:797:THR:HG22	3:J:924:GLY:CA	2.48	0.42
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.99	0.42
5:L:444:ALA:HB1	5:L:457:ILE:CD1	2.46	0.42
5:L:493:LYS:O	5:L:497:VAL:N	2.39	0.42
5:L:602:SER:OG	5:L:603:ARG:N	2.51	0.42
1:A:195:ARG:HG3	1:A:198:LEU:HD21	2.01	0.42
2:C:98:VAL:O	2:C:121:GLU:HA	2.18	0.42
2:C:748:ILE:HD11	2:C:967:LEU:HD12	2.00	0.42
3:D:712:GLN:HB2	3:D:713:GLU:H	1.59	0.42
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.45	0.42
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.35	0.42
4:E:15:ASN:HD22	4:E:18:ASP:CG	2.23	0.42
5:F:561:MET:HE3	5:F:561:MET:HB2	1.68	0.42
1:H:89:ALA:HB1	1:H:210:THR:CG2	2.50	0.42
2:I:147:SER:HB2	2:I:529:ARG:O	2.19	0.42
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.44	0.42
3:J:57:PHE:CE1	3:J:252:LEU:HB2	2.54	0.42
3:J:122:SER:O	3:J:126:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HA	1:A:278:ILE:CD1	2.48	0.42
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.54	0.42
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.42
2:C:884:VAL:HG21	2:C:1050:VAL:HB	2.00	0.42
2:C:943:LYS:HG2	2:C:947:GLU:OE1	2.19	0.42
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.43	0.42
5:F:383:ASN:O	5:F:386:LEU:HB3	2.19	0.42
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.87	0.42
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.84	0.42
2:I:704:MET:HE3	2:I:704:MET:HB3	1.91	0.42
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.54	0.42
3:J:259:ARG:HG2	5:L:505:ILE:HD13	2.00	0.42
5:L:407:GLU:HG3	5:L:442:SER:OG	2.19	0.42
1:A:201:LEU:C	1:A:201:LEU:HD12	2.44	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.90	0.42
1:B:49:SER:O	1:B:151:GLY:HA2	2.19	0.42
3:D:491:LEU:HD23	3:D:498:PRO:HA	2.01	0.42
3:D:501:VAL:CG2	3:D:602:SER:HB2	2.48	0.42
3:D:884:SER:OG	3:D:886:VAL:HG12	2.20	0.42
5:F:585:GLU:O	5:F:589:GLN:HG3	2.19	0.42
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.01	0.42
3:J:416:ILE:HA	3:J:416:ILE:HD12	1.79	0.42
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.85	0.42
3:J:513:MET:SD	3:J:631:TYR:CD2	3.12	0.42
3:J:601:ILE:HD13	3:J:601:ILE:HG21	1.85	0.42
5:L:476:ARG:HD2	5:L:477:GLU:H	1.83	0.42
5:L:603:ARG:HD3	5:L:603:ARG:HA	1.76	0.42
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.90	0.42
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.51	0.42
2:C:946:LEU:HD23	2:C:946:LEU:HA	1.78	0.42
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.20	0.42
3:D:99:ARG:HG3	3:D:249:LEU:HD21	2.00	0.42
3:D:358:GLY:N	3:D:359:PRO:HD3	2.35	0.42
3:D:466:MET:HE2	3:D:466:MET:HB3	1.86	0.42
3:D:859:PRO:HD2	3:D:862:THR:HG21	2.01	0.42
3:D:860:ARG:HB3	3:D:861:ASN:H	1.60	0.42
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.85	0.42
2:I:337:PHE:C	2:I:337:PHE:CD1	2.97	0.42
2:I:745:GLU:HA	2:I:971:LEU:HD12	2.02	0.42
3:J:327:LEU:HD23	3:J:327:LEU:HA	1.82	0.42
3:J:758:PRO:O	3:J:760:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:4:VAL:HG13	4:K:5:THR:HG23	2.00	0.42
5:L:611:LEU:HA	5:L:611:LEU:HD23	1.64	0.42
2:C:119:GLU:CG	2:C:489:PRO:HD2	2.49	0.42
2:C:122:VAL:HG21	2:C:493:ILE:HG23	2.01	0.42
2:C:463:GLN:OE1	2:C:463:GLN:HA	2.19	0.42
1:G:62:ASP:HB2	1:G:141:SER:O	2.19	0.42
1:G:228:LEU:HD12	1:G:228:LEU:HA	1.81	0.42
2:I:184:LEU:HD12	2:I:184:LEU:HA	1.86	0.42
2:I:397:LEU:O	2:I:398:SER:OG	2.35	0.42
2:I:616:ILE:HG22	2:I:617:ALA:O	2.20	0.42
2:I:800:MET:HE3	2:I:800:MET:HB3	1.62	0.42
2:I:803:ALA:CB	2:I:1094:VAL:HG21	2.50	0.42
2:I:850:ILE:O	2:I:850:ILE:HG22	2.19	0.42
3:J:131:PRO:O	3:J:135:ILE:HG13	2.20	0.42
3:J:159:ILE:O	3:J:159:ILE:HG13	2.18	0.42
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.34	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.34	0.42
5:L:493:LYS:HG2	5:L:496:LYS:HE2	2.01	0.42
1:A:162:GLU:HB3	1:A:163:GLU:H	1.68	0.42
1:B:86:LYS:HD3	1:B:174:ASP:HB2	2.01	0.42
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.84	0.42
2:C:494:ASN:ND2	2:C:497:PRO:HD3	2.35	0.42
2:C:1054:LEU:HD12	2:C:1054:LEU:HA	1.75	0.42
3:D:77:ARG:HA	3:D:77:ARG:HD2	1.85	0.42
3:D:148:GLU:H	3:D:156:ARG:HG3	1.85	0.42
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.01	0.42
3:D:822:MET:SD	3:D:838:ARG:HB3	2.60	0.42
3:D:1156:LEU:HA	3:D:1208:ASP:O	2.19	0.42
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.19	0.42
3:D:1274:PHE:CD2	3:D:1274:PHE:C	2.97	0.42
4:E:38:LEU:HB2	4:E:53:GLU:OE1	2.19	0.42
1:G:59:VAL:HG21	1:G:85:LEU:CD1	2.49	0.42
2:I:158:ASP:OD1	2:I:159:SER:N	2.46	0.42
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.83	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	2.00	0.42
2:I:1140:LYS:HD2	2:I:1140:LYS:HA	1.82	0.42
3:J:356:THR:OG1	3:J:357:VAL:N	2.47	0.42
3:J:743:MET:HB2	3:J:759:ILE:O	2.20	0.42
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.34	0.42
1:A:285:THR:HG23	1:A:288:GLU:HG2	2.01	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:GLN:O	2:C:121:GLU:C	2.62	0.42
2:C:582:ASN:O	2:C:585:GLY:N	2.52	0.42
3:D:594:GLN:HB2	3:D:595:ALA:H	1.72	0.42
3:D:926:PRO:CB	3:D:1246:VAL:HG11	2.50	0.42
1:H:147:GLN:HG3	1:H:148:ARG:H	1.84	0.42
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.73	0.42
2:I:149:LEU:HD12	2:I:149:LEU:HA	1.67	0.42
2:I:715:THR:HG23	2:I:717:VAL:HG23	2.01	0.42
2:I:1080:ASN:CB	2:I:1085:MET:HE3	2.49	0.42
2:I:1285:TYR:CD1	3:J:475:GLU:HG2	2.55	0.42
3:J:148:GLU:H	3:J:156:ARG:HG3	1.83	0.42
5:L:377:LYS:O	5:L:381:GLU:HG3	2.20	0.42
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.42
1:A:108:GLY:HA2	1:A:109:PRO:HD2	1.93	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.35	0.42
1:B:125:LYS:HE2	1:B:125:LYS:HB3	1.95	0.42
1:B:205:MET:HE3	1:B:213:PRO:CB	2.48	0.42
2:C:202:ARG:CZ	2:C:368:ARG:HH12	2.32	0.42
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.01	0.42
2:C:681:MET:O	2:C:685:MET:HE2	2.20	0.42
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.60	0.42
3:D:835:LEU:O	3:D:839:VAL:HG23	2.20	0.42
5:F:483:LEU:H	5:F:483:LEU:HD12	1.85	0.42
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.70	0.42
1:G:142:MET:SD	1:G:144:ILE:HD11	2.60	0.42
2:I:61:SER:O	2:I:63:SER:N	2.53	0.42
2:I:497:PRO:HB2	2:I:498:ILE:HD12	2.02	0.42
3:J:466:MET:HE2	3:J:466:MET:HB3	1.85	0.42
4:K:71:GLU:O	4:K:75:GLN:HG3	2.19	0.42
1:A:97:GLU:HA	1:A:146:VAL:O	2.20	0.42
1:A:195:ARG:HB3	1:A:198:LEU:HG	2.01	0.42
2:C:802:VAL:HG11	2:C:1230:MET:HB3	2.02	0.42
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.69	0.42
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.18	0.42
3:D:318:GLY:C	3:D:320:ASN:H	2.27	0.42
3:D:514:THR:HG23	3:D:596:LEU:HB2	2.02	0.42
3:D:901:ARG:HA	3:D:908:ILE:HA	2.02	0.42
5:F:536:THR:O	5:F:540:LEU:N	2.49	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.20	0.42
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.54	0.42
3:J:116:PHE:O	3:J:124:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:O	3:J:654:ILE:HG13	2.20	0.42
3:J:844:THR:HG23	3:J:864:LEU:HD21	2.01	0.42
2:C:73:TYR:HB2	2:C:98:VAL:HG22	2.02	0.41
2:C:185:ASP:HB2	2:C:197:ARG:HG3	2.02	0.41
2:C:582:ASN:C	2:C:585:GLY:H	2.28	0.41
2:C:775:GLU:HA	2:C:776:PRO:HD3	1.86	0.41
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.45	0.41
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.50	0.41
3:D:16:GLU:HA	3:D:16:GLU:OE2	2.20	0.41
3:D:507:VAL:O	3:D:508:LEU:C	2.63	0.41
3:D:1158:GLU:HB3	3:D:1186:TYR:CE1	2.55	0.41
2:I:452:ARG:NH1	2:I:584:TYR:O	2.52	0.41
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.02	0.41
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.20	0.41
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.33	0.41
3:J:594:GLN:HG3	3:J:596:LEU:CD2	2.50	0.41
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.20	0.41
1:A:163:GLU:O	1:A:164:ASP:HB2	2.18	0.41
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.02	0.41
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.55	0.41
2:C:481:LEU:HD22	2:C:481:LEU:N	2.34	0.41
2:C:522:SER:O	2:C:525:THR:HG22	2.19	0.41
2:C:685:MET:HE3	2:C:685:MET:HB2	1.62	0.41
2:C:746:ALA:HB2	2:C:974:ARG:NE	2.35	0.41
2:C:886:LYS:HB3	2:C:917:SER:HA	2.01	0.41
3:D:11:GLN:OE1	3:D:11:GLN:HA	2.20	0.41
3:D:204:GLU:C	3:D:217:LEU:HD21	2.45	0.41
3:D:215:LYS:O	3:D:219:LYS:HE3	2.20	0.41
3:D:349:TYR:CE1	3:D:472:LEU:HD11	2.56	0.41
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.53	0.41
3:D:664:ILE:HD12	3:D:664:ILE:HG23	1.80	0.41
3:D:1372:ARG:HE	3:D:1372:ARG:HB2	1.63	0.41
1:H:83:LEU:HD11	3:J:526:VAL:HG23	2.01	0.41
2:I:60:GLN:O	2:I:476:LYS:HE2	2.19	0.41
2:I:107:ARG:HA	2:I:108:GLU:HA	1.86	0.41
2:I:607:SER:H	2:I:610:GLU:HB2	1.85	0.41
3:J:57:PHE:CE2	3:J:252:LEU:HD12	2.55	0.41
3:J:504:GLN:HG3	3:J:505:ASP:H	1.85	0.41
3:J:901:ARG:HA	3:J:908:ILE:HA	2.01	0.41
1:A:46:ILE:CG2	1:A:223:ILE:HD12	2.50	0.41
1:A:211:ILE:HG21	1:A:216:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.86	0.41
3:D:57:PHE:N	3:D:57:PHE:CD2	2.88	0.41
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.75	0.41
3:D:697:MET:HE1	3:D:737:ILE:CG2	2.46	0.41
3:D:853:THR:O	3:D:854:ALA:HB3	2.20	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.41
5:F:414:LYS:HD3	5:F:434:TRP:CE3	2.55	0.41
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.02	0.41
1:H:178:SER:HA	1:H:179:PRO:HD3	1.82	0.41
2:I:30:ILE:H	2:I:30:ILE:CD1	2.25	0.41
2:I:403:MET:HE3	2:I:403:MET:HB3	1.89	0.41
2:I:470:ARG:HA	2:I:473:ARG:HD2	2.02	0.41
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.40	0.41
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.86	0.41
3:J:418:GLU:H	4:K:45:LYS:HZ3	1.68	0.41
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.41
3:J:678:ARG:HG3	3:J:679:TYR:N	2.34	0.41
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.30	0.41
2:C:490:GLN:HG3	5:F:472:GLN:HG3	2.03	0.41
2:C:629:PHE:HB2	2:C:647:ARG:HG3	2.02	0.41
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.50	0.41
3:D:8:LEU:HD23	3:D:9:LYS:N	2.35	0.41
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.51	0.41
3:D:411:ILE:O	3:D:414:GLU:HB2	2.21	0.41
5:F:412:LEU:HD13	5:F:435:ILE:HD11	2.01	0.41
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.29	0.41
1:G:88:LEU:HD12	1:G:89:ALA:N	2.35	0.41
1:G:187:VAL:CG1	1:G:201:LEU:HD13	2.50	0.41
1:G:218:ARG:HG3	1:H:231:PHE:O	2.21	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
2:I:397:LEU:O	2:I:401:GLY:HA3	2.20	0.41
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.83	0.41
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.56	0.41
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.20	0.41
3:J:705:THR:OG1	3:J:718:SER:HA	2.21	0.41
5:L:299:LYS:HA	5:L:302:PHE:CB	2.49	0.41
1:A:13:LEU:HG	1:A:13:LEU:O	2.20	0.41
1:B:205:MET:HE2	1:B:205:MET:HB3	1.70	0.41
2:C:302:ILE:O	2:C:330:HIS:NE2	2.49	0.41
2:C:903:ARG:NE	2:C:910:ALA:HB2	2.35	0.41
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.53	0.41
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.35	0.41
3:D:184:ALA:O	3:D:187:ALA:HB3	2.21	0.41
3:D:532:GLU:HA	3:D:535:ARG:HB3	2.02	0.41
3:D:556:GLU:C	3:D:558:ASP:H	2.29	0.41
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.47	0.41
5:F:99:ARG:HG3	5:F:103:ARG:HH12	1.85	0.41
5:F:298:PRO:HD2	5:F:326:TRP:CG	2.56	0.41
1:G:59:VAL:HG21	1:G:85:LEU:HD13	2.01	0.41
1:G:168:ILE:HG12	1:G:168:ILE:H	1.57	0.41
2:I:158:ASP:CG	2:I:159:SER:H	2.28	0.41
2:I:234:ASP:OD1	2:I:235:ASN:N	2.53	0.41
2:I:888:THR:OG1	2:I:914:LYS:HB3	2.20	0.41
2:I:1092:THR:HA	2:I:1093:PRO:HD3	1.82	0.41
3:J:156:ARG:NH1	3:J:157:GLN:NE2	2.69	0.41
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.76	0.41
3:J:1163:VAL:HG11	3:J:1198:VAL:HG21	2.03	0.41
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.89	0.41
1:B:113:ALA:HB2	1:B:126:PRO:HB3	2.01	0.41
1:B:196:THR:HG22	1:B:197:ASP:N	2.36	0.41
3:D:45:ASN:O	3:D:46:TYR:CD2	2.73	0.41
3:D:107:LEU:CD2	3:D:299:LEU:HD21	2.50	0.41
3:D:113:HIS:ND1	3:D:113:HIS:C	2.78	0.41
3:D:435:GLN:HB3	3:D:437:PHE:HE2	1.86	0.41
3:D:647:PRO:HG3	3:D:697:MET:N	2.36	0.41
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.02	0.41
5:F:465:ARG:HA	5:F:468:ARG:NH2	2.36	0.41
5:F:560:ARG:HA	5:F:565:ILE:HB	2.03	0.41
2:I:42:ASP:O	2:I:44:GLU:N	2.48	0.41
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.48	0.41
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.55	0.41
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.29	0.41
2:I:1117:LEU:HD21	2:I:1182:ILE:HD12	2.02	0.41
2:I:1234:LYS:CE	2:I:1238:LEU:HD23	2.50	0.41
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.54	0.41
5:L:340:ALA:HA	5:L:343:LYS:HZ2	1.86	0.41
1:B:109:PRO:HG3	1:B:132:HIS:CD2	2.55	0.41
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.94	0.41
3:D:552:ILE:O	3:D:567:THR:HG23	2.21	0.41
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.02	0.41
3:D:795:TYR:CE2	3:D:799:ARG:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:798:ARG:HH22	3:D:1325:PHE:HB3	1.84	0.41
3:D:1280:VAL:HG22	3:D:1284:ARG:HD2	2.02	0.41
5:F:562:ARG:NH2	5:F:573:LEU:HD23	2.36	0.41
2:I:93:SER:OG	2:I:126:GLU:OE1	2.22	0.41
2:I:171:LEU:HA	2:I:171:LEU:HD23	1.77	0.41
2:I:237:LEU:HA	2:I:237:LEU:HD13	1.79	0.41
2:I:397:LEU:HB3	2:I:401:GLY:HA3	2.02	0.41
2:I:559:CYS:HB2	2:I:662:SER:HB3	2.01	0.41
2:I:618:GLN:O	2:I:653:MET:HE3	2.20	0.41
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.03	0.41
2:I:1239:VAL:O	2:I:1242:LYS:N	2.50	0.41
3:J:316:ILE:HA	3:J:323:PRO:HA	2.02	0.41
3:J:723:TYR:CE1	3:J:727:ASP:HB2	2.56	0.41
3:J:735:ALA:O	3:J:739:GLN:HG3	2.21	0.41
3:J:843:VAL:HG13	3:J:883:ARG:HD3	2.02	0.41
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.50	0.41
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.61	0.41
1:A:106:GLY:HA2	1:A:136:GLU:O	2.21	0.41
2:C:149:LEU:CD1	2:C:453:ILE:HG13	2.50	0.41
2:C:358:ASP:OD2	2:C:361:SER:HB2	2.21	0.41
2:C:513:GLN:HE21	2:C:526:HIS:CE1	2.39	0.41
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	2.02	0.41
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.94	0.41
3:D:211:GLU:O	3:D:215:LYS:HB3	2.21	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.21	0.41
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.02	0.41
4:E:30:MET:HE3	4:E:46:THR:HB	2.02	0.41
1:G:166:ARG:O	1:G:167:PRO:C	2.63	0.41
1:H:64:VAL:HG11	1:H:69:SER:HB2	2.03	0.41
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.35	0.41
3:J:161:THR:HG22	3:J:164:GLN:CD	2.46	0.41
3:J:332:LYS:HA	3:J:337:ARG:H	1.85	0.41
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	2.03	0.41
5:L:105:MET:HE1	5:L:385:ARG:HG2	2.02	0.41
5:L:405:ILE:HG21	5:L:405:ILE:HD13	1.79	0.41
1:A:53:GLY:O	1:A:148:ARG:HG3	2.21	0.41
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.20	0.41
1:A:178:SER:HA	1:A:179:PRO:HD3	1.62	0.41
1:A:228:LEU:HA	1:A:231:PHE:HB2	2.03	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.84	0.41
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLN:HG2	1:B:76:GLU:OE1	2.21	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.51	0.41
2:C:55:SER:OG	2:C:56:VAL:N	2.54	0.41
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.03	0.41
2:C:145:ILE:HG21	2:C:456:VAL:HG13	2.03	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.02	0.41
2:C:248:GLY:O	2:C:249:GLU:HG3	2.21	0.41
2:C:481:LEU:HD22	2:C:481:LEU:H	1.86	0.41
2:C:533:LEU:HA	2:C:533:LEU:HD23	1.85	0.41
2:C:1144:PHE:HE1	2:C:1201:LEU:HD11	1.86	0.41
2:C:1207:SER:C	2:C:1209:GLN:N	2.77	0.41
2:C:1232:MET:C	2:C:1233:LEU:HD13	2.46	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.56	0.41
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.35	0.41
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.85	0.41
3:D:317:THR:HG23	3:D:320:ASN:CB	2.49	0.41
3:D:484:MET:HE2	3:D:484:MET:HB3	1.90	0.41
3:D:501:VAL:HG23	3:D:602:SER:HB2	2.03	0.41
3:D:700:ASN:O	3:D:704:GLU:HB2	2.21	0.41
3:D:1160:SER:HA	3:D:1204:VAL:O	2.21	0.41
3:D:1278:GLU:OE1	3:D:1279:GLN:HG2	2.21	0.41
5:F:415:ALA:O	5:F:419:PHE:HB2	2.21	0.41
1:G:232:VAL:C	1:H:218:ARG:HH12	2.28	0.41
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.36	0.41
2:I:90:VAL:HG12	2:I:91:THR:N	2.36	0.41
2:I:519:ASN:HB3	2:I:522:SER:HB2	2.01	0.41
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.21	0.41
2:I:1085:MET:HE2	2:I:1085:MET:HA	2.03	0.41
2:I:1255:THR:O	2:I:1257:GLN:N	2.54	0.41
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.54	0.41
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.21	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.70	0.41
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.41
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.50	0.41
3:J:414:GLU:O	4:K:45:LYS:NZ	2.49	0.41
3:J:702:GLN:HA	3:J:723:TYR:HE2	1.79	0.41
3:J:1154:ALA:HB2	3:J:1213:GLY:O	2.21	0.41
3:J:1292:LEU:O	3:J:1293:GLU:HB2	2.21	0.41
5:L:95:THR:O	5:L:96:ASP:C	2.64	0.41
5:L:117:ILE:O	5:L:121:LYS:N	2.39	0.41
5:L:285:ARG:HA	5:L:288:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:474:MET:C	5:L:476:ARG:N	2.78	0.41
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.03	0.41
5:L:608:ARG:O	5:L:611:LEU:HB2	2.21	0.41
2:C:149:LEU:HD22	2:C:530:ILE:HG21	2.02	0.41
2:C:379:GLU:H	2:C:379:GLU:CD	2.28	0.41
2:C:483:ASP:HB2	2:C:486:THR:HG22	2.01	0.41
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	2.03	0.41
3:D:504:GLN:CG	3:D:505:ASP:H	2.31	0.41
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.86	0.41
3:D:1165:PHE:CD1	3:D:1165:PHE:N	2.88	0.41
5:F:111:LEU:HA	5:F:111:LEU:HD23	1.78	0.41
5:F:269:LEU:HD23	5:F:269:LEU:HA	1.84	0.41
5:F:531:PRO:O	5:F:533:ASP:N	2.54	0.41
1:G:167:PRO:C	1:G:169:GLY:N	2.79	0.41
1:G:190:ALA:O	1:G:191:ARG:HD3	2.20	0.41
2:I:22:LEU:HB3	2:I:655:VAL:HG11	2.03	0.41
2:I:488:MET:HE3	2:I:488:MET:HB2	1.92	0.41
2:I:681:MET:O	2:I:685:MET:HE2	2.21	0.41
2:I:845:LEU:H	2:I:845:LEU:HG	1.56	0.41
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.56	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.21	0.41
5:L:276:MET:O	5:L:280:VAL:HG23	2.20	0.41
5:L:343:LYS:H	5:L:343:LYS:HD2	1.85	0.41
5:L:547:VAL:HG13	5:L:598:LEU:HD22	2.03	0.41
1:A:92:VAL:HB	1:A:120:ASP:HB3	2.04	0.40
1:B:109:PRO:HB3	1:B:132:HIS:HD2	1.86	0.40
2:C:879:GLY:HA2	2:C:920:VAL:HG12	2.03	0.40
2:C:1233:LEU:HD13	2:C:1233:LEU:N	2.35	0.40
2:C:1272:GLU:H	3:D:342:LEU:CB	2.34	0.40
3:D:123:ARG:NH1	3:D:1334:GLU:HG3	2.36	0.40
5:F:599:ARG:O	5:F:604:SER:HB2	2.21	0.40
1:G:73:GLY:C	1:G:134:THR:HG22	2.46	0.40
2:I:5:TYR:CD1	2:I:8:LYS:HD3	2.42	0.40
3:J:162:GLU:O	3:J:163:GLU:C	2.62	0.40
3:J:712:GLN:HB2	3:J:713:GLU:H	1.65	0.40
3:J:1146:GLU:O	3:J:1147:ALA:HB3	2.20	0.40
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.80	0.40
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.20	0.40
1:A:123:ILE:O	1:A:125:LYS:N	2.54	0.40
2:C:4:SER:O	2:C:8:LYS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:ASN:HD22	2:C:139:ASN:HA	1.66	0.40
2:C:210:LEU:O	2:C:215:TYR:HB2	2.21	0.40
2:C:500:ALA:O	2:C:504:GLU:HB2	2.21	0.40
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.22	0.40
3:D:111:THR:HG23	3:D:300:GLN:CD	2.46	0.40
3:D:122:SER:O	3:D:126:LEU:HG	2.22	0.40
3:D:252:LEU:HD23	3:D:252:LEU:HA	1.84	0.40
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.02	0.40
3:D:526:VAL:HA	3:D:549:LYS:O	2.21	0.40
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.86	0.40
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.20	0.40
3:D:1314:LEU:O	3:D:1326:GLN:NE2	2.52	0.40
5:F:540:LEU:HD23	5:F:544:THR:HG23	2.04	0.40
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.56	0.40
1:G:195:ARG:HA	1:G:195:ARG:HD2	1.85	0.40
1:G:224:LEU:O	1:G:228:LEU:HB2	2.21	0.40
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.35	0.40
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.51	0.40
2:I:972:PHE:HD2	2:I:975:ILE:HD12	1.87	0.40
3:J:751:ASP:HB3	3:J:753:SER:H	1.86	0.40
3:J:819:GLY:HA3	3:J:882:VAL:O	2.21	0.40
5:L:394:TYR:OH	5:L:436:ARG:HD2	2.20	0.40
5:L:584:ARG:HD2	5:L:584:ARG:HA	1.84	0.40
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.52	0.40
2:C:395:TYR:HB3	2:C:419:ILE:HG22	2.03	0.40
2:C:403:MET:HB3	2:C:403:MET:HE3	1.64	0.40
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.52	0.40
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.70	0.40
2:C:1142:ARG:HH22	2:C:1165:SER:C	2.19	0.40
3:D:54:ASP:HB2	3:D:61:ILE:HD11	2.03	0.40
5:F:124:GLU:O	5:F:127:ILE:HG13	2.21	0.40
5:F:280:VAL:O	5:F:284:GLU:HG3	2.22	0.40
1:G:47:LEU:HD13	1:G:183:ILE:HG12	2.04	0.40
1:G:79:LEU:HD13	1:G:79:LEU:O	2.20	0.40
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.40
2:I:553:THR:H	2:I:553:THR:HG1	1.52	0.40
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.52	0.40
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.37	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.89	0.40
3:J:526:VAL:HA	3:J:549:LYS:O	2.22	0.40
3:J:709:ARG:HD2	3:J:710:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.43	0.40
5:L:288:MET:CG	5:L:299:LYS:HE2	2.51	0.40
2:C:289:VAL:HG13	2:C:319:LEU:HD11	2.03	0.40
2:C:681:MET:HE2	2:C:681:MET:HB3	1.97	0.40
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.34	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	2.03	0.40
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.37	0.40
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.02	0.40
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.87	0.40
3:D:1319:PHE:CD1	3:D:1319:PHE:C	2.99	0.40
5:F:493:LYS:HA	5:F:496:LYS:HG3	2.03	0.40
2:I:91:THR:HB	2:I:138:ILE:O	2.22	0.40
2:I:448:LEU:HD23	2:I:448:LEU:HA	1.83	0.40
2:I:888:THR:HG23	2:I:916:SER:OG	2.22	0.40
3:J:360:TYR:OH	3:J:442:ILE:HD11	2.21	0.40
3:J:650:LYS:HE2	3:J:654:ILE:HD11	2.03	0.40
3:J:1287:ILE:H	3:J:1287:ILE:HG13	1.79	0.40
1:A:88:LEU:HA	1:A:128:HIS:CD2	2.57	0.40
1:A:315:GLY:C	1:A:316:MET:HG3	2.46	0.40
2:C:46:GLN:O	2:C:47:TYR:C	2.63	0.40
2:C:318:SER:OG	2:C:321:LEU:HB2	2.22	0.40
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.57	0.40
2:C:1252:SER:HB3	2:C:1255:THR:O	2.22	0.40
3:D:392:THR:CG2	5:F:606:VAL:HA	2.51	0.40
4:E:4:VAL:HG13	4:E:5:THR:HG23	2.02	0.40
1:G:77:ASP:O	1:G:81:ILE:HG13	2.22	0.40
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.04	0.40
2:I:534:GLY:HA3	2:I:535:PRO:HD2	1.78	0.40
2:I:582:ASN:HB3	2:I:586:PHE:N	2.33	0.40
2:I:639:LYS:C	2:I:641:GLU:H	2.30	0.40
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.03	0.40
2:I:1164:PHE:O	2:I:1166:ASP:N	2.55	0.40
3:J:104:HIS:HA	3:J:244:VAL:HG13	2.02	0.40
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.86	0.40
5:L:288:MET:HG2	5:L:299:LYS:HE2	2.03	0.40
5:L:320:ILE:O	5:L:327:SER:HB3	2.21	0.40
5:L:384:LEU:HD23	5:L:384:LEU:HA	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:712:GLN:NE2	2:I:862:LEU:O[4_545]	2.14	0.06

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%)	246 (78%)	53 (17%)	18 (6%)	1	15
1	B	213/329 (65%)	193 (91%)	16 (8%)	4 (2%)	6	33
1	G	225/329 (68%)	198 (88%)	18 (8%)	9 (4%)	2	21
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	6	33
2	C	1338/1342 (100%)	1205 (90%)	112 (8%)	21 (2%)	7	35
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	7	35
3	D	1162/1407 (83%)	1030 (89%)	105 (9%)	27 (2%)	5	30
3	J	1151/1407 (82%)	1027 (89%)	98 (8%)	26 (2%)	5	30
4	E	87/91 (96%)	81 (93%)	5 (6%)	1 (1%)	11	42
4	K	77/91 (85%)	71 (92%)	3 (4%)	3 (4%)	2	21
5	F	462/613 (75%)	423 (92%)	32 (7%)	7 (2%)	8	36
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	34
All	All	7045/8222 (86%)	6292 (89%)	604 (9%)	149 (2%)	5	31

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO
1	A	242	VAL
1	A	320	ASN

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Mol	Chain	Res	Type
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	1153	ALA
2	C	1154	ASP
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	89	GLY
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	569	THR
1	G	162	GLU
1	G	167	PRO
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	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	496	GLY
3	J	710	ASP
3	J	712	GLN

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Mol	Chain	Res	Type
3	J	805	GLN
3	J	850	LYS
3	J	1294	ALA
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG
1	A	50	SER
1	A	119	GLY
1	A	164	ASP
1	A	232	VAL
1	A	315	GLY
1	B	13	LEU
2	C	121	GLU
3	D	805	GLN
3	D	1274	PHE
5	F	566	ASP
5	F	584	ARG
1	G	168	ILE
1	H	138	ALA
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	332	LYS
3	J	339	ARG
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	A	319	GLU
1	A	324	ALA
1	B	136	GLU
1	B	138	ALA
2	C	163	LYS
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY

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Mol	Chain	Res	Type
3	D	314	ARG
3	D	417	ARG
3	D	1344	LEU
5	F	602	SER
1	G	229	GLU
1	H	193	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	417	ARG
3	J	745	GLY
4	K	14	GLY
2	C	62	TYR
2	C	813	GLU
2	C	1158	LYS
3	D	828	GLY
3	D	1297	LYS
2	I	201	ARG
2	I	696	ASP
2	I	813	GLU
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
5	L	585	GLU
1	A	318	LEU
2	C	1059	ARG
2	C	1256	GLN
3	D	46	TYR
3	D	345	LYS
1	H	20	SER
2	I	160	ASP
2	I	756	TYR
3	J	338	PHE
3	J	357	VAL
1	A	19	VAL
2	C	983	GLY
3	D	357	VAL
3	D	806	ASP
5	F	96	ASP
1	G	9	LEU
1	G	164	ASP
5	L	395	THR
3	D	120	LEU

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Mol	Chain	Res	Type
3	J	173	GLY
3	J	333	GLY
3	J	639	VAL
3	D	82	GLY
3	D	826	ILE
5	F	361	ILE
1	G	166	ARG
3	J	336	GLY
5	L	475	GLY
3	D	831	VAL
2	I	1202	GLY
1	A	293	PRO
2	C	897	PRO
3	D	1184	ASP
1	G	14	VAL
1	H	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	222 (80%)	56 (20%)	1	8
1	B	186/286 (65%)	163 (88%)	23 (12%)	4	22
1	G	193/286 (68%)	157 (81%)	36 (19%)	1	10
1	H	183/286 (64%)	167 (91%)	16 (9%)	9	34
2	C	1155/1157 (100%)	1021 (88%)	134 (12%)	5	24
2	I	1154/1157 (100%)	1031 (89%)	123 (11%)	6	27
3	D	962/1168 (82%)	853 (89%)	109 (11%)	5	25
3	J	960/1168 (82%)	855 (89%)	105 (11%)	6	26
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	21
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	23
5	F	417/540 (77%)	374 (90%)	43 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L	418/540 (77%)	371 (89%)	47 (11%)	6	25
All	All	6045/7024 (86%)	5336 (88%)	709 (12%)	5	24

All (709) 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	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	32	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	75	GLN
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	110	VAL
1	A	116	THR
1	A	133	LEU
1	A	137	ASN
1	A	159	ILE
1	A	165	GLU
1	A	168	ILE
1	A	171	LEU
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE

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Mol	Chain	Res	Type
1	A	223	ILE
1	A	227	GLN
1	A	231	PHE
1	A	239	GLN
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	252	ILE
1	A	262	LEU
1	A	264	VAL
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	9	LEU
1	B	14	VAL
1	B	16	ILE
1	B	26	VAL
1	B	27	THR
1	B	50	SER
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	72	GLU
1	B	79	LEU
1	B	92	VAL
1	B	95	LYS
1	B	102	LEU
1	B	121	VAL
1	B	124	VAL
1	B	133	LEU
1	B	139	SER
1	B	146	VAL
1	B	183	ILE
1	B	191	ARG
1	B	196	THR

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Mol	Chain	Res	Type
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	22	LEU
2	C	23	ASP
2	C	39	ILE
2	C	46	GLN
2	C	56	VAL
2	C	81	ASP
2	C	90	VAL
2	C	103	VAL
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR
2	C	135	THR
2	C	138	ILE
2	C	145	ILE
2	C	164	THR
2	C	170	VAL
2	C	201	ARG
2	C	208	ILE
2	C	285	ILE
2	C	292	ILE
2	C	302	ILE
2	C	306	THR
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	453	ILE
2	C	455	SER
2	C	456	VAL
2	C	471	VAL
2	C	481	LEU

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Mol	Chain	Res	Type
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	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	550	VAL
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	575	LEU
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	633	LEU
2	C	634	VAL
2	C	657	THR
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	705	GLU
2	C	714	VAL
2	C	723	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	781	ASP
2	C	783	LEU
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	817	LEU
2	C	864	LYS

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Mol	Chain	Res	Type
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	922	ASN
2	C	948	ILE
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1050	VAL
2	C	1054	LEU
2	C	1072	ASN
2	C	1076	ILE
2	C	1078	LYS
2	C	1082	ILE
2	C	1098	LEU
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1145	ILE
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1172	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1222	GLU
2	C	1225	VAL
2	C	1227	VAL
2	C	1233	LEU
2	C	1238	LEU
2	C	1240	ASP

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Mol	Chain	Res	Type
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1291	LEU
2	C	1296	ASP
2	C	1313	HIS
2	C	1327	LEU
3	D	11	GLN
3	D	12	THR
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	80	HIS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	93	THR
3	D	95	THR
3	D	96	LYS
3	D	97	VAL
3	D	154	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	290	ILE
3	D	292	VAL
3	D	306	LEU
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	363	LEU
3	D	374	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR

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Mol	Chain	Res	Type
3	D	394	ILE
3	D	399	LYS
3	D	407	VAL
3	D	413	ASP
3	D	415	VAL
3	D	416	ILE
3	D	423	LEU
3	D	425	ARG
3	D	429	LEU
3	D	442	ILE
3	D	490	ILE
3	D	505	ASP
3	D	507	VAL
3	D	510	LEU
3	D	514	THR
3	D	532	GLU
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	594	GLN
3	D	605	LEU
3	D	615	LYS
3	D	639	VAL
3	D	641	ILE
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	721	SER
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	790	THR
3	D	797	THR
3	D	801	VAL
3	D	810	THR

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Mol	Chain	Res	Type
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	890	THR
3	D	903	LEU
3	D	908	ILE
3	D	918	ILE
3	D	1135	THR
3	D	1146	GLU
3	D	1155	ILE
3	D	1156	LEU
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1194	ARG
3	D	1221	LEU
3	D	1251	LYS
3	D	1255	VAL
3	D	1257	VAL
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
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	18	ASP
4	E	21	LEU
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL

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Mol	Chain	Res	Type
4	E	58	LEU
5	F	98	VAL
5	F	114	GLU
5	F	127	ILE
5	F	152	GLU
5	F	154	GLU
5	F	163	THR
5	F	230	VAL
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	399	LEU
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
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	494	ILE
5	F	507	MET
5	F	516	ASP
5	F	526	THR
5	F	527	THR
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	559	LEU
5	F	561	MET
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	578	LYS
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG

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Mol	Chain	Res	Type
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	27	THR
1	G	33	ARG
1	G	50	SER
1	G	64	VAL
1	G	65	LEU
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	129	VAL
1	G	133	LEU
1	G	137	ASN
1	G	145	LYS
1	G	156	SER
1	G	161	SER
1	G	162	GLU
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	187	VAL
1	G	192	VAL
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	217	ILE
1	G	219	ARG
1	H	16	ILE
1	H	27	THR
1	H	58	GLU
1	H	61	ILE

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Mol	Chain	Res	Type
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	66	HIS
1	H	75	GLN
1	H	90	VAL
1	H	95	LYS
1	H	102	LEU
1	H	121	VAL
1	H	124	VAL
1	H	133	LEU
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	21	VAL
2	I	22	LEU
2	I	39	ILE
2	I	46	GLN
2	I	56	VAL
2	I	86	GLN
2	I	90	VAL
2	I	103	VAL
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	119	GLU
2	I	131	THR
2	I	132	ASP
2	I	135	THR
2	I	138	ILE
2	I	156	PHE
2	I	164	THR
2	I	170	VAL
2	I	208	ILE
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP

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Mol	Chain	Res	Type
2	I	343	HIS
2	I	360	LEU
2	I	384	LEU
2	I	423	ASP
2	I	445	ILE
2	I	453	ILE
2	I	455	SER
2	I	456	VAL
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	492	MET
2	I	493	ILE
2	I	518	ASN
2	I	521	LEU
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	542	ARG
2	I	550	VAL
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	575	LEU
2	I	596	ASP
2	I	600	THR
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	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	705	GLU
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE

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Mol	Chain	Res	Type
2	I	781	ASP
2	I	782	VAL
2	I	800	MET
2	I	817	LEU
2	I	828	PHE
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	922	ASN
2	I	951	MET
2	I	984	VAL
2	I	1002	LEU
2	I	1037	THR
2	I	1050	VAL
2	I	1054	LEU
2	I	1073	LYS
2	I	1078	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1172	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1206	THR
2	I	1210	ILE
2	I	1225	VAL
2	I	1227	VAL
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER

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Mol	Chain	Res	Type
2	I	1254	VAL
2	I	1287	LEU
2	I	1296	ASP
2	I	1299	ASN
2	I	1313	HIS
2	I	1326	LEU
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	96	LYS
3	J	97	VAL
3	J	98	ARG
3	J	162	GLU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	283	LEU
3	J	292	VAL
3	J	306	LEU
3	J	324	LEU
3	J	343	LEU
3	J	357	VAL
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE

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Mol	Chain	Res	Type
3	J	415	VAL
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	514	THR
3	J	532	GLU
3	J	536	LEU
3	J	545	HIS
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	591	ILE
3	J	594	GLN
3	J	605	LEU
3	J	615	LYS
3	J	639	VAL
3	J	641	ILE
3	J	678	ARG
3	J	680	ASN
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	713	GLU
3	J	717	VAL
3	J	721	SER
3	J	754	ILE
3	J	764	ARG
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	827	GLU
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR

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Mol	Chain	Res	Type
3	J	857	LEU
3	J	858	VAL
3	J	877	VAL
3	J	897	HIS
3	J	898	CYS
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN
3	J	913	GLU
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	1194	ARG
3	J	1204	VAL
3	J	1221	LEU
3	J	1243	LEU
3	J	1251	LYS
3	J	1255	VAL
3	J	1257	VAL
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	127	ILE

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Mol	Chain	Res	Type
5	L	152	GLU
5	L	154	GLU
5	L	163	THR
5	L	261	LEU
5	L	277	MET
5	L	305	LEU
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	405	ILE
5	L	429	THR
5	L	445	ASP
5	L	450	ILE
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	494	ILE
5	L	507	MET
5	L	511	ILE
5	L	526	THR
5	L	527	THR
5	L	547	VAL
5	L	552	THR
5	L	558	VAL
5	L	559	LEU
5	L	561	MET
5	L	568	ASN
5	L	569	THR
5	L	572	THR
5	L	573	LEU
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

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Mol	Chain	Res	Type
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	268	ASN
1	B	117	HIS
2	C	46	GLN
2	C	139	ASN
2	C	235	ASN
2	C	406	ASN
2	C	510	GLN
2	C	513	GLN
2	C	618	GLN
2	C	620	ASN
2	C	658	GLN
2	C	677	ASN
2	C	760	ASN
2	C	808	ASN
2	C	952	GLN
2	C	1023	HIS
2	C	1061	GLN
2	C	1116	HIS
2	C	1146	GLN
2	C	1220	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1299	ASN
2	C	1314	GLN
3	D	200	GLN
3	D	294	ASN
3	D	365	GLN
3	D	419	HIS
3	D	424	ASN
3	D	504	GLN
3	D	690	ASN
3	D	712	GLN
3	D	716	GLN
3	D	805	GLN
3	D	907	HIS
3	D	1218	HIS

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Mol	Chain	Res	Type
3	D	1235	ASN
3	D	1366	HIS
5	F	129	GLN
5	F	131	GLN
5	F	147	GLN
5	F	246	GLN
5	F	258	GLN
5	F	294	GLN
5	F	301	ASN
5	F	383	ASN
5	F	406	GLN
5	F	446	GLN
5	F	455	HIS
5	F	469	GLN
5	F	579	GLN
5	F	600	HIS
1	G	41	ASN
1	G	66	HIS
1	G	186	ASN
2	I	20	GLN
2	I	41	GLN
2	I	46	GLN
2	I	139	ASN
2	I	150	HIS
2	I	165	HIS
2	I	314	ASN
2	I	510	GLN
2	I	604	HIS
2	I	620	ASN
2	I	673	HIS
2	I	766	ASN
2	I	799	ASN
2	I	1017	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	1288	GLN
2	I	1299	ASN

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Mol	Chain	Res	Type
2	I	1336	ASN
3	J	157	GLN
3	J	200	GLN
3	J	206	ASN
3	J	430	HIS
3	J	435	GLN
3	J	450	HIS
3	J	489	ASN
3	J	594	GLN
3	J	606	ASN
3	J	716	GLN
3	J	817	HIS
3	J	1197	ASN
3	J	1235	ASN
3	J	1279	GLN
3	J	1295	ASN
3	J	1366	HIS
5	L	258	GLN
5	L	301	ASN
5	L	345	GLN
5	L	357	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	455	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.84	0 100 100	84, 129, 182, 196	0
1	B	217/329 (65%)	-0.72	0 100 100	91, 164, 203, 214	0
1	G	227/329 (68%)	-0.79	0 100 100	126, 154, 181, 218	0
1	H	216/329 (65%)	-0.74	0 100 100	118, 174, 198, 207	0
2	C	1340/1342 (99%)	-0.78	0 100 100	58, 114, 218, 253	0
2	I	1340/1342 (99%)	-0.75	0 100 100	93, 148, 222, 378	0
3	D	1166/1407 (82%)	-0.83	0 100 100	63, 107, 168, 218	0
3	J	1155/1407 (82%)	-0.76	0 100 100	85, 128, 189, 228	0
4	E	89/91 (97%)	-0.90	0 100 100	67, 116, 140, 152	0
4	K	79/91 (86%)	-0.80	0 100 100	99, 139, 205, 222	0
5	F	468/613 (76%)	-0.70	0 100 100	93, 160, 273, 305	0
5	L	469/613 (76%)	-0.73	0 100 100	114, 172, 279, 307	0
All	All	7085/8222 (86%)	-0.77	0 100 100	58, 135, 209, 378	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	I	1401	1/1	0.71	0.19	94,94,94,94	0
6	MG	C	1401	1/1	0.85	0.13	94,94,94,94	0
6	MG	J	2001	1/1	0.97	0.05	94,94,94,94	0
6	MG	D	2001	1/1	0.98	0.05	94,94,94,94	0
7	ZN	D	2002	1/1	0.99	0.03	113,113,113,113	0
7	ZN	J	2002	1/1	0.99	0.02	105,105,105,105	0
7	ZN	D	2003	1/1	1.00	0.02	94,94,94,94	0
7	ZN	J	2003	1/1	1.00	0.01	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.