



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:31 AM UTC

PDB ID : 4YFK / pdb_00004yfk
Title : Escherichia coli RNA polymerase in complex with squaramide compound 8.
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.;
McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

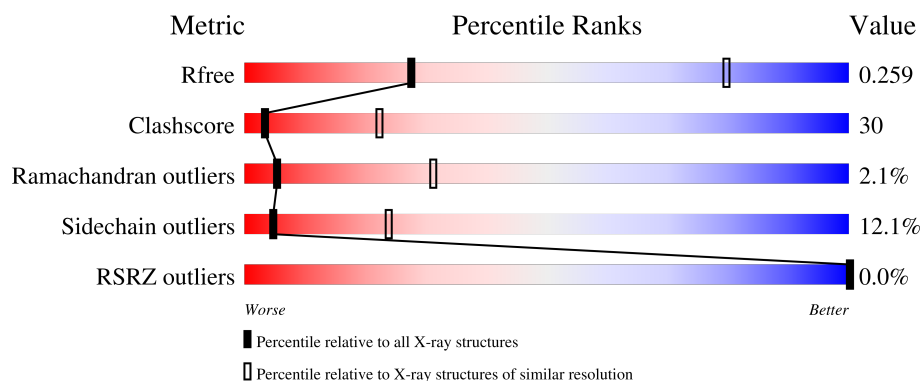
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	35% 45% 16% ••
1	B	329	27% 31% 7% • 34%
1	G	329	30% 32% 7% 31%
1	H	329	25% 34% 6% 34%
2	C	1342	44% 46% 9% •

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

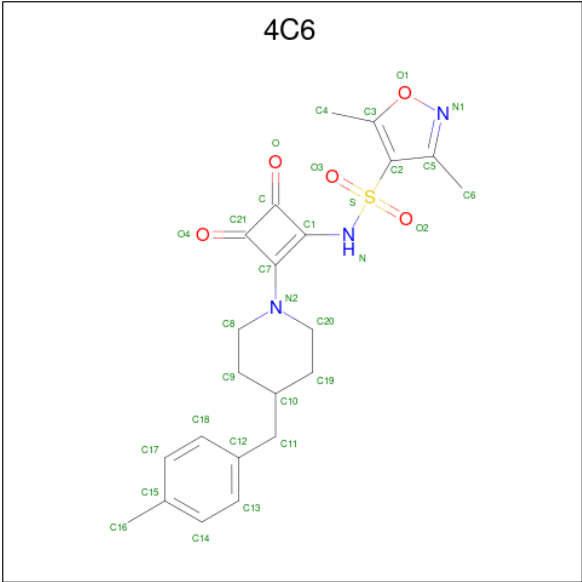
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

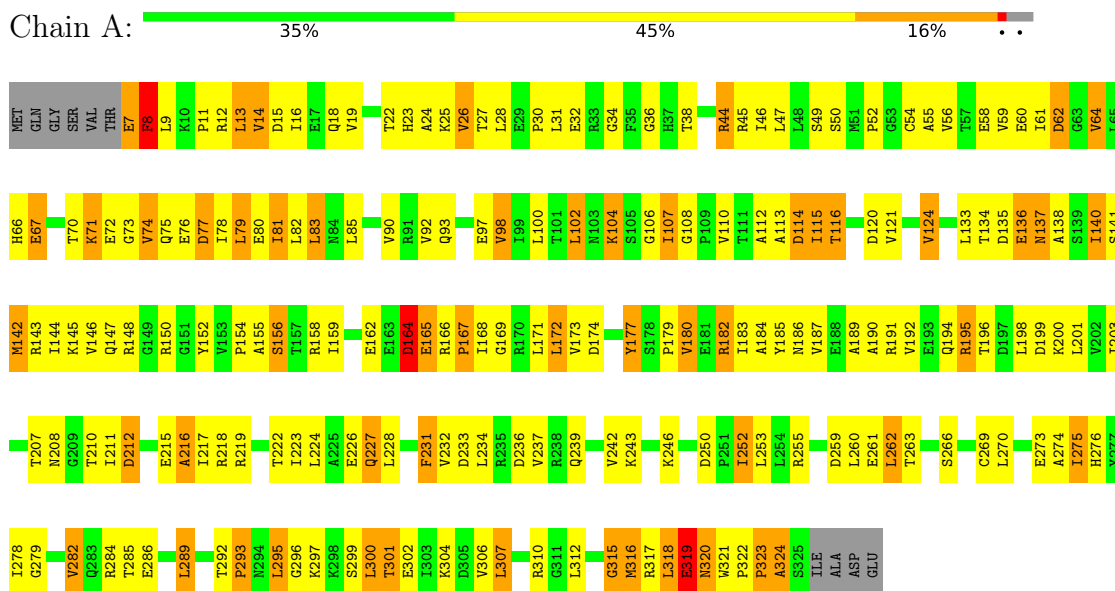


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			31	22	3	5	1		
8	J	1	Total	C	N	O	S	0	0
			31	22	3	5	1		

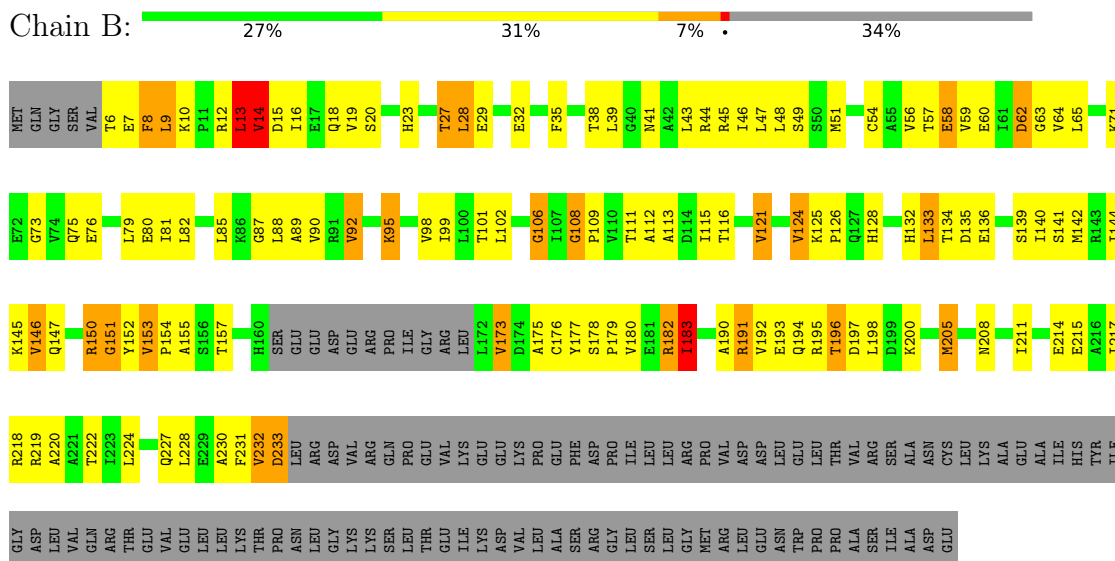
3 Residue-property plots

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.

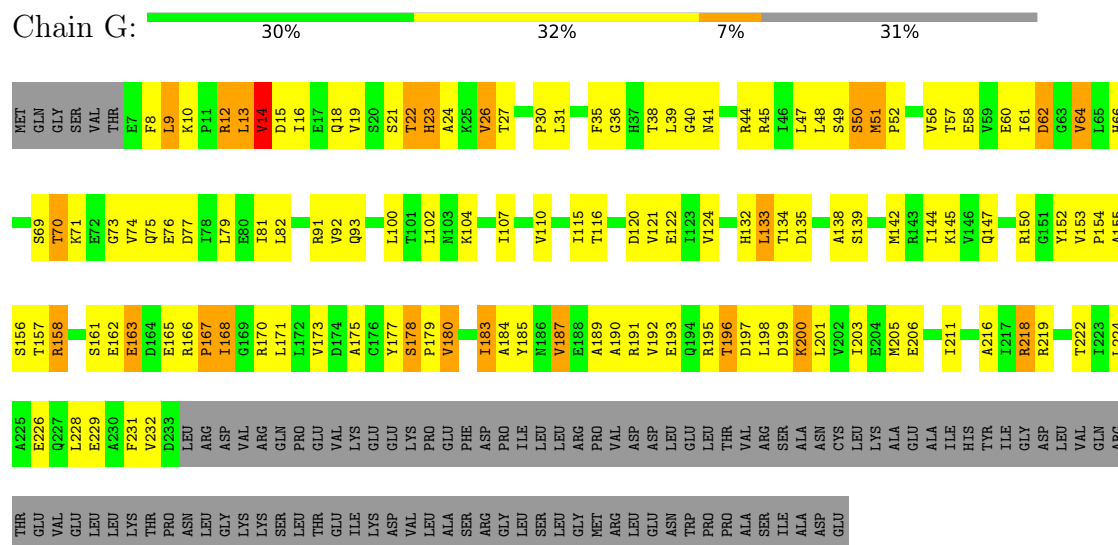
• Molecule 1: DNA-directed RNA polymerase subunit alpha



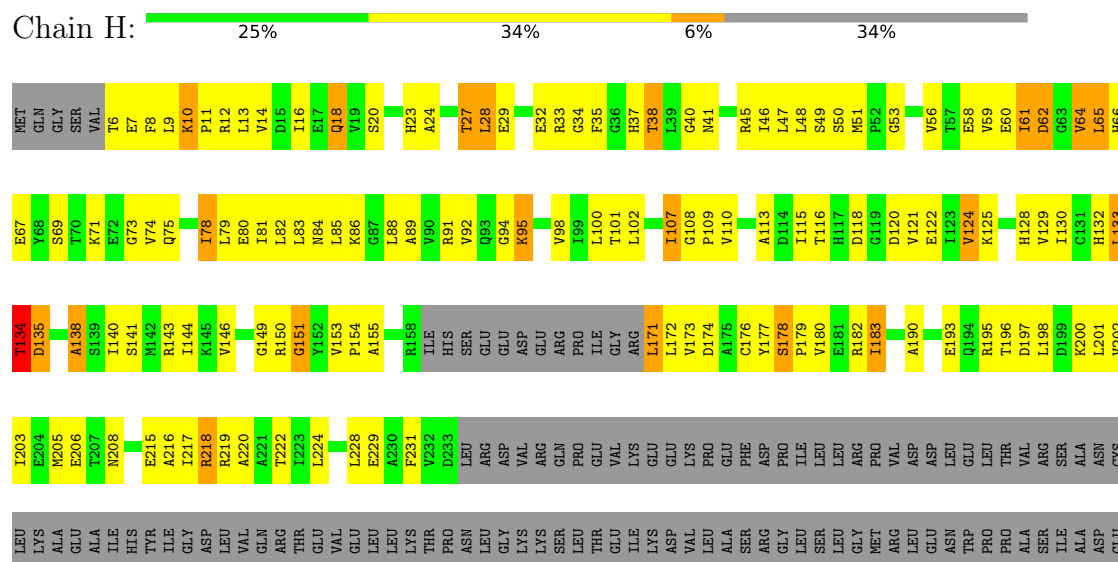
• Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

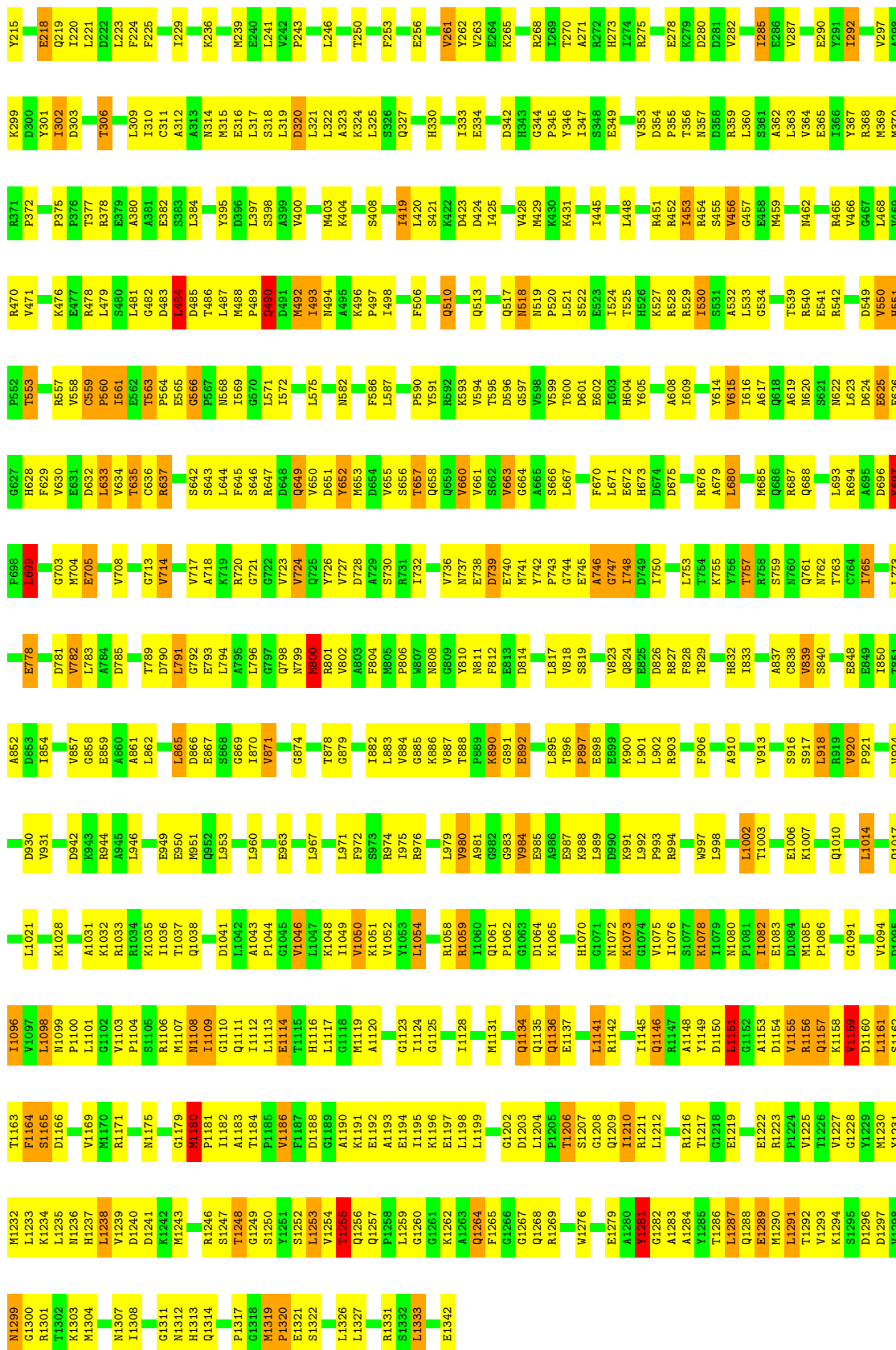


- Molecule 1: DNA-directed RNA polymerase subunit alpha

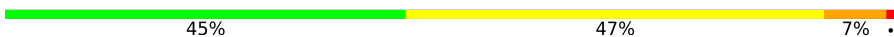


- Molecule 2: DNA-directed RNA polymerase subunit beta

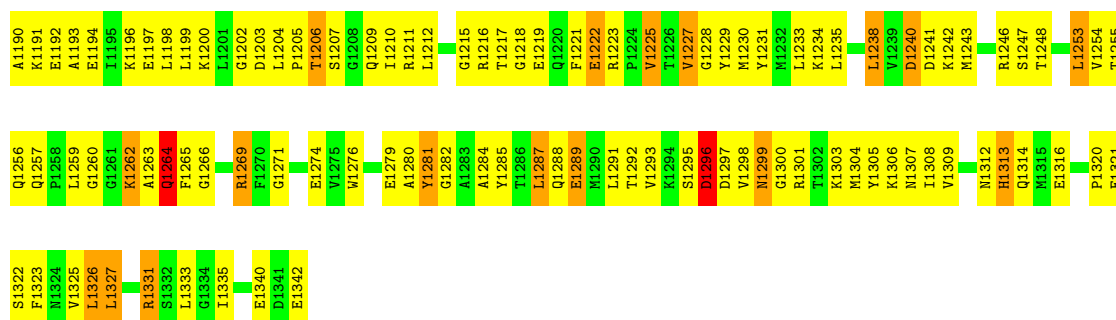




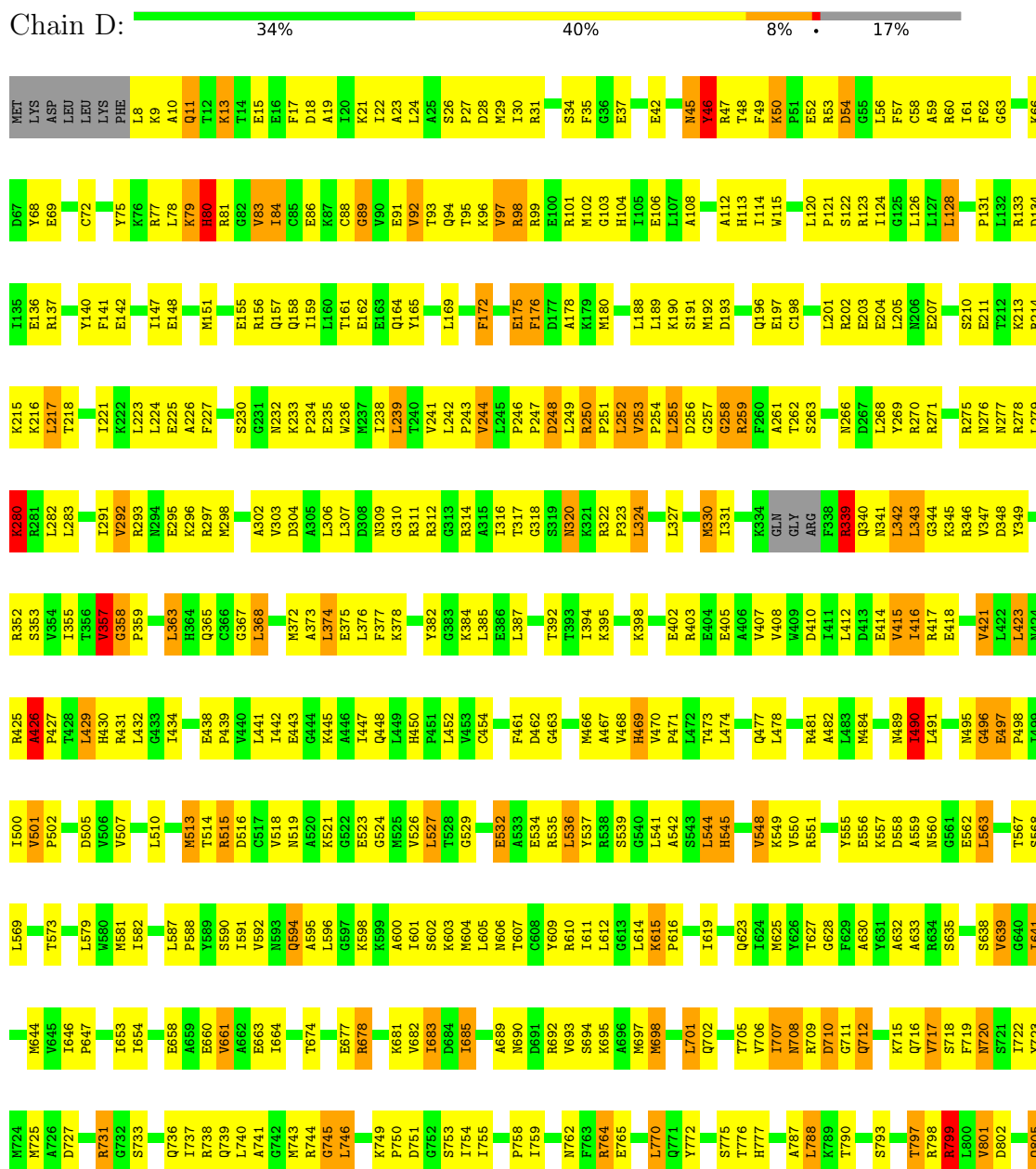
- Molecule 2: DNA-directed RNA polymerase subunit beta

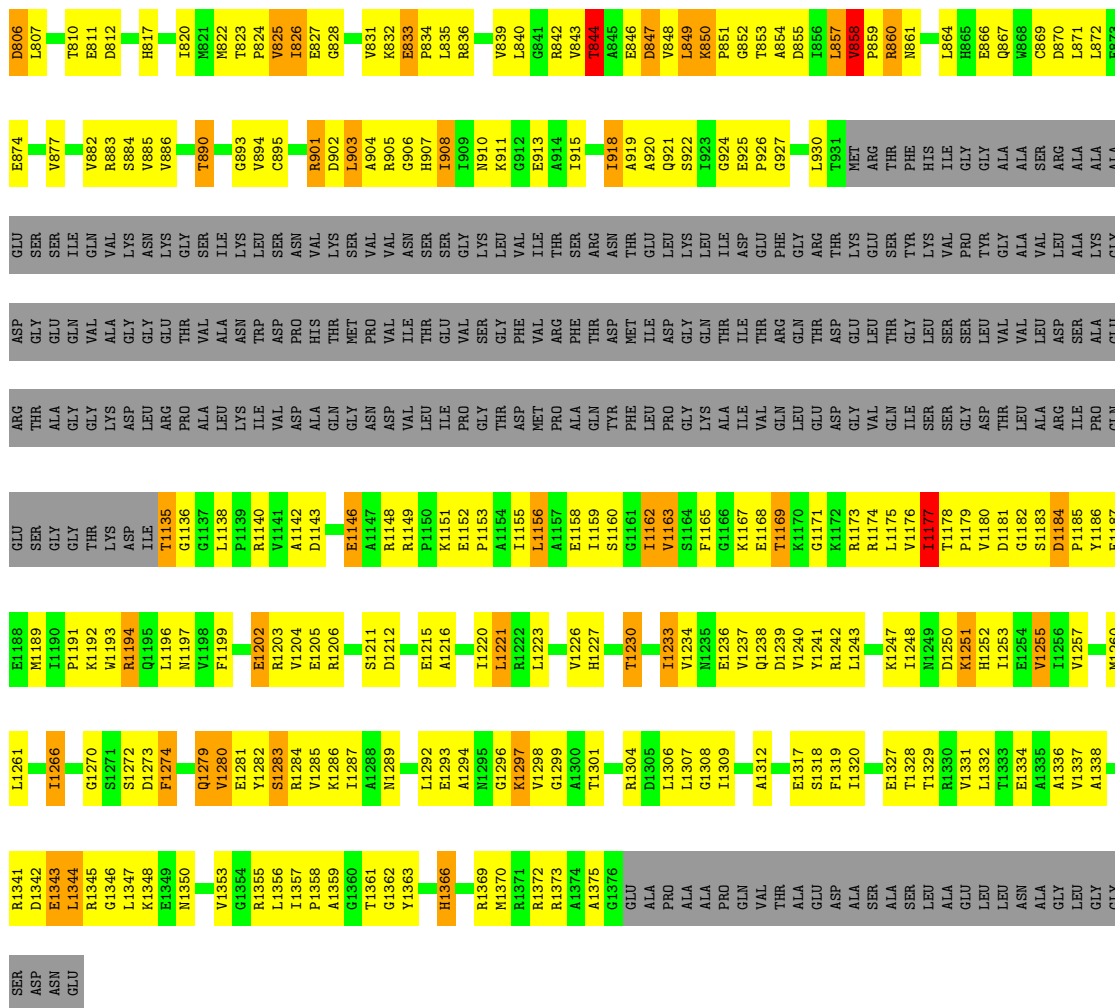
Chain I:  45% 47% 7%

VAL	Y3	Y4	Y5	K8	K9	R10	I11	R12	K13	D14	F15	G16	K17	V21	L22	D23	V24	P25	Y26	L27	L28	S29	L30	Q31	L32	F35	Q36	K37	F38	D42	P43	E44	G45	Q46	Y47	G48	L49	E50	F57	P58	L59	Q60	S61	Y62	S63	G64	N65	V71	S72	Y73	R74				
F80	E84	C85	Q86	T91	Y92		P95	L96	K97	Y98	K99	V103	I104	I105	E106	R107	E108	A109	P110	E111	K115	D116	I117	K118	E119	Q120	E121	V122	Y123	M124	G125	E126	I127	P128	L129	M130	T131	D132	T136	V137	I138	N139	L143	S147	Q148	L149	R151	S152	P153						
F156	F157	D158	S159	D160	K161	G168	K169	V170	L171	Y172	N173	A174	R175	I176	P178	S182	W183	L184	D185	F186	E187	F188	L194	F195	E196	R197	I198	D199	R200	R201	R202	K203	A206	T207	L208	L209	L210	R211	A212	L213	Q219	I220	L221	D222	H227	V228	F230	E231	L232						
K236	L237	Q238	M239	E240	L241	V242	P243	E244	R245	L246	T250	R268	R176	I269	R272	H273	L277	V282	K283	L284	L285	E290	V291	L292	I302	T306	I310	R314	K315	E316	L319	D320	L321	L322	H330	K331	R332	T335	L336	F337	T338														
D342	H343	G344	P345	Y346	L351	D354	P355	T356	N357	R358	K359	L360	S361	A362	L363	V364	E365	L366	Y367	K368	K369	K370	E374	P375	P376	T377	K378	A380	A381	S382	L384	F385	K386	N387	L388	F389	F390	Y396	D396	L397	S398	A399	V400	G401	R402	F405	L409	L492	L493	G416	L419				
L420	S421	K422	D423	D424	L425	V428	M429	K430	T431	L432	L435	D443	D444	L445	L448	R451	R452	L453	V456	G457	N462	R465	V466	G467	L468	V469	R470	E471	F472	R473	A474	V475	K476	H477	R478	L479	G482	D483	L484	D485	T486	L487	P489	Q490	D491	K492	L493	N494	A495	K496					
P497	L498	S499	V502	L503	F506	L511	T512	K513	D514	E515	H516	D517	N518	N519	P520	L521	S522	E523	L524	H525	K526	K527	H528	R529	L530	P535	L538	T539	H542	V543	H544	V545	H546	H547	H548	H549	H550	H551	P552	H553	H554	H555	H556	H557	V558	C559	P560	I561	T563	P564	N568	L569	L571	L572	L575
S576	A579	Q580	T581	N582	G585	F586	L587	E588	T589	P590	K593	V594	T595	D596	G597	T600	D601	E602	L603	H604	Y605	L606	S607	A608	L609	E610	G611	L612	N613	V614	H615	T616	A617	Q618	P619	L623	D624	E625	F629	V630	E631	D632	L633	V634	T635	C636	R637	F645	S646	R647	D648	Q649			
V650	D651	V652	D654	V655	S656	Q658	Q659	V660	V661	S662	V663	G664	S665	S666	L667	F670	L671	E672	H673	D674	D675	A676	H677	A679	L680	N681	G682	M685	Q686	Q687	Q688	A689	T692	D696	K697	L698	V700	G703	M704	D705	V714	T715	A716	G717	Q718	K719	R720	G721							
V724	Q725	Y726	Y727	D728	A729	T732	V733	I734	K735	V736	V737	E738	D739	E740	M741	Y742	G743	G744	E745	A746	G747	I748	Y751	K755	Y756	R757	R758	S759	I765	P769	G770	V771	S772	L773	G774	E775	V782	L783	A784	L791	G792	E793	L794	A795	L796	G797	Q798	R800	R801	V802					
N808	G809	N810	N811	F812	E813	D814	S815	V816	V817	V818	S819	E820	Q824	R827	F828	T829	T830	E832	L836	V839	L845	E848	K849	L850	T851	A852	L853	R854	P855	N856	V857	L862	E867	S868	V871	I882	L883	V884	G885	K886	V887	T888	S893	K890	G891	E892									
T896	P897	E898	R903	E908	R909	A910	V913	K914	D915	S916	S917	L918	R919	V920	P921	V924	L1000	G1001	L1002	T1003	K1007	Q1010	L1011	E1012	Q1013	L1014	A1015	E1016	Q1017	P1018	L1021	K1022	H1023	E1024	F1025	E1026	K1027	E1030	L1033	R1034	I966	L967	E968	L971	G972	M1043	R974	I975	R976	I1049					
V1050	L1054	R1059	P1062	K1065	M1066	A1067	K1073	T1076	S1077	K1078	I1079	N1080	P1081	L1082	E1083	G1085	P1086	Y1087	G1091	V1094	I1096	V1097	L1098	N1099	F1164	L1101	G1102	V1103	R1106	M1107	L1108	I1109	G1110	Q1111	L1112	L1113	E1114	T1115	H1116	L1117	G1118	M1119	A1120	P1121	K1122	G1123	L1124	G1189							
I1128	M1129	A1130	M1131	L1132	K1133	Q1134	L1135	Q1136	E1137	V1138	A1139	K1140	L1141	R1142	E1143	Q1146	Y1149	D1150	L1151	G1152	A1153	D1154	V1155	K1156	Q1157	K1158	V1159	D1160	L1161	T1162	N1163	F1164	S1165	D1166	V1169	M1170	R1171	L1172	A1173	E1174	M1175	L1176	R1177	K1178	G1179	R1181	I1182	A1183	T1184	P1185	V1186	F1187	D1188	G1189	

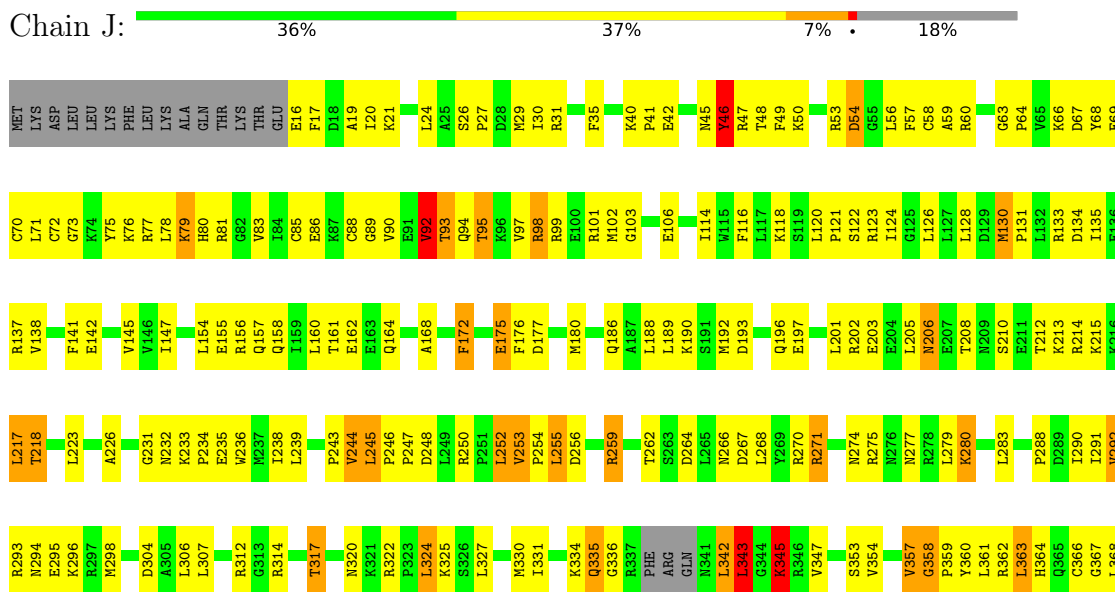


• Molecule 3: DNA-directed RNA polymerase subunit beta'





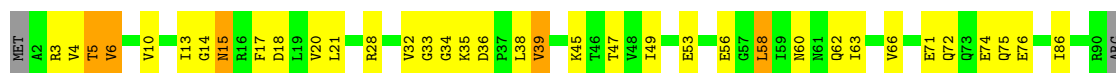
- Molecule 3: DNA-directed RNA polymerase subunit beta'



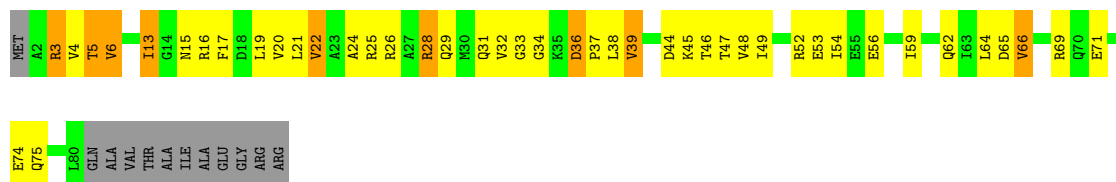
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SER	L1306	I1233	E1188	ASP	PHE	VAL	I908	V831	L746	M680	K599	C517	K445	K370
LEU	ALA	I1234	E1189	MET	VAL	ILE	I909	V832	A748	K681	A600	V518	Q448	L374
LEU	LEU	M1235	I1182	PRO	ARG	THR	N910	K832	A749	V682	I601	N519	L449	E375
LEU	LEU	E1236	V1163	GLN	PHE	THR	K911	E833	P750	I683	S602	K520	H450	L376
ASN	LEU	V1237	S1164	TYR	ASP	ASN	G912	P834	D751	D684	K603	A521	P451	
ALA	ALA	Q1238	F1165	PHE	MET	THR	I915	L835	G752	I685	M604	G522	L452	P379
GLY	GLY	E1166	G1166	LEU	ILE	GLU	G916	V839	S753	A689	L605	M525	A459	F380
GLY	GLY	K1167	K1167	PRO	ASP	LEU	I917	R842	I754	M690	Y609	V527	I381	I381
GLY	GLY	E1168	E1168	GLY	GLY	LYS	I918	R843	P758	D691	R610	L527	G383	G383
SER	GLY	M1169	T1169	LYS	GLN	LEU	I923	T844		R692	I611	T528	D462	K384
SER	GLY	K1170	G1171	ILE	THR	ILE	G924	A845	A761	V693	L612	E532	D464	L385
ASP	ASP	R1172	K1172	VAL	THR	ASP	P926	E846	N762	S694	G613		Q465	
ASN	ASN	R1173	R1173	GLN	THR	GLU	P926	D847	N763	K695	L614		Q466	
GLU	GLU	R1174	S1174	GLN	ARG	PHE		V848	R764	K697	K615		M466	
GLU	GLU	L1175	L1175	THR	THR	ARG	L930	L849		M698	P616		V468	
ASP	ASP	V1176	T1176	ASP	ASP	THR	T931	K850	L767	D699	I619		H469	
GLY	GLY	I1177	I1177	GLU	GLU	LYS	MET	P851	N768	N700	F620		V470	
VAL	VAL	T1178	T1178	LEU	LEU	GLU	ARG	G852	N769	L701			P471	
GLN	GLN	P1179	P1179	THR	THR	THR	THR	T853	L770	Q702	Q623		L472	
ILE	ILE	V1180	V1180	GLY	GLY	TYR	PHE	A854	Q771	T703	I624		T473	
SER	SER	D1181	D1181	LEU	LEU	VAL	HIS	D855	F772	E704	M625		L474	
GLY	GLY	G1182	G1182	SER	SER	VAL	ILE	T856	F773	T705			E475	
ASP	ASP	S1183	S1183	GLY	SER	PRO	GLY	L857	I774	V706	G628		A476	
ASP	ASP	D1184	D1184	LEU	LEU	TYR	GLY	P858	S775	I707			Q477	
THR	THR	P1185	P1185	VAL	VAL	GLY	ALA	R860	T776	N708	Y631		L478	
ALA	ALA	Y1186	Y1186	VAL	VAL	ALA	ALA	R861	H777	R709	V550		E479	
ARG	ARG	M1189	M1189	ASP	ASP	LEU	ARG	T862	R780	D710	R634		V408	
ILE	ILE	K1192	K1192	SER	SER	ALA	ALA	L863		G711	S635		W409	
PRO	PRO	V1193	V1193	GLU	GLU	LYS	ALA	L864	L788	Q712	G636		A482	
GLN	GLN	R1194	R1194	ARG	ARG	GLY	ALA	H865		Q716	A637		L483	
GLU	GLU	Q1195	Q1195	THR	THR	ASP	GLU	E866	S793	V717	S638		M484	
SER	SER	L1196	L1196	GLY	GLY	GLY	SER	Q867		S718	V639		M485	
GLY	GLY	F1199	F1199	GLY	GLY	GLN	ILE	L796	L796	F719	G640		S486	
THR	THR	E1202	E1202	THR	THR	VAL	ILE	L872	T797	N720	I641		T487	
ASP	ASP	R1203	R1203	ILE	LYS	VAL	GLN	V877	R799	S721	M644		W488	
THR	THR	V1204	V1204	GLY	LYS	ALA	VAL	R882	L800	I722	V645		M489	
GLY	GLY	E1205	E1205	ARG	ARG	GLY	ASN	V883	P647	W723	I646		I490	
ALA	ALA	G1207	G1207	PRO	PRO	VAL	LYS	S884	B802	M724	P647		L491	
ALA	ALA	A1208	A1208	ALA	ALA	THR	GLY	V885	V803	M725	E648		M495	
ALA	ALA	N1289	N1289	LEU	LEU	VAL	ILE	G893	Q805		K649		G496	
ASN	ASN	I1210	I1210	ILE	ILE	ASP	LEU	V894	D806	I654	K650		E497	
ALA	ALA	E1215	E1215	VAL	VAL	ASP	SER	C895	V809	S733	I654		P498	
ALA	ALA	H1218	H1218	ASP	ASP	PRO	ASN	A896	T810	A734	A657		I500	
GLN	GLN	D1219	D1219	GLN	GLN	HIS	VAL	H897	E811	A735	E658		S503	
VAL	VAL	I1220	I1220	ASN	ASN	THR	LYS	C898	D812	Q736	A659		Q504	
THR	THR	K1297	K1297	ASP	ASP	MET	SER	Y899	D813	I737	E660		D505	
ALA	ALA	R1222	R1222	VAL	VAL	PRO	VAL	G900	R738	R738	V661		V506	
GLU	GLU	V1226	V1226	LEU	LEU	ILE	ASN	R901	H817	Q739	I591		L510	
ASP	ASP	T1301	T1301	ILE	ILE	THR	SER	D902	L740	W592	K593		Y511	
ALA	ALA	R1304	R1304	PRO	PRO	GLU	SER	L903	A741	Q594	Q594		Y512	
SER	SER			GLY	GLY	VAL	GLY	A904	G742	A595	L596		M513	
								G906	W825	M743	G597		T514	
									I826	R744	R678		E443	

● Molecule 4: DNA-directed RNA polymerase subunit omega

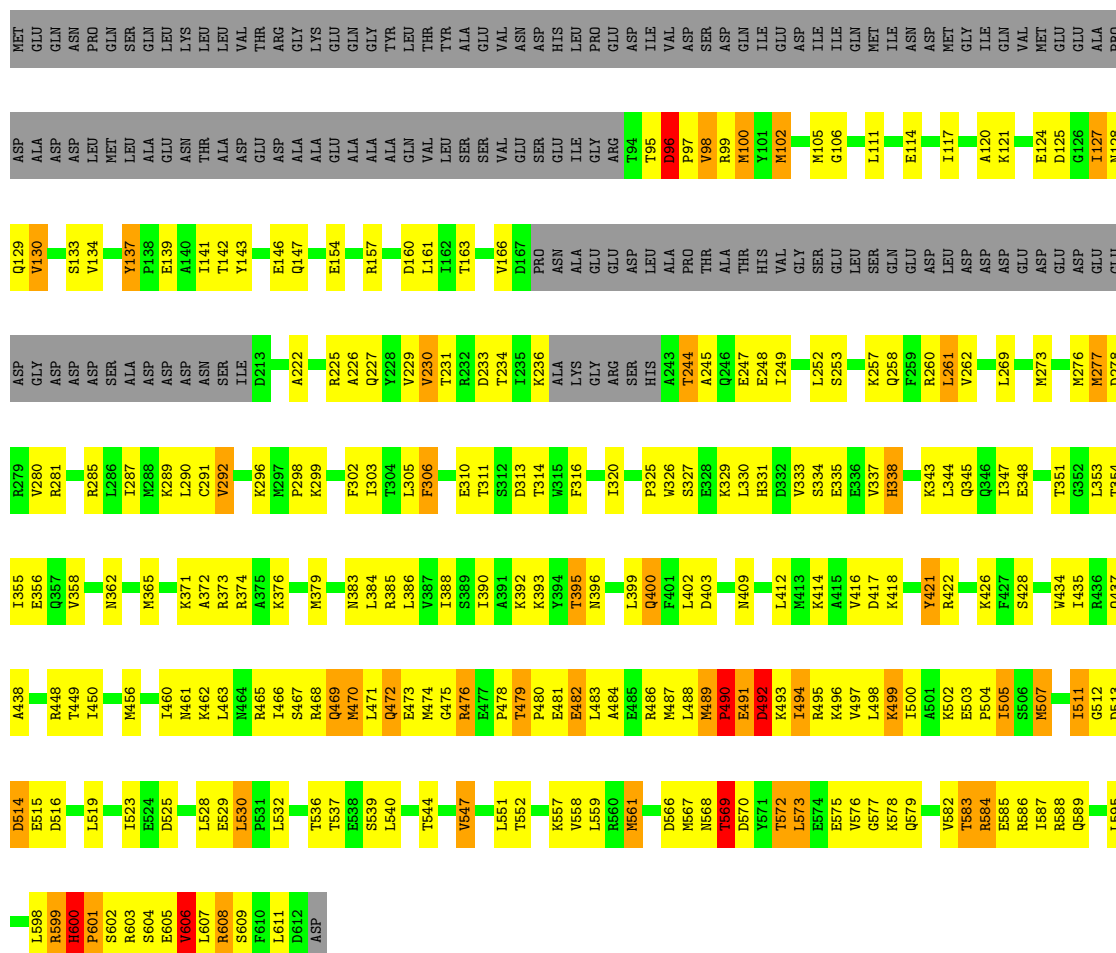
Chain E: 58% 34% 5%



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD



V558	E473	A391	K329	R260	GLU	ASP
L559	M474	K392	V333	L261	GLU	ALA
M560	G475	K393	V334	V262	ASP	ASP
R561	R476	Y394	P263	P264	GLY	ASP
R562	E477	T395	E335	K265	ASP	LEU
	P478	N396	E336	Q265	ASP	MET
I565	T479	R397	F266	F266	ASP	LEU
D566		H398			ASP	ALA
M567	E482	L399	N271	N271	SER	ALA
N568	L483	A340	S272	S272	ALA	GLU
T569	A484	L341	M273	M273	ASP	ASN
D570	E485	K342	R274	R274	ASP	THR
Y571	R486	D403	R275	R275	ALA	ALA
T572	M487	K343	V276	V276	ASP	ALA
L573	L488	L344	M276	M276	ASP	ASP
E574	M489	Q345	M277	M277	SER	GLU
E575	P490	Q346			ILE	ASP
V576	E491	I347	V280	V280	ALA	ALA
G577	D492	E348	R281	R281	ALA	ALA
K578	K493	E349	T282	T282	GLU	GLU
Q579	I494	E350	Q283	Q283	ALA	ALA
F580		T351	E284	E284	ALA	ALA
D581	K499	G352	R285	R285	ALA	ALA
V582	I500	L353	L286	L286	GLN	GLN
T583		T354	L287	L287	VAL	VAL
R584	E503	I355	M288	M288	LEU	LEU
E585	P504	E356	K289	K289	SER	SER
R586	F505	Q357	L290	L290	SER	SER
T587	L506	V358	C291	C291	VAL	VAL
R588	E508	K359	V292	V292	GLU	GLU
Q589		D360	E293	E293	GLU	GLU
		I361			ILE	ILE
	I511	N362	M297	M297	GLY	GLY
K597	G512	R363	P298	P298	ARG	ARG
L598	D513	R364	K299	K299	T94	T94
R599	D514	N365			T95	T95
H600	E515	I443	F302	F302	D96	D96
	D516	I367	I303	I303	P97	P97
		R448	T304	T304	V98	V98
	L519	T449	L305	L305	ALA	ALA
	D525	I450	F306	F306	PRO	PRO
L607	T526	A370			R99	R99
R608	T527	K371	E310	E310	THR	THR
S609		A372	S311	S311	ALA	ALA
F610	P531	R373	D312	D312	THR	THR
L611	L532	A375	T314	T314	ALA	ALA
D612		K376	W315	W315	Y101	Y101
D613	A535	E378	F316	F316	M102	M102
	T536	N379	N317	N317	M105	M105
		I460	V380	V380	VAL	VAL
	L540	L463	A318	A318	GLY	GLY
	T544	R464	L320	L320	SER	SER
	V547	R465	A321	A321	GLU	GLU
		L466	L384	L384	GLN	GLN
		S467	R385	R385	ASP	ASP
		R468	L386	L386	ASP	ASP
	L551	Q469	K324	K324	ASP	ASP
	T552	M470	P325	P325	GLU	GLU
		L471	W326	W326	ASP	ASP
		K557	S327	S327	GLU	GLU
			I390	I390	ASP	ASP
					E124	E124

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.10Å 206.44Å 307.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.57 29.96 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.96-3.57) 92.1 (29.96-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.252 0.228 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55782	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4C6, 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	1.03	0/2524	1.26	12/3421 (0.4%)
1	B	1.15	9/1697 (0.5%)	1.34	14/2300 (0.6%)
1	G	1.02	1/1777 (0.1%)	1.25	8/2408 (0.3%)
1	H	1.11	3/1681 (0.2%)	1.34	16/2278 (0.7%)
2	C	1.12	18/10739 (0.2%)	1.27	73/14489 (0.5%)
2	I	1.01	9/10735 (0.1%)	1.25	59/14484 (0.4%)
3	D	1.19	16/9188 (0.2%)	1.32	68/12404 (0.5%)
3	J	1.04	16/9128 (0.2%)	1.28	63/12322 (0.5%)
4	E	0.89	0/693	1.12	2/935 (0.2%)
4	K	1.45	4/629 (0.6%)	1.37	2/847 (0.2%)
5	F	1.10	5/3864 (0.1%)	1.27	22/5194 (0.4%)
5	L	1.08	9/3872 (0.2%)	1.21	10/5205 (0.2%)
All	All	1.09	90/56527 (0.2%)	1.28	349/76287 (0.5%)

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

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

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1296	ASP	CG-OD2	10.00	1.44	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	799	ARG	CB-CG	-9.11	1.25	1.52
1	H	14	VAL	CA-CB	9.02	1.65	1.54
2	C	1112	ILE	CA-CB	-8.57	1.43	1.54
2	I	975	ILE	CA-CB	8.24	1.63	1.54
5	L	337	VAL	CA-CB	8.23	1.64	1.54
3	D	339	ARG	CZ-NH2	8.15	1.44	1.33
3	J	831	VAL	CA-CB	8.07	1.65	1.54
5	L	292	VAL	CA-CB	7.84	1.64	1.54
1	B	232	VAL	CA-CB	7.69	1.62	1.54
5	F	569	THR	CA-CB	7.44	1.66	1.53
4	K	36	ASP	CA-C	7.39	1.59	1.52
3	D	339	ARG	CB-CG	-7.24	1.30	1.52
3	J	208	THR	CA-CB	7.24	1.63	1.53
1	G	14	VAL	CA-CB	7.21	1.64	1.54
1	B	233	ASP	CA-CB	7.20	1.67	1.53
2	I	984	VAL	CA-CB	7.00	1.64	1.54
2	C	1096	ILE	CA-CB	-6.97	1.45	1.54
3	D	799	ARG	CG-CD	6.85	1.73	1.52
2	I	1269	ARG	NE-CZ	-6.77	1.25	1.33
1	B	232	VAL	CA-C	-6.72	1.44	1.52
5	F	476	ARG	CA-C	6.60	1.55	1.52
2	C	1255	THR	CA-C	-6.42	1.45	1.52
5	L	479	THR	CA-CB	6.37	1.62	1.53
2	I	488	MET	CA-C	6.37	1.58	1.52
1	H	134	THR	CA-CB	6.36	1.64	1.53
3	D	468	VAL	CA-CB	-6.33	1.45	1.54
3	J	917	VAL	CA-CB	-6.28	1.47	1.54
2	I	1003	THR	CA-CB	6.23	1.63	1.53
2	C	364	VAL	CA-CB	6.20	1.61	1.54
3	D	470	VAL	CA-C	-6.16	1.48	1.53
2	C	663	VAL	CA-CB	-6.11	1.46	1.54
2	C	1186	VAL	CA-CB	-6.11	1.46	1.54
3	J	470	VAL	CA-CB	-6.05	1.47	1.53
3	J	674	THR	CA-CB	6.04	1.61	1.53
5	L	582	VAL	CA-CB	6.03	1.61	1.53
2	C	839	VAL	CA-CB	-6.01	1.47	1.54
1	B	146	VAL	CA-CB	6.00	1.62	1.54
5	F	314	THR	CA-CB	5.96	1.63	1.53
3	J	212	THR	CA-CB	5.83	1.62	1.53
2	I	980	VAL	CA-CB	5.83	1.62	1.54
2	C	282	VAL	CA-CB	5.75	1.59	1.53
3	J	92	VAL	CA-CB	5.74	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	476	ARG	CA-C	5.72	1.55	1.52
4	K	66	VAL	CA-CB	5.68	1.61	1.54
3	D	470	VAL	CA-CB	-5.66	1.47	1.53
3	J	345	LYS	CE-NZ	-5.64	1.32	1.49
5	L	569	THR	CA-CB	5.61	1.62	1.53
5	L	347	ILE	CA-CB	5.58	1.61	1.54
3	J	853	THR	CA-CB	5.58	1.62	1.53
3	J	1253	ILE	CA-CB	-5.54	1.46	1.54
3	D	339	ARG	CG-CD	-5.53	1.35	1.52
2	I	594	VAL	CA-C	5.52	1.58	1.53
3	D	342	LEU	CA-C	-5.50	1.45	1.52
4	K	22	VAL	CA-CB	5.50	1.60	1.54
4	K	47	THR	CA-CB	5.44	1.62	1.53
3	J	317	THR	CA-CB	5.41	1.62	1.53
5	L	303	ILE	CA-CB	5.40	1.61	1.54
2	C	871	VAL	CA-CB	-5.39	1.49	1.54
3	D	1331	VAL	CA-C	-5.38	1.46	1.52
3	D	242	LEU	C-O	-5.37	1.20	1.25
2	C	717	VAL	CA-CB	-5.35	1.48	1.54
1	B	111	THR	CA-CB	5.35	1.60	1.53
1	B	153	VAL	CA-CB	5.34	1.60	1.54
1	B	182	ARG	CA-C	5.33	1.59	1.52
3	D	731	ARG	CA-C	-5.31	1.46	1.52
1	H	107	ILE	CA-CB	5.31	1.59	1.53
3	J	682	VAL	CA-CB	5.29	1.61	1.54
2	C	261	VAL	CA-CB	5.28	1.59	1.53
2	C	1320	PRO	CA-C	-5.28	1.45	1.52
1	B	173	VAL	CA-CB	5.27	1.64	1.55
2	C	724	VAL	CA-CB	-5.26	1.47	1.54
3	D	1287	ILE	CA-CB	5.25	1.61	1.54
3	J	354	VAL	CA-CB	-5.23	1.48	1.54
2	C	833	ILE	CA-CB	-5.18	1.47	1.54
3	D	1253	ILE	CA-CB	-5.18	1.47	1.54
3	J	208	THR	CA-C	5.18	1.59	1.52
1	B	125	LYS	CA-C	5.18	1.58	1.52
3	D	1177	ILE	CA-CB	5.18	1.60	1.54
2	C	496	LYS	CA-C	5.17	1.57	1.52
2	I	1269	ARG	N-CA	-5.16	1.39	1.46
2	C	87	ILE	CA-CB	-5.13	1.48	1.54
3	J	1287	ILE	CA-CB	5.12	1.61	1.54
2	C	1255	THR	CA-CB	-5.12	1.46	1.53
3	D	607	THR	CA-CB	-5.08	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	127	ILE	CA-CB	5.08	1.60	1.54
5	F	296	LYS	CA-C	5.05	1.59	1.53
2	C	170	VAL	CA-CB	5.04	1.61	1.54
3	J	705	THR	CA-CB	5.02	1.61	1.53
5	L	319	ALA	CA-C	5.02	1.59	1.52

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ALA	CA-C-N	-12.96	103.64	119.84
3	D	426	ALA	C-N-CA	-12.96	103.64	119.84
2	C	920	VAL	CA-C-N	11.63	131.74	119.76
2	C	920	VAL	C-N-CA	11.63	131.74	119.76
3	D	833	GLU	CA-C-N	11.32	131.08	120.21
3	D	833	GLU	C-N-CA	11.32	131.08	120.21
5	F	600	HIS	CA-C-N	-9.94	110.35	120.98
5	F	600	HIS	C-N-CA	-9.94	110.35	120.98
3	J	426	ALA	CA-C-N	-9.94	107.87	120.79
3	J	426	ALA	C-N-CA	-9.94	107.87	120.79
2	I	812	PHE	N-CA-C	9.74	121.85	111.03
1	B	108	GLY	CA-C-N	9.14	129.71	119.93
1	B	108	GLY	C-N-CA	9.14	129.71	119.93
1	H	10	LYS	CA-C-N	9.05	131.15	119.84
1	H	10	LYS	C-N-CA	9.05	131.15	119.84
3	J	253	VAL	CA-C-N	8.98	128.92	120.03
3	J	253	VAL	C-N-CA	8.98	128.92	120.03
3	D	368	LEU	CA-C-N	8.90	128.98	119.90
3	D	368	LEU	C-N-CA	8.90	128.98	119.90
3	J	1266	ILE	N-CA-C	8.87	119.71	110.05
2	C	559	CYS	CA-C-N	8.84	128.49	119.56
2	C	559	CYS	C-N-CA	8.84	128.49	119.56
5	L	96	ASP	CA-C-N	8.78	130.81	119.84
5	L	96	ASP	C-N-CA	8.78	130.81	119.84
2	I	1269	ARG	CD-NE-CZ	8.69	136.57	124.40
2	I	374	GLU	CA-C-N	8.64	129.28	120.38
2	I	374	GLU	C-N-CA	8.64	129.28	120.38
1	H	172	LEU	N-CA-C	8.52	122.73	109.96
2	C	1157	GLN	N-CA-C	8.46	120.27	111.14
3	D	470	VAL	N-CA-C	8.41	116.26	107.76
3	J	419	HIS	CA-C-N	8.32	128.35	119.78
3	J	419	HIS	C-N-CA	8.32	128.35	119.78
3	J	497	GLU	CA-C-N	8.24	128.73	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	497	GLU	C-N-CA	8.24	128.73	119.83
5	L	489	MET	CA-C-N	8.14	130.02	119.84
5	L	489	MET	C-N-CA	8.14	130.02	119.84
2	I	98	VAL	N-CA-C	8.11	119.79	108.12
2	I	1262	LYS	N-CA-C	-7.99	102.85	112.59
3	D	1152	GLU	CA-C-N	7.87	127.83	120.03
3	D	1152	GLU	C-N-CA	7.87	127.83	120.03
3	J	1149	ARG	CA-C-N	7.75	128.19	120.52
3	J	1149	ARG	C-N-CA	7.75	128.19	120.52
3	D	1240	VAL	N-CA-C	7.70	117.77	110.53
3	D	799	ARG	N-CA-C	-7.69	101.88	111.11
3	D	1296	GLY	N-CA-C	-7.68	103.34	112.64
3	J	470	VAL	N-CA-C	7.66	115.50	107.76
3	D	469	HIS	CA-C-N	-7.54	117.16	122.59
3	D	469	HIS	C-N-CA	-7.54	117.16	122.59
2	C	1180	MET	CA-C-N	7.53	127.97	119.83
2	C	1180	MET	C-N-CA	7.53	127.97	119.83
3	D	515	ARG	N-CA-C	-7.50	97.67	109.07
3	D	587	LEU	CA-C-N	7.43	128.02	120.14
3	D	587	LEU	C-N-CA	7.43	128.02	120.14
2	C	1319	MET	N-CA-C	7.34	121.41	110.32
2	C	746	ALA	CB-CA-C	-7.34	108.10	116.54
2	I	929	ILE	N-CA-C	7.33	120.21	113.10
5	F	489	MET	CA-C-N	7.26	128.91	119.84
5	F	489	MET	C-N-CA	7.26	128.91	119.84
3	D	799	ARG	CB-CG-CD	7.15	127.74	111.30
1	A	212	ASP	CA-C-N	7.14	128.76	119.84
1	A	212	ASP	C-N-CA	7.14	128.76	119.84
2	C	717	VAL	N-CA-C	7.07	118.47	108.36
4	K	66	VAL	N-CA-C	7.05	117.84	110.72
5	F	530	LEU	CA-C-N	7.02	126.85	119.05
5	F	530	LEU	C-N-CA	7.02	126.85	119.05
3	J	506	VAL	N-CA-C	7.02	117.81	110.72
3	D	490	ILE	N-CA-C	-7.00	105.80	113.43
1	G	21	SER	N-CA-C	-6.99	103.72	111.82
3	D	80	HIS	CA-C-N	-6.96	113.14	121.90
3	D	80	HIS	C-N-CA	-6.96	113.14	121.90
5	F	244	THR	N-CA-C	-6.94	104.78	113.18
5	F	137	TYR	CA-C-N	6.94	126.19	118.97
5	F	137	TYR	C-N-CA	6.94	126.19	118.97
2	C	490	GLN	N-CA-C	-6.91	106.75	114.62
3	J	515	ARG	N-CA-C	-6.91	98.52	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	752	GLY	N-CA-C	-6.90	104.98	114.64
2	I	1180	MET	CA-C-N	6.87	127.25	119.83
2	I	1180	MET	C-N-CA	6.87	127.25	119.83
2	I	1241	ASP	N-CA-C	-6.87	104.90	113.55
1	H	178	SER	CA-C-N	6.86	126.49	119.56
1	H	178	SER	C-N-CA	6.86	126.49	119.56
3	D	239	LEU	N-CA-C	6.85	119.73	109.25
3	J	177	ASP	N-CA-C	6.83	120.78	108.69
3	D	257	GLY	N-CA-C	-6.80	105.50	115.30
3	D	253	VAL	CA-C-N	6.79	127.33	120.14
3	D	253	VAL	C-N-CA	6.79	127.33	120.14
1	B	150	ARG	N-CA-C	-6.76	102.29	111.55
1	B	28	LEU	N-CA-C	6.75	118.51	107.23
2	C	206	ALA	N-CA-C	6.74	119.49	111.33
1	B	8	PHE	N-CA-C	6.72	119.37	109.69
2	I	818	VAL	N-CA-C	6.72	118.16	108.48
5	L	137	TYR	CA-C-N	6.72	125.96	118.97
5	L	137	TYR	C-N-CA	6.72	125.96	118.97
1	G	180	VAL	N-CA-C	6.70	118.46	108.54
2	C	800	MET	N-CA-C	6.69	119.11	109.14
2	C	518	ASN	N-CA-C	-6.67	104.45	112.59
2	C	109	ALA	CA-C-N	-6.65	112.05	120.23
2	C	109	ALA	C-N-CA	-6.65	112.05	120.23
2	C	1241	ASP	N-CA-C	-6.63	105.72	113.88
2	I	223	LEU	N-CA-C	6.61	118.28	111.14
2	I	965	GLN	N-CA-C	6.61	118.28	111.14
3	J	817	HIS	N-CA-C	-6.58	105.25	113.28
1	B	151	GLY	N-CA-C	6.57	122.30	111.59
2	I	1269	ARG	NE-CZ-NH1	6.54	128.04	121.50
2	I	1295	SER	N-CA-C	6.51	124.66	110.80
3	D	45	ASN	N-CA-C	6.50	119.36	111.82
2	I	1335	ILE	N-CA-C	6.43	117.56	108.36
2	I	742	TYR	CA-C-N	6.37	125.60	118.97
2	I	742	TYR	C-N-CA	6.37	125.60	118.97
2	C	1161	LEU	CA-CB-CG	-6.37	94.01	116.30
2	C	812	PHE	N-CA-C	6.36	118.09	111.03
3	J	1246	VAL	N-CA-C	6.36	117.07	108.17
1	B	183	ILE	N-CA-C	6.36	117.27	108.12
1	A	289	LEU	N-CA-C	6.35	121.16	113.41
3	J	206	ASN	N-CA-C	6.33	118.26	111.36
2	C	218	GLU	N-CA-C	6.30	117.95	111.14
3	D	1308	GLY	N-CA-C	-6.26	104.73	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1112	ILE	N-CA-C	6.26	116.89	110.82
1	B	153	VAL	N-CA-C	6.23	114.83	107.73
3	J	587	LEU	CA-C-N	6.22	126.74	120.14
3	J	587	LEU	C-N-CA	6.22	126.74	120.14
2	C	1208	GLY	N-CA-C	-6.22	107.38	115.59
3	D	799	ARG	CA-CB-CG	6.22	126.54	114.10
1	H	149	GLY	N-CA-C	6.21	120.17	110.91
2	I	127	ILE	CA-C-N	6.21	127.06	120.11
2	I	127	ILE	C-N-CA	6.21	127.06	120.11
2	C	34	SER	N-CA-C	6.20	117.70	111.07
3	D	358	GLY	CA-C-N	6.19	125.89	119.82
3	D	358	GLY	C-N-CA	6.19	125.89	119.82
3	J	611	ILE	CB-CA-C	-6.19	105.54	111.05
3	D	1230	THR	N-CA-C	-6.17	104.56	111.28
5	F	96	ASP	CA-C-N	6.15	127.53	119.84
5	F	96	ASP	C-N-CA	6.15	127.53	119.84
3	D	852	GLY	N-CA-C	-6.15	103.17	112.89
3	J	358	GLY	CA-C-N	6.15	126.27	119.87
3	J	358	GLY	C-N-CA	6.15	126.27	119.87
2	I	1316	GLU	CA-C-N	6.13	127.50	119.84
2	I	1316	GLU	C-N-CA	6.13	127.50	119.84
2	I	24	VAL	CA-C-N	-6.09	114.37	120.21
2	I	24	VAL	C-N-CA	-6.09	114.37	120.21
3	J	368	LEU	CA-C-N	6.08	126.43	119.93
3	J	368	LEU	C-N-CA	6.08	126.43	119.93
2	C	375	PRO	N-CA-C	6.06	118.10	110.70
3	J	343	LEU	N-CA-C	6.06	118.78	110.24
2	C	652	TYR	N-CA-C	6.05	117.39	108.86
2	I	1266	GLY	N-CA-C	-6.05	104.97	111.93
3	D	1293	GLU	N-CA-C	6.04	114.55	108.75
4	E	14	GLY	N-CA-C	6.04	120.50	112.77
3	J	645	VAL	N-CA-C	6.03	117.46	108.23
1	G	64	VAL	N-CA-C	6.02	116.96	108.17
2	C	375	PRO	CA-C-N	6.02	125.93	119.85
2	C	375	PRO	C-N-CA	6.02	125.93	119.85
2	I	1242	LYS	N-CA-C	6.00	119.79	112.23
2	C	1333	LEU	N-CA-C	-5.99	102.76	110.19
2	C	1103	VAL	CA-C-N	-5.97	112.38	119.84
2	C	1103	VAL	C-N-CA	-5.97	112.38	119.84
3	J	130	MET	CA-C-N	5.97	126.31	119.92
3	J	130	MET	C-N-CA	5.97	126.31	119.92
2	C	1281	TYR	N-CA-C	-5.95	102.14	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	GLU	N-CA-C	-5.95	104.88	111.36
3	J	483	LEU	N-CA-C	-5.93	105.12	112.72
3	D	1211	SER	N-CA-C	-5.93	99.52	107.88
1	A	142	MET	N-CA-C	5.88	118.05	108.76
3	J	657	ALA	CA-C-N	5.87	129.24	120.31
3	J	657	ALA	C-N-CA	5.87	129.24	120.31
3	D	755	ILE	N-CA-C	5.87	117.19	109.21
1	B	106	GLY	N-CA-C	5.86	119.20	111.70
3	J	1161	GLY	N-CA-C	5.85	118.01	112.04
1	A	8	PHE	N-CA-C	5.85	117.86	109.14
2	I	1157	GLN	N-CA-C	5.85	117.33	111.07
2	I	976	ARG	N-CA-C	5.84	117.72	111.36
2	C	699	LEU	N-CA-C	-5.83	105.00	111.36
2	C	453	ILE	N-CA-C	5.83	116.26	107.80
2	C	1046	VAL	N-CA-C	5.83	116.51	107.99
2	C	64	GLY	N-CA-C	-5.83	106.46	115.73
2	C	112	GLY	N-CA-C	-5.83	104.03	110.96
2	I	484	LEU	CA-CB-CG	5.82	136.69	116.30
3	D	1273	ASP	N-CA-C	5.81	119.89	113.21
5	F	499	LYS	N-CA-C	5.81	117.41	111.14
2	I	1281	TYR	N-CA-C	-5.81	102.99	110.19
3	J	362	ARG	N-CA-C	-5.80	102.31	110.50
3	J	611	ILE	N-CA-C	5.80	116.21	111.62
1	B	205	MET	N-CA-C	5.80	118.22	109.23
1	A	292	THR	CA-C-N	5.80	127.09	119.84
1	A	292	THR	C-N-CA	5.80	127.09	119.84
3	D	524	GLY	N-CA-C	5.80	123.07	115.36
3	D	258	GLY	N-CA-C	5.80	123.07	115.36
5	L	483	LEU	CA-C-N	5.79	128.62	120.28
5	L	483	LEU	C-N-CA	5.79	128.62	120.28
3	J	1210	ILE	N-CA-C	-5.79	107.10	112.83
3	D	1162	ILE	N-CA-C	5.79	117.08	109.21
3	D	858	VAL	CA-C-N	5.77	127.05	119.84
3	D	858	VAL	C-N-CA	5.77	127.05	119.84
3	J	203	GLU	N-CA-C	5.76	117.36	111.14
2	C	496	LYS	CA-C-N	5.76	125.44	119.05
2	C	496	LYS	C-N-CA	5.76	125.44	119.05
3	D	470	VAL	CB-CA-C	-5.76	104.55	110.71
2	I	703	GLY	N-CA-C	-5.75	107.64	114.48
3	D	339	ARG	CB-CG-CD	5.73	124.47	111.30
3	J	775	SER	CA-C-N	5.71	127.87	120.44
3	J	775	SER	C-N-CA	5.71	127.87	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	280	LYS	N-CA-C	-5.71	104.42	111.33
3	D	844	THR	N-CA-C	5.71	118.52	109.96
2	I	746	ALA	CB-CA-C	-5.71	109.98	116.54
2	C	110	PRO	N-CA-C	-5.70	101.55	110.50
5	F	460	ILE	N-CA-C	5.68	115.88	110.42
2	I	375	PRO	N-CA-C	5.68	117.63	110.70
1	B	113	ALA	N-CA-C	-5.67	106.32	113.18
2	C	746	ALA	N-CA-C	5.67	116.92	108.31
3	J	1162	ILE	N-CA-C	5.67	116.92	109.21
4	E	15	ASN	N-CA-C	5.66	118.18	111.33
2	C	806	PRO	CA-C-O	-5.66	115.33	121.27
3	J	67	ASP	N-CA-C	5.66	118.56	110.24
5	F	583	THR	N-CA-C	5.65	118.00	109.41
3	D	293	ARG	N-CA-C	-5.65	104.76	111.03
2	I	1298	VAL	N-CA-C	-5.65	104.86	110.62
1	A	44	ARG	N-CA-C	-5.64	105.28	111.82
1	H	135	ASP	N-CA-C	5.63	118.15	110.55
3	D	1375	ALA	N-CA-C	5.63	115.67	108.24
3	D	339	ARG	CA-CB-CG	-5.63	102.85	114.10
1	H	53	GLY	N-CA-C	5.63	121.58	110.83
2	I	1264	GLN	N-CA-C	-5.63	101.05	109.15
3	J	1278	GLU	N-CA-C	5.61	117.71	109.24
2	C	804	PHE	N-CA-C	5.58	117.39	108.41
2	C	818	VAL	N-CA-C	5.58	116.51	108.48
3	D	339	ARG	CB-CA-C	-5.58	99.33	110.42
1	H	218	ARG	N-CA-C	-5.57	104.42	111.11
1	A	323	PRO	CA-C-O	-5.57	115.28	122.13
2	C	287	VAL	CA-C-N	5.55	125.75	120.31
2	C	287	VAL	C-N-CA	5.55	125.75	120.31
3	D	527	LEU	N-CA-C	5.54	118.26	109.50
2	C	560	PRO	CA-C-N	-5.54	115.58	121.84
2	C	560	PRO	C-N-CA	-5.54	115.58	121.84
2	C	865	LEU	N-CA-C	5.54	118.52	109.59
2	I	490	GLN	N-CA-C	-5.54	108.30	114.62
2	I	734	ILE	N-CA-C	5.54	115.83	107.80
3	D	746	LEU	N-CA-C	-5.52	100.18	109.07
1	H	94	GLY	N-CA-C	-5.52	107.05	115.66
2	I	182	SER	N-CA-C	5.51	118.27	110.50
2	C	98	VAL	N-CA-C	5.51	115.82	108.11
2	I	1263	ALA	N-CA-C	-5.50	106.95	113.38
2	C	649	GLN	N-CA-C	-5.49	106.42	114.39
3	J	1273	ASP	N-CA-C	5.48	116.99	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	854	ALA	N-CA-C	-5.47	106.98	113.38
3	J	245	LEU	CA-C-N	5.47	126.01	120.38
3	J	245	LEU	C-N-CA	5.47	126.01	120.38
1	H	29	GLU	C-N-CD	-5.47	108.58	120.60
3	D	250	ARG	CA-C-N	5.44	125.44	120.21
3	D	250	ARG	C-N-CA	5.44	125.44	120.21
3	J	1344	LEU	CA-CB-CG	-5.44	97.25	116.30
1	G	165	GLU	N-CA-C	-5.44	107.21	112.97
5	L	477	GLU	CA-C-N	5.44	125.45	119.90
5	L	477	GLU	C-N-CA	5.44	125.45	119.90
3	J	737	ILE	N-CA-C	-5.44	104.65	110.36
2	C	6	THR	N-CA-C	-5.42	106.25	112.92
2	I	1320	PRO	CA-C-O	-5.42	115.16	121.34
3	D	497	GLU	CA-C-N	5.40	125.66	119.83
3	D	497	GLU	C-N-CA	5.40	125.66	119.83
3	D	1239	ASP	N-CA-C	-5.39	104.64	111.11
3	J	1296	GLY	N-CA-C	-5.39	106.12	112.64
3	J	1266	ILE	CB-CA-C	-5.38	105.67	111.59
2	C	145	ILE	N-CA-C	5.38	115.33	107.37
2	C	354	ASP	CA-C-N	5.37	125.46	119.87
2	C	354	ASP	C-N-CA	5.37	125.46	119.87
3	D	501	VAL	N-CA-C	5.37	114.87	108.96
3	J	347	VAL	N-CA-C	5.36	116.00	108.17
3	J	477	GLN	N-CA-C	-5.36	105.51	111.36
3	J	487	THR	N-CA-C	5.36	118.92	112.38
5	F	373	ARG	N-CA-C	-5.35	105.34	111.07
2	I	571	LEU	N-CA-C	-5.34	106.61	113.02
2	I	612	GLY	N-CA-C	5.34	119.10	112.64
5	F	292	VAL	N-CA-C	5.34	116.00	110.82
2	I	854	ILE	N-CA-C	5.34	113.96	107.61
5	F	492	ASP	N-CA-C	-5.33	106.62	113.23
1	G	51	MET	CA-C-N	5.33	125.58	119.83
1	G	51	MET	C-N-CA	5.33	125.58	119.83
2	C	566	GLY	CA-C-N	5.32	124.99	119.56
2	C	566	GLY	C-N-CA	5.32	124.99	119.56
2	C	657	THR	N-CA-C	-5.29	106.09	112.54
3	D	176	PHE	N-CA-C	-5.27	100.02	108.55
3	D	825	VAL	N-CA-C	5.26	118.49	111.44
2	C	1151	LEU	CA-CB-CG	-5.26	97.88	116.30
5	F	606	VAL	N-CA-C	5.26	115.36	110.42
1	B	9	LEU	N-CA-C	5.26	117.09	108.52
2	I	345	PRO	CA-C-O	-5.26	117.42	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1326	LEU	N-CA-C	-5.26	105.63	111.36
3	J	1261	LEU	N-CA-C	-5.26	105.10	112.25
1	H	78	ILE	N-CA-C	5.25	115.98	110.62
3	J	609	TYR	N-CA-C	-5.24	105.47	111.07
2	I	747	GLY	N-CA-C	5.24	121.80	112.22
2	I	800	MET	N-CA-C	5.23	116.76	108.96
3	J	271	ARG	N-CA-C	5.23	117.66	111.33
2	C	664	GLY	N-CA-C	-5.23	106.44	112.50
1	B	198	LEU	N-CA-C	-5.23	102.17	109.69
3	J	894	VAL	N-CA-C	5.23	115.65	108.12
2	C	747	GLY	N-CA-C	5.22	125.56	113.18
2	I	1271	GLY	N-CA-C	5.21	120.60	112.31
2	C	113	THR	N-CA-C	5.21	117.89	109.40
1	B	155	ALA	N-CA-C	-5.20	105.79	111.82
2	C	1184	THR	CA-C-N	-5.20	114.29	120.11
2	C	1184	THR	C-N-CA	-5.20	114.29	120.11
2	I	1296	ASP	CA-C-O	5.20	125.57	119.28
3	D	365	GLN	N-CA-C	5.20	116.19	108.86
2	C	82	VAL	N-CA-C	5.19	115.33	110.30
1	G	13	LEU	N-CA-C	5.19	117.19	109.25
2	I	1139	ALA	N-CA-C	5.18	116.62	110.97
2	C	532	ALA	N-CA-C	-5.18	106.80	113.02
1	H	113	ALA	N-CA-C	-5.17	106.92	113.18
3	D	128	LEU	N-CA-C	-5.17	106.97	113.28
2	I	456	VAL	N-CA-C	5.17	115.79	110.36
2	C	73	TYR	N-CA-C	5.17	117.04	109.24
2	C	661	VAL	N-CA-C	5.16	120.07	109.34
5	F	507	MET	N-CA-C	-5.15	105.78	111.71
1	A	301	THR	CA-C-N	5.14	127.16	120.28
1	A	301	THR	C-N-CA	5.14	127.16	120.28
4	K	22	VAL	N-CA-C	5.12	115.34	110.42
3	J	1174	ARG	N-CA-C	5.12	117.65	110.23
3	J	1151	LYS	N-CA-C	5.12	116.67	111.14
1	H	28	LEU	N-CA-C	5.12	116.65	107.80
3	J	797	THR	N-CA-C	-5.10	105.72	111.28
3	D	548	VAL	N-CA-C	5.09	115.07	108.35
3	J	99	ARG	N-CA-C	-5.09	107.10	113.72
5	F	505	ILE	N-CA-C	5.08	116.67	108.85
2	I	110	PRO	CA-C-O	-5.07	114.98	120.92
3	D	253	VAL	N-CA-C	5.07	119.83	108.88
3	D	1293	GLU	CB-CA-C	-5.07	109.08	116.53
3	J	231	GLY	N-CA-C	-5.07	101.18	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1067	ALA	N-CA-C	5.06	116.76	108.76
2	C	1041	ASP	N-CA-C	5.06	116.99	109.25
2	I	1184	THR	CA-C-N	-5.06	114.44	120.11
2	I	1184	THR	C-N-CA	-5.06	114.44	120.11
3	D	320	ASN	N-CA-C	-5.05	100.94	109.07
2	I	1222	GLU	N-CA-C	-5.05	103.12	110.24
2	C	223	LEU	N-CA-C	5.05	117.56	111.40
2	C	1075	VAL	N-CA-C	5.05	115.31	107.28
1	H	151	GLY	N-CA-C	5.05	119.82	111.59
3	D	50	LYS	CA-C-N	5.05	125.20	119.90
3	D	50	LYS	C-N-CA	5.05	125.20	119.90
1	G	177	TYR	CA-CB-CG	5.05	122.98	113.90
1	A	13	LEU	N-CA-C	5.04	116.73	108.52
2	C	551	HIS	CA-C-N	5.03	125.31	119.47
2	C	551	HIS	C-N-CA	5.03	125.31	119.47
5	F	514	ASP	CA-C-N	5.03	129.37	120.87
5	F	514	ASP	C-N-CA	5.03	129.37	120.87
2	C	1054	LEU	N-CA-C	5.03	118.01	109.76
1	H	40	GLY	N-CA-C	5.02	118.33	112.50
2	I	237	LEU	N-CA-C	5.01	121.48	110.80
2	I	1097	VAL	N-CA-C	5.01	113.96	106.85
2	I	109	ALA	N-CA-C	5.00	117.41	109.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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	208	0
1	B	1677	0	1703	108	0
1	G	1755	0	1773	126	0
1	H	1662	0	1687	135	0
2	C	10570	0	10582	636	0
2	I	10566	0	10576	647	0
3	D	9050	0	9218	670	0
3	J	8990	0	9173	615	0
4	E	691	0	695	25	0
4	K	627	0	634	47	0
5	F	3813	0	3880	216	0
5	L	3821	0	3884	258	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	0	25	1	0
8	J	31	0	25	2	0
All	All	55782	0	56397	3392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (3392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.29	1.14
1:A:45:ARG:HG2	1:B:38:THR:HB	1.31	1.12
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.30	1.08
2:I:1269:ARG:HD3	3:J:343:LEU:HD21	1.35	1.08
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.17	1.07
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.33	1.06
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.39	1.04
1:G:12:ARG:H	1:G:30:PRO:HD2	1.24	1.02
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.40	1.00
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.23	0.99
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.45	0.99
1:A:156:SER:HB3	2:C:1059:ARG:HH22	1.30	0.96
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.47	0.96
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.48	0.95
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.46	0.94
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.49	0.94
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.13	0.94
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.48	0.94
2:C:324:LYS:O	2:C:327:GLN:NE2	1.99	0.93
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.50	0.93
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.49	0.93
2:I:17:LYS:HZ1	2:I:1154:ASP:HB3	1.30	0.92
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.05	0.92
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.52	0.92
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.47	0.92
1:G:45:ARG:HG2	1:H:38:THR:HB	1.51	0.92
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.49	0.92
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.52	0.92
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.51	0.91
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.53	0.91
1:G:187:VAL:HG12	1:G:201:LEU:HD13	1.52	0.90
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.53	0.90
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.07	0.90
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.37	0.90
2:I:148:GLN:NE2	2:I:535:PRO:O	2.04	0.89
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.54	0.89
3:D:156:ARG:NH2	3:D:191:SER:OG	2.05	0.89
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.55	0.88
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.87	0.88
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.54	0.87
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.54	0.87
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.08	0.87
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.56	0.87
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.38	0.87
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.55	0.87
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.55	0.86
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1269:ARG:CD	3:J:343:LEU:HD21	2.05	0.86
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.58	0.86
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.41	0.86
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.41	0.86
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.38	0.86
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.41	0.86
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.57	0.86
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.57	0.86
1:H:9:LEU:HD12	1:H:195:ARG:HH21	1.41	0.86
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.11	0.86
2:I:1296:ASP:OD2	2:I:1322:SER:N	2.08	0.85
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.58	0.85
1:A:77:ASP:OD1	1:A:77:ASP:N	2.09	0.85
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.10	0.85
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.38	0.85
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.40	0.85
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.38	0.85
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.59	0.85
3:D:339:ARG:HD3	3:D:798:ARG:HH11	1.42	0.84
3:D:418:GLU:HG3	4:E:45:LYS:H	1.40	0.84
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.60	0.84
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.49	0.84
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.59	0.84
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.58	0.84
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.59	0.84
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.56	0.84
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.58	0.84
1:A:296:GLY:H	1:A:299:SER:HB2	1.43	0.84
1:B:102:LEU:O	1:B:141:SER:HA	1.78	0.83
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.60	0.83
1:A:133:LEU:HD21	1:A:140:ILE:HD11	1.59	0.83
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.59	0.83
2:C:810:TYR:HE1	2:C:1078:LYS:HZ3	1.24	0.83
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.59	0.83
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.42	0.83
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.60	0.83
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.12	0.83
3:D:128:LEU:HA	3:D:192:MET:HE1	1.59	0.83
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.60	0.82
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.44	0.82
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.60	0.82
3:D:425:ARG:HG2	3:D:426:ALA:H	1.42	0.82
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.61	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.25	0.82
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.59	0.82
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.61	0.82
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	1.93	0.82
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.14	0.82
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.13	0.82
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.13	0.82
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.60	0.81
5:L:316:PHE:HZ	5:L:334:SER:HA	1.44	0.81
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.63	0.81
2:C:703:GLY:N	2:C:705:GLU:OE2	2.11	0.81
3:D:317:THR:HG22	3:D:322:ARG:O	1.81	0.81
2:I:30:ILE:HD12	2:I:30:ILE:H	1.44	0.81
1:G:166:ARG:HH11	1:G:168:ILE:HG12	1.46	0.81
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.63	0.81
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.62	0.80
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.16	0.80
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.61	0.80
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.14	0.80
2:I:17:LYS:NZ	2:I:1154:ASP:HB3	1.96	0.80
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.62	0.80
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.61	0.80
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.28	0.80
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.64	0.80
1:G:229:GLU:HA	1:G:231:PHE:CE2	2.17	0.80
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.64	0.80
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.64	0.80
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.62	0.80
3:D:339:ARG:HD2	3:D:798:ARG:HD3	1.64	0.79
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.64	0.79
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.28	0.79
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.63	0.79
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.62	0.79
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.64	0.79
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.63	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.64	0.79
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:LEU:HA	3:J:192:MET:HE1	1.65	0.79
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.64	0.78
2:I:600:THR:HG21	2:I:602:GLU:HG2	1.63	0.78
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.63	0.78
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.16	0.78
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.12	0.78
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.17	0.78
1:A:166:ARG:O	1:A:168:ILE:N	2.17	0.78
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.19	0.78
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.16	0.78
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.66	0.78
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.64	0.78
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.66	0.78
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.17	0.78
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.66	0.77
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	1.98	0.77
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.00	0.77
3:J:722:ILE:HA	3:J:725:MET:HE3	1.66	0.77
1:H:98:VAL:HG21	1:H:121:VAL:HG23	1.67	0.77
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.49	0.77
5:F:281:ARG:O	5:F:285:ARG:HG3	1.85	0.77
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.65	0.77
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.66	0.77
2:I:227:LYS:O	2:I:245:ARG:NH2	2.18	0.77
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.67	0.76
1:G:218:ARG:NH1	1:H:231:PHE:O	2.18	0.76
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.67	0.76
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.20	0.76
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.66	0.76
2:I:170:VAL:HG21	2:I:172:TYR:CZ	2.20	0.76
1:H:61:ILE:HB	1:H:64:VAL:O	1.85	0.76
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.67	0.76
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.67	0.76
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.14	0.76
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.76
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.67	0.76
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.66	0.76
3:J:425:ARG:HG2	3:J:426:ALA:H	1.51	0.76
3:D:414:GLU:O	4:E:45:LYS:NZ	2.18	0.75
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.68	0.75
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:TYR:HD1	2:C:112:GLY:H	1.31	0.75
3:D:844:THR:OG1	3:D:860:ARG:O	2.02	0.75
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.51	0.75
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.21	0.75
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.52	0.75
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.68	0.75
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.67	0.75
2:I:724:VAL:HG23	2:I:775:GLU:H	1.52	0.75
1:A:92:VAL:O	1:A:148:ARG:NH1	2.18	0.75
3:D:1191:PRO:HB3	3:D:1194:ARG:HH11	1.52	0.75
3:D:1320:ILE:HG23	8:D:2004:4C6:H9	1.68	0.75
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.69	0.75
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.68	0.75
5:F:547:VAL:HG13	5:F:598:LEU:HD22	1.69	0.75
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.16	0.75
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.67	0.75
1:H:108:GLY:O	1:H:133:LEU:HB2	1.86	0.74
1:A:115:ILE:HG22	1:A:116:THR:H	1.52	0.74
3:J:201:LEU:O	3:J:217:LEU:HD11	1.87	0.74
1:A:49:SER:OG	1:A:50:SER:N	2.17	0.74
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.69	0.74
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.18	0.74
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.68	0.74
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.50	0.74
3:D:1345:ARG:HG2	3:D:1370:MET:HE1	1.68	0.74
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.23	0.74
3:J:747:MET:HE2	3:J:775:SER:HA	1.68	0.74
2:I:892:GLU:OE2	3:J:66:LYS:NZ	2.19	0.74
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.68	0.74
5:L:281:ARG:O	5:L:285:ARG:HG3	1.88	0.74
1:A:76:GLU:N	1:A:76:GLU:OE2	2.21	0.74
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.69	0.74
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.53	0.74
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.70	0.73
3:D:722:ILE:HA	3:D:725:MET:HE3	1.70	0.73
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.52	0.73
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.52	0.73
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.23	0.73
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.68	0.73
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.70	0.73
3:J:846:GLU:HA	3:J:860:ARG:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.16	0.73
2:C:1281:TYR:CE2	3:D:431:ARG:HB2	2.23	0.73
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.70	0.73
3:D:392:THR:HG21	5:F:606:VAL:HA	1.69	0.73
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.24	0.73
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.23	0.73
2:C:197:ARG:NH1	2:C:201:ARG:O	2.21	0.73
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.71	0.73
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.70	0.73
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.53	0.73
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.15	0.73
3:J:19:ALA:HB2	3:J:1373:ARG:HH22	1.53	0.73
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.18	0.73
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.69	0.73
2:I:600:THR:HG22	2:I:602:GLU:H	1.53	0.73
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.70	0.73
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.54	0.72
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.19	0.72
3:D:1227:HIS:HB2	3:J:1293:GLU:CD	2.14	0.72
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.71	0.72
3:J:708:ASN:HB3	3:J:712:GLN:O	1.87	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.21	0.72
3:D:860:ARG:HB3	3:D:860:ARG:HH11	1.55	0.72
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.22	0.72
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.54	0.72
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.71	0.72
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.52	0.72
1:G:75:GLN:HA	2:I:729:ALA:N	2.05	0.72
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.24	0.72
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.72
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.70	0.72
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.23	0.72
1:H:51:MET:HB3	1:H:178:SER:HB2	1.71	0.72
1:H:101:THR:H	1:H:116:THR:HG22	1.54	0.72
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.53	0.72
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.72	0.72
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.54	0.72
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.54	0.72
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.72	0.72
2:C:201:ARG:NH2	2:C:370:MET:O	2.21	0.72
1:G:12:ARG:N	1:G:30:PRO:HD2	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:CD	1:A:143:ARG:HH21	1.96	0.71
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.72	0.71
1:H:18:GLN:HA	1:H:24:ALA:HA	1.72	0.71
1:A:73:GLY:O	1:A:134:THR:HG22	1.89	0.71
1:A:190:ALA:HB2	1:A:200:LYS:HE3	1.71	0.71
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.73	0.71
3:D:515:ARG:NH2	3:D:717:VAL:O	2.23	0.71
5:F:311:THR:HG21	5:F:348:GLU:OE2	1.91	0.71
1:G:61:ILE:HG22	1:G:62:ASP:H	1.55	0.71
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.72	0.71
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.72	0.71
5:F:354:THR:O	5:F:358:VAL:HG23	1.91	0.71
5:F:532:LEU:O	5:F:536:THR:HG23	1.91	0.71
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.24	0.71
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.71	0.71
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.71	0.71
2:I:963:GLU:O	2:I:967:LEU:HB2	1.91	0.71
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.72	0.71
3:D:707:ILE:HD12	3:D:707:ILE:H	1.56	0.71
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.53	0.71
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.72	0.71
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.55	0.70
1:A:158:ARG:NH2	1:A:172:LEU:HB3	2.05	0.70
2:I:123:TYR:OH	2:I:126:GLU:HG3	1.91	0.70
3:J:70:CYS:SG	3:J:71:LEU:N	2.63	0.70
5:L:262:VAL:HG11	5:L:264:LYS:NZ	2.06	0.70
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.73	0.70
2:C:1269:ARG:HD3	3:D:343:LEU:HD11	1.72	0.70
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.07	0.70
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.70
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.55	0.70
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.25	0.70
5:F:320:ILE:HG21	5:F:331:HIS:CE1	2.25	0.70
2:I:499:SER:HA	2:I:502:VAL:HG12	1.74	0.70
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.74	0.70
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.24	0.70
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.72	0.70
3:J:48:THR:O	3:J:50:LYS:N	2.25	0.70
3:J:210:SER:O	3:J:214:ARG:HG2	1.91	0.70
3:D:495:ASN:O	3:D:497:GLU:N	2.23	0.70
2:I:206:ALA:O	2:I:209:ILE:HG22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:OE1	1:B:150:ARG:NH1	2.25	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.23	0.70
3:D:805:GLN:O	3:D:807:LEU:N	2.25	0.70
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.74	0.70
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.72	0.70
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.73	0.70
5:F:575:GLU:O	5:F:579:GLN:HG2	1.91	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.72	0.70
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.25	0.70
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.74	0.69
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.92	0.69
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.72	0.69
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.22	0.69
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.56	0.69
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.74	0.69
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.27	0.69
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.25	0.69
2:C:1269:ARG:CD	3:D:343:LEU:HD11	2.22	0.69
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.74	0.69
3:D:918:ILE:O	3:D:922:SER:OG	2.09	0.69
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.75	0.69
3:D:853:THR:HG22	3:D:854:ALA:H	1.56	0.69
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.05	0.69
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.75	0.69
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.73	0.69
3:J:1260:MET:HE3	3:J:1306:LEU:HD21	1.75	0.69
2:C:5:TYR:O	2:C:8:LYS:HG2	1.93	0.69
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.16	0.69
1:G:92:VAL:HA	1:G:120:ASP:O	1.92	0.69
5:L:395:THR:OG1	5:L:396:ASN:N	2.26	0.69
5:L:561:MET:HA	5:L:567:MET:HE1	1.73	0.69
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.75	0.69
2:C:615:VAL:HG13	2:C:651:ASP:H	1.58	0.69
2:C:930:ASP:OD2	2:C:931:VAL:N	2.26	0.69
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.91	0.69
3:D:210:SER:O	3:D:214:ARG:HG2	1.92	0.69
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.75	0.69
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.57	0.69
1:A:32:GLU:HG2	1:A:198:LEU:HD22	1.75	0.69
1:H:61:ILE:HG12	1:H:171:LEU:HD12	1.75	0.69
3:J:259:ARG:HD2	5:L:505:ILE:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.58	0.69
1:A:113:ALA:O	1:A:115:ILE:N	2.25	0.68
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.73	0.68
3:D:1174:ARG:HE	3:D:1189:MET:HE2	1.58	0.68
2:C:566:GLY:O	2:C:569:ILE:HG13	1.94	0.68
3:D:709:ARG:HD2	3:D:710:ASP:H	1.58	0.68
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.75	0.68
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.75	0.68
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.26	0.68
5:F:469:GLN:O	5:F:473:GLU:HB2	1.93	0.68
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.93	0.68
5:L:134:VAL:HA	5:L:273:MET:HE1	1.76	0.68
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.07	0.68
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.74	0.68
3:J:902:ASP:OD1	3:J:903:LEU:N	2.26	0.68
1:A:66:HIS:HD2	2:C:874:GLY:HA2	1.59	0.68
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.74	0.68
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.76	0.68
1:H:109:PRO:HA	1:H:132:HIS:HA	1.73	0.68
5:L:233:ASP:O	5:L:236:LYS:HE2	1.93	0.68
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.28	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.76	0.68
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.76	0.68
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.29	0.68
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.58	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
2:C:1281:TYR:HE2	3:D:431:ARG:HB2	1.59	0.68
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.76	0.68
3:J:1157:ALA:HB3	3:J:1207:GLY:H	1.59	0.68
3:D:75:TYR:HD2	3:D:80:HIS:HD2	1.41	0.67
1:H:35:PHE:HA	1:H:38:THR:HG22	1.76	0.67
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.76	0.67
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.10	0.67
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.75	0.67
2:I:1124:ILE:O	2:I:1128:ILE:HG13	1.94	0.67
3:J:1193:TRP:HB2	3:J:1194:ARG:HH12	1.60	0.67
2:I:871:VAL:O	2:I:944:ARG:NH1	2.27	0.67
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.75	0.67
5:F:163:THR:O	5:F:260:ARG:NH2	2.28	0.67
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.20	0.67
1:A:250:ASP:HA	5:F:605:GLU:HG3	1.77	0.67
2:C:854:ILE:O	2:C:857:VAL:HG22	1.95	0.67
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.76	0.67
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.77	0.67
3:D:339:ARG:HD3	3:D:798:ARG:NH1	2.08	0.67
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.29	0.67
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.77	0.67
2:C:98:VAL:HB	2:C:124:MET:HE3	1.76	0.67
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.75	0.67
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.60	0.67
2:C:744:GLY:C	2:C:746:ALA:H	2.03	0.67
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.28	0.67
4:K:52:ARG:O	4:K:56:GLU:HG2	1.95	0.67
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.77	0.67
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.09	0.67
3:D:515:ARG:O	3:D:545:HIS:HB3	1.94	0.67
1:G:161:SER:O	1:G:163:GLU:N	2.28	0.67
2:I:1197:GLU:HA	2:I:1200:LYS:HD2	1.75	0.67
3:J:425:ARG:HG2	3:J:426:ALA:N	2.09	0.67
3:J:797:THR:O	3:J:801:VAL:HG12	1.94	0.67
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.60	0.67
2:I:998:LEU:H	2:I:998:LEU:HD12	1.59	0.66
2:I:1013:GLN:O	2:I:1017:GLN:HG2	1.95	0.66
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.77	0.66
3:D:510:LEU:O	3:D:514:THR:HG22	1.95	0.66
2:I:499:SER:O	2:I:503:LYS:HB2	1.95	0.66
1:A:31:LEU:HB2	1:A:199:ASP:O	1.95	0.66
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.10	0.66
2:C:303:ASP:HB3	2:C:306:THR:HG23	1.78	0.66
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.77	0.66
3:J:45:ASN:HB3	3:J:48:THR:O	1.95	0.66
1:A:135:ASP:O	1:A:138:ALA:N	2.27	0.66
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.77	0.66
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.66
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.59	0.66
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.77	0.66
3:J:903:LEU:HB3	3:J:905:ARG:HG3	1.77	0.66
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.27	0.66
5:L:453:PRO:O	5:L:456:MET:HB2	1.95	0.66
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:276:MET:O	5:F:280:VAL:HG23	1.95	0.66
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.76	0.66
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.31	0.66
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.78	0.66
3:J:853:THR:HG22	3:J:854:ALA:H	1.60	0.66
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.08	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.77	0.66
5:F:261:LEU:H	5:F:261:LEU:HD12	1.60	0.66
2:I:4:SER:OG	2:I:5:TYR:N	2.27	0.66
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.78	0.66
5:L:386:LEU:O	5:L:389:SER:OG	2.10	0.66
3:J:16:GLU:HG3	3:J:17:PHE:H	1.61	0.66
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.77	0.66
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.77	0.66
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.77	0.66
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.77	0.66
3:J:1167:LYS:HZ3	3:J:1170:LYS:HB2	1.60	0.66
1:B:196:THR:CG2	3:D:443:GLU:HG3	2.26	0.66
2:C:721:GLY:N	2:C:740:GLU:OE1	2.25	0.66
2:I:799:ASN:HB3	2:I:1231:TYR:HD1	1.61	0.66
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.61	0.66
2:C:27:LEU:O	2:C:528:ARG:NH1	2.29	0.65
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.25	0.65
5:F:134:VAL:HA	5:F:273:MET:HE1	1.77	0.65
3:J:700:ASN:O	3:J:704:GLU:HB2	1.97	0.65
3:D:594:GLN:HG3	3:D:596:LEU:HD22	1.78	0.65
3:D:709:ARG:HD2	3:D:710:ASP:N	2.11	0.65
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.22	0.65
5:F:343:LYS:O	5:F:347:ILE:HG13	1.97	0.65
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.76	0.65
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.77	0.65
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.11	0.65
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.32	0.65
1:H:69:SER:HB2	1:H:78:ILE:HD11	1.76	0.65
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.78	0.65
3:J:596:LEU:HD11	3:J:604:MET:HE1	1.78	0.65
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.79	0.65
2:C:600:THR:HG22	2:C:602:GLU:H	1.61	0.65
2:C:624:ASP:OD1	2:C:625:GLU:N	2.26	0.65
2:C:1243:MET:HA	3:D:353:SER:HB3	1.78	0.65
3:J:827:GLU:CB	3:J:832:LYS:HD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.32	0.65
3:D:709:ARG:O	3:D:711:GLY:N	2.30	0.65
2:C:4:SER:OG	2:C:5:TYR:N	2.30	0.65
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.77	0.65
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.77	0.65
1:H:27:THR:HB	1:H:202:VAL:HG22	1.79	0.65
1:H:101:THR:HG22	1:H:116:THR:HB	1.79	0.65
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.28	0.65
3:J:479:GLU:HG2	4:K:20:VAL:HG11	1.77	0.65
3:J:495:ASN:O	3:J:497:GLU:N	2.30	0.65
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.77	0.65
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.62	0.65
2:C:1017:GLN:O	2:C:1021:LEU:HG	1.97	0.65
1:H:81:ILE:HG23	1:H:130:ILE:O	1.97	0.65
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.78	0.65
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.43	0.65
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.79	0.65
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.31	0.65
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.79	0.65
5:L:343:LYS:O	5:L:347:ILE:HG13	1.96	0.65
5:L:476:ARG:HB3	5:L:476:ARG:HH11	1.61	0.65
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.77	0.65
5:F:483:LEU:H	5:F:483:LEU:HD12	1.62	0.65
2:I:596:ASP:CG	2:I:597:GLY:H	2.05	0.65
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.30	0.65
1:G:23:HIS:HB2	1:G:205:MET:O	1.97	0.65
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.78	0.65
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.78	0.65
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.29	0.65
3:D:425:ARG:HG2	3:D:426:ALA:N	2.03	0.64
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.37	0.64
5:F:125:ASP:O	5:F:129:GLN:HG3	1.97	0.64
5:F:466:ILE:CG2	5:F:486:ARG:HG3	2.27	0.64
1:H:13:LEU:HA	1:H:28:LEU:HD13	1.79	0.64
1:H:62:ASP:OD1	1:H:62:ASP:N	2.30	0.64
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.30	0.64
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	1.96	0.64
3:D:1191:PRO:HB3	3:D:1194:ARG:NH1	2.11	0.64
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.80	0.64
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.32	0.64
2:I:746:ALA:HA	2:I:974:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HD3	1:A:114:ASP:OD2	1.98	0.64
2:C:367:TYR:HA	2:C:384:LEU:HD22	1.78	0.64
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.78	0.64
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.98	0.64
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.79	0.64
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.64
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.77	0.64
2:C:40:GLU:HG2	2:C:41:GLN:N	2.12	0.64
1:H:35:PHE:HA	1:H:38:THR:CG2	2.28	0.64
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.79	0.64
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.10	0.64
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.33	0.64
5:L:573:LEU:HD23	5:L:573:LEU:H	1.61	0.64
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.80	0.64
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.13	0.64
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.32	0.64
2:I:888:THR:OG1	2:I:914:LYS:HB3	1.97	0.64
2:C:619:ALA:HB1	2:C:657:THR:HA	1.80	0.64
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.29	0.64
5:F:298:PRO:HD2	5:F:326:TRP:CG	2.33	0.64
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.78	0.64
3:J:770:LEU:H	3:J:770:LEU:HD22	1.63	0.64
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.79	0.64
3:D:140:TYR:HB3	5:F:100:MET:SD	2.37	0.64
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.79	0.64
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.80	0.64
3:D:66:LYS:HE2	3:D:69:GLU:OE1	1.97	0.64
5:F:463:LEU:HD21	5:F:487:MET:HG3	1.81	0.64
1:G:45:ARG:NH2	1:H:37:HIS:HB3	2.13	0.64
1:H:9:LEU:HD12	1:H:195:ARG:NH2	2.10	0.64
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.63
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.13	0.63
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.78	0.63
3:D:60:ARG:HA	3:D:89:GLY:O	1.99	0.63
3:D:327:LEU:HA	3:D:330:MET:HG3	1.81	0.63
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.33	0.63
1:H:102:LEU:O	1:H:141:SER:HA	1.98	0.63
2:I:617:ALA:HA	2:I:636:CYS:SG	2.37	0.63
1:B:112:ALA:HA	1:B:115:ILE:HG13	1.80	0.63
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.79	0.63
2:I:705:GLU:HB2	2:I:794:LEU:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.80	0.63
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.34	0.63
2:I:1065:LYS:HE2	3:J:462:ASP:O	1.98	0.63
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.63	0.63
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.63	0.63
1:A:14:VAL:HG22	1:A:15:ASP:H	1.63	0.63
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.34	0.63
3:D:1280:VAL:CG2	3:D:1304:ARG:HH21	2.04	0.63
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.60	0.63
2:C:510:GLN:NE2	2:C:534:GLY:HA2	2.14	0.63
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.14	0.63
3:J:510:LEU:O	3:J:514:THR:HG22	1.99	0.63
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.81	0.63
3:D:902:ASP:OD1	3:D:903:LEU:N	2.32	0.63
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.24	0.63
3:J:432:LEU:HD21	3:J:489:ASN:HB3	1.79	0.63
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.81	0.63
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.81	0.63
2:C:1255:THR:O	2:C:1257:GLN:N	2.32	0.63
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.79	0.63
5:L:244:THR:O	5:L:247:GLU:HG2	1.99	0.63
1:A:55:ALA:HB3	1:A:177:TYR:HD1	1.61	0.63
2:C:356:THR:HG21	2:C:362:ALA:HA	1.81	0.63
3:D:48:THR:C	3:D:50:LYS:H	2.06	0.63
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.80	0.63
3:D:1179:PRO:HG2	3:D:1183:SER:O	1.99	0.63
2:I:857:VAL:HG21	2:I:862:LEU:HD21	1.80	0.63
2:C:325:LEU:O	2:C:330:HIS:HB2	1.98	0.62
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.81	0.62
4:E:38:LEU:HB2	4:E:53:GLU:OE1	1.99	0.62
5:F:470:MET:HA	5:F:473:GLU:HB3	1.81	0.62
5:L:245:ALA:O	5:L:249:ILE:HG13	1.99	0.62
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.80	0.62
3:D:491:LEU:HD22	3:D:496:GLY:O	1.99	0.62
3:D:507:VAL:HG11	3:D:598:LYS:HG3	1.81	0.62
3:D:701:LEU:HD12	3:D:723:TYR:HD2	1.64	0.62
2:I:975:ILE:HD13	2:I:998:LEU:HG	1.80	0.62
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.11	0.62
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.81	0.62
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.64	0.62
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:771:VAL:HG21	2:I:783:LEU:HD13	1.82	0.62
3:J:515:ARG:NH2	3:J:717:VAL:O	2.32	0.62
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.81	0.62
5:L:322:MET:HE2	5:L:324:LYS:HZ3	1.63	0.62
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.14	0.62
3:D:271:ARG:HG2	3:D:302:ALA:HB1	1.80	0.62
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.98	0.62
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.35	0.62
5:L:470:MET:O	5:L:478:PRO:HD3	1.99	0.62
1:A:156:SER:HB3	2:C:1059:ARG:NH2	2.08	0.62
1:H:41:ASN:O	1:H:45:ARG:HG3	1.99	0.62
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.81	0.62
2:I:1192:GLU:O	2:I:1196:LYS:HG2	1.98	0.62
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.30	0.62
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.32	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.65	0.62
3:D:432:LEU:HD21	3:D:489:ASN:HB3	1.80	0.62
2:I:358:ASP:OD2	2:I:361:SER:HB2	2.00	0.62
2:I:498:ILE:H	2:I:498:ILE:HD12	1.65	0.62
3:J:600:ALA:O	3:J:603:LYS:HG2	1.99	0.62
3:D:197:GLU:O	3:D:201:LEU:HG	1.99	0.62
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.81	0.62
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.35	0.62
1:A:54:CYS:HA	1:A:148:ARG:HA	1.82	0.62
2:C:138:ILE:O	2:C:139:ASN:ND2	2.33	0.62
2:C:421:SER:H	2:C:424:ASP:HB2	1.64	0.62
1:H:9:LEU:HB3	1:H:32:GLU:HG2	1.81	0.62
2:I:490:GLN:HA	2:I:493:ILE:HG23	1.82	0.62
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.34	0.62
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.82	0.62
5:L:544:THR:HG22	5:L:607:LEU:HD11	1.81	0.62
1:A:145:LYS:HZ2	1:A:147:GLN:HG3	1.64	0.62
2:C:377:THR:HB	2:C:380:ALA:H	1.65	0.62
2:C:561:ILE:O	2:C:680:LEU:HD12	2.00	0.62
2:C:796:LEU:H	2:C:796:LEU:HD12	1.64	0.62
3:D:339:ARG:CD	3:D:798:ARG:HD3	2.30	0.62
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.82	0.62
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.82	0.62
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.15	0.62
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.33	0.61
3:D:248:ASP:O	3:D:251:PRO:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.30	0.61
1:G:93:GLN:H	1:G:120:ASP:HB3	1.63	0.61
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.80	0.61
2:I:356:THR:HG21	2:I:362:ALA:HA	1.82	0.61
2:I:560:PRO:O	3:J:780:ARG:NH2	2.32	0.61
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.81	0.61
3:D:203:GLU:O	3:D:207:GLU:HG2	1.99	0.61
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.15	0.61
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.65	0.61
2:I:519:ASN:O	2:I:523:GLU:HG3	1.99	0.61
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.32	0.61
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.29	0.61
3:D:661:VAL:CG1	3:D:685:ILE:HD11	2.30	0.61
3:D:1344:LEU:O	3:D:1346:GLY:N	2.27	0.61
1:G:14:VAL:HG22	1:G:15:ASP:H	1.66	0.61
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.83	0.61
2:I:582:ASN:HB3	2:I:586:PHE:H	1.65	0.61
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.31	0.61
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.83	0.61
5:F:311:THR:HB	5:F:345:GLN:HG2	1.81	0.61
2:I:232:ILE:HD12	2:I:330:HIS:O	2.00	0.61
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.34	0.61
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.00	0.61
5:L:515:GLU:HG2	5:L:516:ASP:H	1.66	0.61
2:C:448:LEU:HB2	2:C:553:THR:HB	1.81	0.61
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.83	0.61
1:G:156:SER:HB2	2:I:1059:ARG:HH22	1.65	0.61
1:H:101:THR:H	1:H:116:THR:CG2	2.14	0.61
2:I:518:ASN:OD1	2:I:518:ASN:N	2.33	0.61
3:D:244:VAL:HA	3:D:269:TYR:OH	2.01	0.61
1:H:151:GLY:O	1:H:177:TYR:HB2	1.99	0.61
2:I:360:LEU:O	2:I:364:VAL:HG23	1.99	0.61
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.82	0.61
3:J:812:ASP:HB2	3:J:911:LYS:HE3	1.83	0.61
5:L:465:ARG:HD2	5:L:468:ARG:HH22	1.65	0.61
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.82	0.61
2:C:55:SER:OG	2:C:465:ARG:NH1	2.34	0.61
2:C:149:LEU:HD12	2:C:452:ARG:O	2.01	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.66	0.61
3:D:632:ALA:O	3:D:635:SER:OG	2.18	0.61
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
3:J:514:THR:HG21	3:J:596:LEU:HG	1.82	0.61
5:L:299:LYS:HA	5:L:302:PHE:CB	2.28	0.61
5:L:414:LYS:HD3	5:L:434:TRP:HZ3	1.66	0.61
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.82	0.61
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.33	0.61
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.83	0.61
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.82	0.61
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.15	0.61
5:F:244:THR:O	5:F:247:GLU:HG2	2.00	0.60
5:F:573:LEU:HD23	5:F:573:LEU:H	1.66	0.60
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.82	0.60
3:J:751:ASP:HB3	3:J:753:SER:H	1.66	0.60
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.84	0.60
2:C:582:ASN:HB3	2:C:586:PHE:H	1.66	0.60
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.18	0.60
1:G:8:PHE:O	1:G:9:LEU:HB2	2.00	0.60
2:I:797:GLY:O	2:I:1231:TYR:OH	2.19	0.60
2:I:798:GLN:HB2	2:I:828:PHE:CE1	2.35	0.60
3:J:215:LYS:O	3:J:218:THR:HG22	2.01	0.60
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.16	0.60
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.31	0.60
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.35	0.60
1:H:49:SER:O	1:H:151:GLY:HA2	2.00	0.60
3:J:267:ASP:HA	3:J:270:ARG:HH21	1.66	0.60
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.83	0.60
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.01	0.60
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.00	0.60
3:J:551:ARG:HA	3:J:568:SER:O	2.01	0.60
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.66	0.60
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.83	0.60
2:C:1191:LYS:O	2:C:1195:ILE:HG13	1.99	0.60
5:F:466:ILE:HG23	5:F:486:ARG:HG3	1.83	0.60
2:I:941:LYS:HD3	2:I:949:GLU:OE1	2.01	0.60
1:B:73:GLY:CA	1:B:134:THR:HG22	2.27	0.60
2:C:148:GLN:NE2	2:C:533:LEU:O	2.26	0.60
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.15	0.60
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.18	0.60
3:D:224:LEU:O	3:D:227:PHE:N	2.34	0.60
3:D:427:PRO:HB2	3:D:429:LEU:HD22	1.84	0.60
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:649:LYS:O	3:J:653:ILE:HG13	2.01	0.60
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.83	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.33	0.60
5:F:277:MET:HE3	5:F:281:ARG:HH21	1.66	0.60
5:F:513:ASP:C	5:F:515:GLU:H	2.09	0.60
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.82	0.60
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.17	0.60
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.42	0.60
5:F:130:VAL:HB	5:F:365:MET:HG3	1.83	0.60
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.83	0.60
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.84	0.60
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.02	0.60
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.60
2:I:971:LEU:HD21	2:I:1014:LEU:O	2.02	0.60
3:J:473:THR:HG23	3:J:476:ALA:H	1.66	0.60
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.83	0.60
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.01	0.60
2:C:1207:SER:C	2:C:1209:GLN:H	2.08	0.60
3:D:27:PRO:O	3:D:31:ARG:HG3	2.02	0.60
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.35	0.60
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.67	0.60
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.17	0.60
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.83	0.60
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.84	0.60
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.32	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.83	0.59
3:D:825:VAL:HG22	3:D:833:GLU:H	1.67	0.59
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.67	0.59
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.83	0.59
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.67	0.59
3:J:405:GLU:O	3:J:408:VAL:HG22	2.02	0.59
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.84	0.59
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.17	0.59
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.14	0.59
1:G:195:ARG:HG3	1:G:198:LEU:HG	1.84	0.59
2:I:57:PHE:CD1	2:I:58:PRO:HA	2.37	0.59
2:I:169:LYS:O	2:I:170:VAL:HG22	2.02	0.59
2:I:528:ARG:NH2	2:I:576:SER:O	2.35	0.59
3:J:619:ILE:O	3:J:623:GLN:HG2	2.03	0.59
5:L:465:ARG:HB3	5:L:468:ARG:HH12	1.67	0.59
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:421:VAL:CG1	3:D:439:PRO:HG3	2.32	0.59
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.83	0.59
2:I:462:ASN:O	2:I:466:VAL:HG23	2.02	0.59
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.84	0.59
3:J:1163:VAL:HG21	3:J:1175:LEU:HD21	1.83	0.59
1:A:49:SER:HG	1:A:50:SER:HG	1.51	0.59
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.03	0.59
5:F:299:LYS:O	5:F:303:ILE:HG12	2.02	0.59
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.84	0.59
5:L:290:LEU:HD22	5:L:333:VAL:HG21	1.83	0.59
1:A:71:LYS:HD3	1:A:72:GLU:N	2.17	0.59
1:B:47:LEU:O	1:B:180:VAL:HG21	2.02	0.59
2:C:41:GLN:NE2	2:C:73:TYR:O	2.34	0.59
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.59
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.83	0.59
5:L:340:ALA:HA	5:L:343:LYS:HZ2	1.66	0.59
5:L:390:ILE:O	5:L:393:LYS:HB2	2.03	0.59
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.59
2:I:12:ARG:NH2	2:I:698:PRO:O	2.27	0.59
3:J:418:GLU:H	4:K:45:LYS:NZ	2.01	0.59
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.84	0.59
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.83	0.59
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.36	0.59
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.64	0.59
2:I:685:MET:HA	2:I:688:GLN:HE21	1.66	0.59
1:A:253:LEU:HA	1:A:278:ILE:HG13	1.85	0.59
2:C:62:TYR:O	2:C:64:GLY:N	2.36	0.59
2:I:384:LEU:O	2:I:388:LEU:HG	2.03	0.59
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.85	0.59
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.36	0.59
2:C:1161:LEU:HG	2:C:1161:LEU:O	1.91	0.59
3:D:1191:PRO:CB	3:D:1194:ARG:HH11	2.16	0.59
5:F:245:ALA:O	5:F:249:ILE:HG13	2.03	0.59
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.67	0.59
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.19	0.59
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.85	0.59
5:L:139:GLU:HG2	5:L:351:THR:HA	1.84	0.59
1:A:296:GLY:N	1:A:299:SER:HB2	2.16	0.59
2:C:705:GLU:HB2	2:C:794:LEU:H	1.68	0.59
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.03	0.59
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:854:ALA:HB2	3:J:1372:ARG:CG	2.33	0.59
2:I:168:GLY:O	2:I:170:VAL:N	2.24	0.59
3:J:735:ALA:O	3:J:739:GLN:HG3	2.03	0.59
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.85	0.59
5:L:320:ILE:HG23	5:L:327:SER:O	2.02	0.59
5:L:348:GLU:HA	5:L:353:LEU:O	2.03	0.59
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.85	0.59
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.83	0.58
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.58
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.36	0.58
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.38	0.58
2:C:486:THR:HG23	2:C:487:LEU:N	2.18	0.58
3:J:733:SER:O	3:J:737:ILE:HG12	2.04	0.58
1:B:35:PHE:HA	1:B:38:THR:HG22	1.84	0.58
3:D:26:SER:HA	3:D:236:TRP:NE1	2.19	0.58
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.84	0.58
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.03	0.58
1:A:236:ASP:HA	1:B:14:VAL:O	2.02	0.58
3:D:678:ARG:O	3:D:682:VAL:HG23	2.03	0.58
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.36	0.58
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.85	0.58
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.69	0.58
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.85	0.58
3:J:689:ALA:O	3:J:693:VAL:HG23	2.03	0.58
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.85	0.58
1:B:101:THR:H	1:B:116:THR:CG2	2.15	0.58
2:C:517:GLN:O	2:C:517:GLN:HG2	2.02	0.58
2:C:998:LEU:H	2:C:998:LEU:HD12	1.68	0.58
3:D:490:ILE:HA	3:D:500:ILE:CG1	2.33	0.58
5:F:379:MET:O	5:F:383:ASN:ND2	2.37	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58
3:J:102:MET:HE2	3:J:244:VAL:O	2.03	0.58
4:K:32:VAL:O	4:K:34:GLY:N	2.34	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.85	0.58
5:L:230:VAL:O	5:L:234:THR:HG23	2.03	0.58
1:B:49:SER:O	1:B:151:GLY:HA2	2.04	0.58
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.84	0.58
2:C:323:ALA:O	2:C:327:GLN:HG3	2.04	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
5:F:226:ALA:O	5:F:229:VAL:HG22	2.03	0.58
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1269:ARG:NE	3:J:343:LEU:HD21	2.17	0.58
3:J:155:GLU:CB	3:J:158:GLN:HB2	2.25	0.58
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.69	0.58
3:J:1167:LYS:CE	3:J:1174:ARG:HD2	2.34	0.58
5:L:561:MET:HA	5:L:567:MET:CE	2.33	0.58
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.85	0.58
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.19	0.58
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	1.85	0.58
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.34	0.58
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.38	0.58
2:C:643:SER:HG	2:C:645:PHE:HE1	1.52	0.58
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.58
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.19	0.58
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.85	0.58
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.85	0.58
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.36	0.58
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.34	0.58
5:L:515:GLU:HG2	5:L:516:ASP:N	2.18	0.58
1:B:101:THR:H	1:B:116:THR:HG21	1.69	0.58
2:C:70:TYR:HA	2:C:100:LEU:HD23	1.85	0.58
2:C:696:ASP:O	2:C:697:LYS:HB3	2.03	0.58
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.38	0.58
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	1.85	0.58
3:D:374:LEU:HD23	3:D:412:LEU:HD12	1.85	0.58
3:J:57:PHE:CE1	3:J:252:LEU:HB2	2.38	0.58
3:J:810:THR:HG23	3:J:811:GLU:H	1.69	0.58
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.85	0.58
3:D:161:THR:H	3:D:164:GLN:HB2	1.69	0.58
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.85	0.58
1:H:50:SER:HA	1:H:150:ARG:O	2.04	0.58
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.69	0.58
2:I:80:PHE:HZ	2:I:1038:GLN:HE22	1.52	0.58
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.34	0.58
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.04	0.58
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.86	0.58
2:C:685:MET:HA	2:C:688:GLN:HE21	1.69	0.57
3:D:215:LYS:HE3	3:D:216:LYS:HG3	1.86	0.57
1:G:12:ARG:H	1:G:30:PRO:CD	2.09	0.57
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.85	0.57
5:L:357:GLN:O	5:L:361:ILE:HG13	2.04	0.57
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.84	0.57
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.85	0.57
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.43	0.57
3:D:474:LEU:HA	3:D:477:GLN:HG3	1.85	0.57
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.19	0.57
3:D:268:LEU:HG	3:D:324:LEU:HD22	1.86	0.57
3:D:438:GLU:OE2	3:D:481:ARG:NH2	2.28	0.57
3:D:787:ALA:O	3:D:790:THR:HB	2.04	0.57
5:F:462:LYS:HD2	5:F:487:MET:HE1	1.86	0.57
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.34	0.57
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.86	0.57
2:I:519:ASN:ND2	2:I:689:ALA:O	2.37	0.57
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.86	0.57
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.86	0.57
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.69	0.57
3:D:161:THR:HG23	3:D:164:GLN:H	1.69	0.57
3:D:653:ILE:HG23	3:D:692:ARG:CZ	2.35	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.69	0.57
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.33	0.57
2:I:800:MET:O	2:I:1229:TYR:HA	2.04	0.57
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.85	0.57
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.85	0.57
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.85	0.57
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.34	0.57
3:D:279:LEU:HD12	3:D:295:GLU:HG3	1.85	0.57
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.35	0.57
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.69	0.57
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.29	0.57
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.40	0.57
1:A:234:LEU:N	1:B:218:ARG:HH12	2.02	0.57
2:C:1160:ASP:HB2	2:C:1161:LEU:HD12	1.86	0.57
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.68	0.57
1:G:189:ALA:HB1	1:G:191:ARG:CZ	2.35	0.57
1:H:100:LEU:HD23	1:H:116:THR:O	2.05	0.57
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.86	0.57
1:A:71:LYS:HB3	1:A:74:VAL:HG13	1.86	0.57
2:C:211:ARG:NH1	2:C:357:ASN:O	2.38	0.57
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.04	0.57
3:D:697:MET:HE2	3:D:698:MET:HG2	1.87	0.57
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.87	0.57
5:F:494:ILE:O	5:F:498:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LEU:O	1:G:180:VAL:HG11	2.04	0.57
1:H:64:VAL:HG12	1:H:66:HIS:H	1.68	0.57
2:I:32:LEU:HD23	2:I:130:MET:SD	2.45	0.57
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.05	0.57
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.28	0.57
5:L:288:MET:HG2	5:L:299:LYS:HE2	1.86	0.57
2:I:5:TYR:O	2:I:8:LYS:HG2	2.04	0.57
3:J:26:SER:HA	3:J:236:TRP:NE1	2.20	0.57
5:L:474:MET:O	5:L:476:ARG:N	2.28	0.57
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.69	0.57
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.39	0.57
5:F:484:ALA:O	5:F:491:GLU:HB2	2.05	0.57
1:G:36:GLY:C	1:G:187:VAL:HG11	2.30	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.86	0.57
3:J:79:LYS:HB2	5:L:569:THR:H	1.70	0.57
5:L:148:TYR:OH	5:L:218:ARG:HA	2.04	0.57
5:L:465:ARG:CD	5:L:468:ARG:HH22	2.18	0.57
3:D:45:ASN:HB3	3:D:48:THR:O	2.04	0.57
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.02	0.57
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.04	0.57
1:A:106:GLY:O	1:A:108:GLY:N	2.38	0.56
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.85	0.56
1:G:10:LYS:NZ	1:H:229:GLU:OE1	2.36	0.56
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.69	0.56
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.20	0.56
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.86	0.56
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.86	0.56
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.45	0.56
3:D:825:VAL:C	3:D:826:ILE:HG13	2.30	0.56
2:I:5:TYR:HD1	2:I:8:LYS:HD3	1.70	0.56
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.27	0.56
2:I:157:PHE:O	2:I:443:ASP:N	2.36	0.56
1:A:112:ALA:O	1:A:115:ILE:HG13	2.05	0.56
1:B:35:PHE:HA	1:B:38:THR:CG2	2.35	0.56
2:C:541:GLU:OE1	2:C:541:GLU:N	2.36	0.56
2:C:898:GLU:OE1	2:C:898:GLU:N	2.30	0.56
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.87	0.56
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.71	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
1:G:195:ARG:HD2	1:G:196:THR:H	1.69	0.56
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.87	0.56
1:H:216:ALA:O	1:H:220:ALA:N	2.37	0.56
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.88	0.56
3:J:48:THR:C	3:J:50:LYS:H	2.13	0.56
3:J:147:ILE:O	3:J:147:ILE:HG13	2.05	0.56
3:J:522:GLY:O	3:J:525:MET:HG2	2.06	0.56
3:J:749:LYS:HG2	3:J:753:SER:O	2.05	0.56
4:K:54:ILE:HD13	4:K:59:ILE:HG22	1.87	0.56
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.68	0.56
5:L:313:ASP:CG	5:L:338:HIS:HE2	2.13	0.56
5:L:456:MET:O	5:L:460:ILE:HG13	2.05	0.56
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.35	0.56
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.87	0.56
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.87	0.56
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.06	0.56
1:G:224:LEU:CD2	1:G:228:LEU:HD22	2.35	0.56
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.21	0.56
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.05	0.56
2:I:1269:ARG:HD3	3:J:343:LEU:CD2	2.24	0.56
3:J:393:THR:HG23	3:J:396:ALA:H	1.71	0.56
2:C:359:ARG:CZ	2:C:363:LEU:HD11	2.36	0.56
2:C:498:ILE:H	2:C:498:ILE:HD12	1.70	0.56
2:C:778:GLU:O	2:C:781:ASP:HB2	2.05	0.56
2:C:976:ARG:HB2	2:C:997:TRP:CZ3	2.41	0.56
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.41	0.56
1:H:60:GLU:HG3	1:H:143:ARG:O	2.06	0.56
2:I:1247:SER:HB3	3:J:375:GLU:O	2.05	0.56
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.87	0.56
5:L:277:MET:SD	5:L:359:LYS:HG2	2.46	0.56
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.86	0.56
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.86	0.56
1:H:78:ILE:O	1:H:82:LEU:HG	2.06	0.56
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.87	0.56
2:I:149:LEU:HD12	2:I:452:ARG:O	2.06	0.56
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.86	0.56
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.88	0.56
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.34	0.56
1:A:219:ARG:O	1:A:222:THR:HB	2.06	0.56
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.21	0.56
2:C:486:THR:HG23	2:C:487:LEU:H	1.70	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.06	0.56
3:D:797:THR:O	3:D:801:VAL:HG12	2.05	0.56
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.69	0.56
1:G:166:ARG:NH1	1:G:168:ILE:HG12	2.19	0.56
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.70	0.56
3:J:805:GLN:NE2	3:J:1348:LYS:HD3	2.21	0.56
5:L:314:THR:O	5:L:318:ALA:HB3	2.06	0.56
1:A:318:LEU:O	1:A:320:ASN:N	2.38	0.56
1:B:88:LEU:HD12	1:B:89:ALA:H	1.71	0.56
3:D:1226:VAL:HG21	3:J:1292:LEU:HA	1.86	0.56
5:F:277:MET:HE3	5:F:281:ARG:NH2	2.20	0.56
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.87	0.56
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.41	0.56
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.87	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.88	0.56
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.88	0.56
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.40	0.56
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.30	0.56
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.87	0.56
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.06	0.56
2:I:1131:MET:HB3	2:I:1141:LEU:HD11	1.88	0.56
2:I:1225:VAL:HG12	3:J:636:GLY:O	2.06	0.56
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.06	0.56
2:C:76:GLY:O	2:C:94:ALA:HB1	2.05	0.56
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.88	0.56
3:D:619:ILE:O	3:D:623:GLN:HG2	2.05	0.56
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.35	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
3:J:844:THR:HG21	3:J:858:VAL:HG21	1.87	0.56
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.21	0.56
3:J:1167:LYS:HD3	3:J:1174:ARG:HH11	1.71	0.56
3:J:1170:LYS:C	3:J:1172:LYS:H	2.13	0.56
1:A:212:ASP:O	1:A:215:GLU:HB3	2.06	0.55
1:B:219:ARG:HA	1:B:222:THR:HB	1.87	0.55
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.87	0.55
3:D:707:ILE:HD12	3:D:707:ILE:N	2.20	0.55
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.87	0.55
5:F:320:ILE:HG23	5:F:327:SER:O	2.05	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.20	0.55
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
3:D:210:SER:HB2	3:D:213:LYS:CB	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.89	0.55
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.42	0.55
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.70	0.55
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.88	0.55
2:I:425:ILE:O	2:I:429:MET:HG3	2.05	0.55
3:J:418:GLU:HG3	4:K:45:LYS:H	1.72	0.55
3:J:1320:ILE:HG23	8:J:2004:4C6:H9	1.87	0.55
1:A:194:GLN:OE1	1:A:195:ARG:N	2.40	0.55
1:B:81:ILE:O	1:B:85:LEU:HG	2.05	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.21	0.55
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.89	0.55
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.88	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55
3:D:810:THR:HG23	3:D:811:GLU:H	1.71	0.55
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.22	0.55
1:H:102:LEU:HD11	1:H:130:ILE:HG21	1.88	0.55
2:I:168:GLY:C	2:I:170:VAL:H	2.13	0.55
5:L:280:VAL:O	5:L:284:GLU:HG3	2.06	0.55
1:A:145:LYS:NZ	1:A:147:GLN:HG3	2.21	0.55
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.86	0.55
2:C:320:ASP:OD1	2:C:324:LYS:HE3	2.05	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.38	0.55
2:C:1281:TYR:HE2	3:D:431:ARG:CB	2.20	0.55
3:D:54:ASP:OD1	3:D:54:ASP:N	2.39	0.55
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.34	0.55
5:L:346:GLN:HA	5:L:349:GLU:OE2	2.07	0.55
1:A:47:LEU:O	1:A:180:VAL:HG11	2.07	0.55
1:A:253:LEU:HA	1:A:278:ILE:CG1	2.37	0.55
1:A:282:VAL:O	1:A:315:GLY:N	2.40	0.55
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.88	0.55
3:D:11:GLN:HE21	3:D:15:GLU:CD	2.15	0.55
3:D:327:LEU:O	3:D:330:MET:HB2	2.06	0.55
3:D:557:LYS:HA	3:D:563:LEU:HA	1.89	0.55
3:D:638:SER:OG	3:D:639:VAL:N	2.39	0.55
5:F:465:ARG:CD	5:F:468:ARG:HH22	2.20	0.55
2:I:431:LYS:O	2:I:435:ILE:HG13	2.07	0.55
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.47	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.22	0.55
3:J:598:LYS:O	3:J:601:ILE:HG22	2.06	0.55
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:LYS:HD2	2:C:791:LEU:HD11	1.89	0.55
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.07	0.55
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.05	0.55
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.87	0.55
5:F:230:VAL:O	5:F:234:THR:HG23	2.05	0.55
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.40	0.55
5:F:372:ALA:O	5:F:376:LYS:HG3	2.07	0.55
2:I:1080:ASN:CB	2:I:1085:MET:HE3	2.36	0.55
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.72	0.55
3:J:580:TRP:HH2	3:J:587:LEU:O	1.89	0.55
3:J:638:SER:OG	3:J:639:VAL:N	2.39	0.55
3:J:1140:ARG:HH21	3:J:1236:GLU:HG3	1.71	0.55
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.36	0.55
3:D:161:THR:CG2	3:D:164:GLN:H	2.20	0.55
3:D:799:ARG:HG2	3:D:1309:ILE:HD12	1.89	0.55
3:D:1193:TRP:HB2	3:D:1194:ARG:CZ	2.37	0.55
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.72	0.55
1:G:190:ALA:CB	1:G:200:LYS:HB2	2.20	0.55
1:H:134:THR:HG23	1:H:135:ASP:H	1.70	0.55
2:I:888:THR:HG23	2:I:916:SER:OG	2.07	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.15	0.55
3:J:197:GLU:O	3:J:201:LEU:HG	2.06	0.55
4:K:62:GLN:O	4:K:66:VAL:HG23	2.07	0.55
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.87	0.55
1:B:12:ARG:O	1:B:13:LEU:HB3	2.06	0.55
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	0.55
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.89	0.55
3:D:514:THR:O	3:D:595:ALA:HA	2.07	0.55
3:D:535:ARG:O	3:D:539:SER:OG	2.24	0.55
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.87	0.55
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.40	0.55
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.40	0.55
5:F:137:TYR:O	5:F:141:ILE:HG12	2.06	0.55
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.55
2:I:715:THR:OG1	2:I:782:VAL:HG12	2.06	0.55
2:I:715:THR:HG23	2:I:717:VAL:HG23	1.89	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.22	0.55
1:A:113:ALA:C	1:A:115:ILE:H	2.14	0.55
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.22	0.55
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.89	0.55
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.42	0.55
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.88	0.55
2:C:494:ASN:HB3	2:C:497:PRO:HG2	1.89	0.54
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.88	0.54
5:F:143:TYR:CE2	5:F:147:GLN:HG3	2.43	0.54
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.07	0.54
2:C:1142:ARG:NH1	2:C:1165:SER:HA	2.15	0.54
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.07	0.54
3:J:1262:ARG:HD2	3:J:1279:GLN:NE2	2.21	0.54
5:L:470:MET:HA	5:L:473:GLU:HB3	1.88	0.54
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.88	0.54
5:F:400:GLN:HB2	5:F:403:ASP:OD2	2.07	0.54
1:G:76:GLU:OE1	1:G:132:HIS:N	2.36	0.54
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.72	0.54
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.42	0.54
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.88	0.54
2:I:971:LEU:HD22	2:I:1018:TYR:CD1	2.43	0.54
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.89	0.54
3:J:517:CYS:HA	3:J:716:GLN:NE2	2.21	0.54
3:D:79:LYS:HE3	3:D:80:HIS:HA	1.90	0.54
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.89	0.54
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.54
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.42	0.54
3:J:1167:LYS:HD3	3:J:1174:ARG:NH1	2.22	0.54
1:A:133:LEU:HD11	1:A:140:ILE:HG12	1.89	0.54
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.43	0.54
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.90	0.54
3:D:848:VAL:O	3:D:857:LEU:HD12	2.08	0.54
5:F:343:LYS:H	5:F:343:LYS:HD2	1.72	0.54
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.90	0.54
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.89	0.54
2:I:896:THR:HB	2:I:897:PRO:HD2	1.89	0.54
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.90	0.54
3:J:694:SER:O	3:J:698:MET:HB2	2.07	0.54
5:L:511:ILE:HG13	5:L:512:GLY:H	1.73	0.54
1:B:62:ASP:OD1	1:B:142:MET:HE2	2.07	0.54
1:B:92:VAL:CG1	1:B:95:LYS:HB3	2.37	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.40	0.54
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.22	0.54
1:H:65:LEU:HD22	1:H:171:LEU:HD21	1.89	0.54
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.22	0.54
3:J:850:LYS:HB2	3:J:852:GLY:O	2.07	0.54
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.23	0.54
5:L:577:GLY:O	5:L:581:ASP:N	2.40	0.54
1:A:124:VAL:HG11	1:A:210:THR:HG23	1.89	0.54
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.89	0.54
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.72	0.54
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.90	0.54
3:D:560:ASN:O	3:D:560:ASN:ND2	2.40	0.54
3:J:279:LEU:HD12	3:J:295:GLU:HG3	1.89	0.54
3:J:793:SER:O	3:J:797:THR:HG23	2.08	0.54
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.08	0.54
4:K:71:GLU:O	4:K:75:GLN:HG3	2.08	0.54
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.90	0.54
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.89	0.54
3:D:48:THR:HB	3:D:50:LYS:HG3	1.90	0.54
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.89	0.54
2:I:131:THR:HG22	2:I:132:ASP:H	1.71	0.54
2:I:930:ASP:OD2	2:I:931:VAL:N	2.40	0.54
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.90	0.54
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.22	0.54
1:A:135:ASP:O	1:A:137:ASN:N	2.41	0.54
3:D:903:LEU:HB3	3:D:905:ARG:H	1.71	0.54
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.90	0.54
2:I:1305:TYR:CD2	5:L:531:PRO:HB2	2.43	0.54
3:J:122:SER:O	3:J:126:LEU:HG	2.07	0.54
1:A:137:ASN:N	1:A:137:ASN:OD1	2.41	0.54
1:A:310:ARG:NE	1:A:310:ARG:HA	2.23	0.54
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.43	0.54
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.89	0.54
3:D:871:LEU:HA	3:D:874:GLU:HG3	1.89	0.54
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.43	0.54
2:I:389:PHE:HD1	2:I:395:TYR:HE1	1.54	0.54
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.43	0.54
2:I:1131:MET:HB3	2:I:1141:LEU:CD1	2.37	0.54
2:C:759:SER:OG	2:C:763:THR:N	2.41	0.53
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	1.89	0.53
1:H:37:HIS:CD2	2:I:1216:ARG:HD2	2.43	0.53
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.43	0.53
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.90	0.53
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.43	0.53
5:F:225:ARG:O	5:F:229:VAL:HG13	2.08	0.53
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.42	0.53
2:C:976:ARG:HB2	2:C:997:TRP:HZ3	1.73	0.53
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.43	0.53
2:C:1236:ASN:HB2	2:C:1238:LEU:HD11	1.90	0.53
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.91	0.53
1:G:39:LEU:HD21	1:H:224:LEU:HD11	1.89	0.53
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.38	0.53
2:I:615:VAL:HG13	2:I:651:ASP:H	1.72	0.53
3:J:647:PRO:HG3	3:J:697:MET:N	2.23	0.53
3:J:697:MET:HG3	3:J:698:MET:N	2.23	0.53
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.42	0.53
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.89	0.53
3:D:223:LEU:O	3:D:226:ALA:HB3	2.09	0.53
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.91	0.53
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.88	0.53
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.09	0.53
3:J:81:ARG:C	3:J:83:VAL:H	2.16	0.53
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.91	0.53
3:J:363:LEU:HD21	3:J:487:THR:HG22	1.90	0.53
2:C:1192:GLU:OE2	3:D:764:ARG:HD3	2.09	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.53
1:H:62:ASP:HB3	1:H:141:SER:O	2.08	0.53
1:H:182:ARG:HD3	1:H:206:GLU:OE2	2.09	0.53
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.44	0.53
5:L:377:LYS:O	5:L:381:GLU:HG3	2.09	0.53
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.91	0.53
1:A:263:THR:HG22	1:A:302:GLU:HG2	1.89	0.53
3:D:54:ASP:HB2	3:D:61:ILE:HD11	1.90	0.53
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.90	0.53
5:F:395:THR:OG1	5:F:396:ASN:N	2.42	0.53
2:I:1243:MET:HA	3:J:353:SER:HB3	1.90	0.53
3:J:773:PHE:O	3:J:776:THR:HB	2.09	0.53
5:L:306:PHE:CE1	5:L:310:GLU:HG3	2.44	0.53
1:A:319:GLU:O	1:A:320:ASN:HB2	2.08	0.53
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.90	0.53
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.09	0.53
3:D:751:ASP:HB3	3:D:753:SER:H	1.73	0.53
5:F:233:ASP:O	5:F:236:LYS:HE2	2.07	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:SER:HB2	2:I:1059:ARG:NH2	2.24	0.53
1:H:215:GLU:OE1	1:H:219:ARG:NH1	2.41	0.53
3:J:322:ARG:HB2	3:J:322:ARG:HH11	1.72	0.53
3:J:720:ASN:OD1	3:J:722:ILE:HG22	2.09	0.53
3:J:845:ALA:O	3:J:860:ARG:NE	2.40	0.53
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.43	0.53
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.91	0.53
2:C:425:ILE:O	2:C:429:MET:HG3	2.09	0.53
2:C:510:GLN:CD	2:C:534:GLY:HA2	2.34	0.53
3:D:500:ILE:HG22	3:D:500:ILE:O	2.08	0.53
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.26	0.53
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.09	0.53
1:H:82:LEU:O	1:H:86:LYS:HG3	2.09	0.53
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.39	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.91	0.53
3:J:660:GLU:O	3:J:664:ILE:HG12	2.08	0.53
3:J:709:ARG:HD2	3:J:710:ASP:N	2.24	0.53
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.89	0.53
1:A:27:THR:C	1:A:28:LEU:HD12	2.33	0.53
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.91	0.53
3:D:211:GLU:O	3:D:215:LYS:HB3	2.08	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.08	0.53
5:F:166:VAL:HG23	5:F:258:GLN:O	2.09	0.53
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.22	0.53
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.74	0.53
1:G:154:PRO:HG2	1:G:157:THR:OG1	2.08	0.53
1:H:98:VAL:HG11	1:H:121:VAL:CG2	2.39	0.53
3:J:588:PRO:O	3:J:591:ILE:HG22	2.09	0.53
3:J:761:ALA:H	3:J:771:GLN:HE22	1.56	0.53
3:J:903:LEU:HD22	3:J:909:ILE:HD12	1.91	0.53
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.90	0.53
2:C:150:HIS:CE1	2:C:454:ARG:HE	2.27	0.53
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.53
2:C:720:ARG:CZ	2:C:736:VAL:HG21	2.38	0.53
5:F:316:PHE:HZ	5:F:334:SER:HA	1.74	0.53
1:G:195:ARG:CG	1:G:198:LEU:HG	2.38	0.53
2:I:646:SER:HB3	2:I:649:GLN:CD	2.34	0.53
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.91	0.53
2:I:692:THR:OG1	2:I:827:ARG:O	2.27	0.53
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.53
3:J:903:LEU:HB3	3:J:905:ARG:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.90	0.53
3:J:1174:ARG:HE	3:J:1189:MET:HE2	1.74	0.53
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.08	0.53
3:D:600:ALA:O	3:D:603:LYS:HG2	2.09	0.52
3:D:733:SER:O	3:D:737:ILE:HG12	2.09	0.52
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.74	0.52
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.90	0.52
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.74	0.52
3:J:156:ARG:HH12	3:J:157:GLN:NE2	2.07	0.52
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.91	0.52
3:J:537:TYR:CZ	3:J:544:LEU:HD22	2.44	0.52
3:J:872:LEU:O	3:J:877:VAL:HG12	2.09	0.52
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.23	0.52
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.08	0.52
5:L:419:PHE:HD1	5:L:430:TYR:CD2	2.27	0.52
2:C:98:VAL:O	2:C:121:GLU:HA	2.08	0.52
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.74	0.52
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.91	0.52
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.44	0.52
3:D:705:THR:OG1	3:D:718:SER:HA	2.09	0.52
1:G:60:GLU:HB2	1:G:170:ARG:CG	2.39	0.52
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.91	0.52
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.09	0.52
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.52
3:J:903:LEU:CB	3:J:905:ARG:HG3	2.39	0.52
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.38	0.52
1:A:190:ALA:CB	1:A:200:LYS:HB2	2.39	0.52
2:C:565:GLU:HG2	2:C:565:GLU:O	2.09	0.52
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.92	0.52
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.35	0.52
3:D:706:VAL:HG12	3:D:715:LYS:HB2	1.91	0.52
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.44	0.52
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.92	0.52
1:G:76:GLU:OE2	1:G:76:GLU:N	2.42	0.52
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.24	0.52
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.10	0.52
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.73	0.52
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.91	0.52
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.92	0.52
1:A:44:ARG:NH2	2:C:1091:GLY:O	2.42	0.52
3:D:347:VAL:HG12	3:D:348:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:529:GLY:HA2	3:D:551:ARG:O	2.09	0.52
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.91	0.52
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.90	0.52
3:D:1260:MET:HE3	3:D:1306:LEU:HD21	1.91	0.52
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.90	0.52
5:F:557:LYS:O	5:F:561:MET:HB2	2.09	0.52
1:H:92:VAL:HG13	1:H:120:ASP:O	2.10	0.52
2:I:517:GLN:O	2:I:517:GLN:HG2	2.09	0.52
2:I:521:LEU:O	2:I:525:THR:HB	2.09	0.52
3:J:436:ALA:HB3	3:J:485:MET:HA	1.91	0.52
5:L:460:ILE:O	5:L:463:LEU:HB2	2.10	0.52
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.52
5:L:608:ARG:O	5:L:611:LEU:N	2.30	0.52
1:A:73:GLY:HA2	2:C:726:TYR:OH	2.10	0.52
1:A:102:LEU:HD23	1:A:115:ILE:HA	1.91	0.52
2:C:466:VAL:O	2:C:470:ARG:HG2	2.09	0.52
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.45	0.52
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.90	0.52
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.91	0.52
2:I:143:ARG:NH2	2:I:512:SER:O	2.42	0.52
3:J:363:LEU:HG	3:J:363:LEU:O	2.10	0.52
2:C:169:LYS:HE2	2:C:190:PRO:O	2.09	0.52
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.93	0.52
3:D:84:ILE:HG22	3:D:91:GLU:HB3	1.90	0.52
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.34	0.52
3:D:490:ILE:HA	3:D:500:ILE:HG12	1.91	0.52
3:D:1160:SER:HA	3:D:1204:VAL:O	2.10	0.52
5:F:311:THR:HG21	5:F:348:GLU:CD	2.35	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.91	0.52
2:I:159:SER:O	2:I:160:ASP:HB2	2.09	0.52
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.23	0.52
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.74	0.52
3:J:266:ASN:O	3:J:270:ARG:HB2	2.10	0.52
3:J:1168:GLU:O	3:J:1170:LYS:N	2.43	0.52
1:A:233:ASP:O	1:A:234:LEU:HG	2.09	0.52
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.92	0.52
2:C:1148:ALA:HB1	2:C:1180:MET:HE1	1.91	0.52
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	1.90	0.52
3:D:772:TYR:O	3:D:775:SER:HB3	2.10	0.52
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.37	0.52
4:E:60:ASN:OD1	4:E:63:ILE:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.91	0.52
2:I:320:ASP:OD1	2:I:324:LYS:HE3	2.08	0.52
2:I:796:LEU:H	2:I:796:LEU:HD12	1.74	0.52
2:I:908:GLU:OE1	5:L:611:LEU:HD22	2.09	0.52
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.23	0.52
3:J:1265:THR:HG22	3:J:1277:GLY:CA	2.34	0.52
5:L:288:MET:HA	5:L:302:PHE:CZ	2.45	0.52
1:A:195:ARG:HG2	1:A:198:LEU:HD11	1.91	0.52
1:B:56:VAL:HG11	1:B:144:ILE:HD11	1.92	0.52
2:C:637:ARG:HA	2:C:642:SER:HA	1.92	0.52
2:C:667:LEU:CD2	2:C:704:MET:HB2	2.40	0.52
5:F:354:THR:OG1	5:F:356:GLU:HB3	2.10	0.52
2:I:158:ASP:OD1	2:I:159:SER:N	2.42	0.52
2:I:721:GLY:N	2:I:740:GLU:OE1	2.38	0.52
2:I:757:THR:O	2:I:765:ILE:HG23	2.10	0.52
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.10	0.52
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.52
1:A:66:HIS:CD2	2:C:874:GLY:HA2	2.44	0.52
2:C:182:SER:O	2:C:395:TYR:HE1	1.93	0.52
2:C:550:VAL:HG11	3:D:776:THR:CG2	2.39	0.52
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.52
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.52
5:F:569:THR:OG1	5:F:570:ASP:N	2.43	0.52
3:J:611:ILE:HB	3:J:612:LEU:HD12	1.92	0.52
3:J:705:THR:OG1	3:J:718:SER:HA	2.10	0.52
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.90	0.52
3:J:1344:LEU:O	3:J:1346:GLY:N	2.40	0.52
5:L:261:LEU:H	5:L:261:LEU:HD12	1.75	0.52
5:L:262:VAL:HG11	5:L:264:LYS:HZ1	1.72	0.52
5:L:421:TYR:CE2	5:L:422:ARG:HG3	2.44	0.52
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.92	0.52
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.73	0.52
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.25	0.52
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.92	0.52
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.91	0.52
2:C:635:THR:HG23	2:C:644:LEU:HD22	1.92	0.52
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.92	0.52
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.92	0.52
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.20	0.52
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.91	0.52
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.75	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:CA	2.40	0.52
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.91	0.52
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.42	0.52
4:K:49:ILE:O	4:K:53:GLU:HG3	2.10	0.52
1:B:75:GLN:HG2	1:B:76:GLU:OE1	2.10	0.51
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.90	0.51
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.40	0.51
3:D:227:PHE:O	3:D:230:SER:HB3	2.10	0.51
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.35	0.51
3:D:537:TYR:CE2	3:D:544:LEU:HD22	2.45	0.51
3:D:598:LYS:O	3:D:601:ILE:HG22	2.09	0.51
5:F:348:GLU:HA	5:F:353:LEU:O	2.10	0.51
5:F:465:ARG:HA	5:F:468:ARG:NH2	2.24	0.51
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.25	0.51
2:I:362:ALA:O	2:I:366:ILE:HG13	2.10	0.51
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.45	0.51
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.91	0.51
5:L:135:ALA:HB1	5:L:253:SER:HB3	1.91	0.51
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.43	0.51
1:A:55:ALA:HB3	1:A:177:TYR:CD1	2.44	0.51
1:B:99:ILE:HD12	1:B:145:LYS:HB2	1.90	0.51
1:B:151:GLY:O	1:B:177:TYR:HB2	2.10	0.51
2:C:62:TYR:C	2:C:64:GLY:H	2.18	0.51
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.92	0.51
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.92	0.51
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.25	0.51
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.10	0.51
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.08	0.51
3:J:419:HIS:HB2	4:K:45:LYS:HE2	1.92	0.51
3:J:503:SER:H	3:J:506:VAL:HG11	1.75	0.51
3:J:1149:ARG:NH2	3:J:1153:PRO:HG2	2.26	0.51
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.45	0.51
2:C:817:LEU:CD1	2:C:1085:MET:HE1	2.40	0.51
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.11	0.51
2:C:1247:SER:HB3	3:D:375:GLU:O	2.10	0.51
5:F:471:LEU:HD23	5:F:476:ARG:O	2.09	0.51
1:G:13:LEU:HD23	1:G:13:LEU:H	1.74	0.51
1:G:190:ALA:C	1:G:191:ARG:HD3	2.36	0.51
1:H:73:GLY:CA	1:H:134:THR:HG22	2.33	0.51
2:I:228:VAL:HB	2:I:335:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:277:LEU:HD23	2:I:282:VAL:HG21	1.92	0.51
2:I:448:LEU:HB2	2:I:553:THR:HB	1.93	0.51
1:A:134:THR:HG23	2:C:726:TYR:CE1	2.45	0.51
1:A:187:VAL:HG23	1:A:187:VAL:O	2.10	0.51
1:A:218:ARG:HG3	1:B:231:PHE:O	2.09	0.51
1:B:205:MET:HE1	1:B:217:ILE:HG13	1.92	0.51
3:D:596:LEU:HD11	3:D:604:MET:HE1	1.91	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.92	0.51
5:F:325:PRO:HG2	5:F:326:TRP:CD1	2.45	0.51
1:G:197:ASP:O	1:G:198:LEU:HD23	2.09	0.51
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.46	0.51
2:I:468:LEU:O	2:I:471:VAL:HG12	2.09	0.51
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.45	0.51
3:J:412:LEU:O	3:J:415:VAL:HG22	2.09	0.51
3:J:697:MET:O	3:J:701:LEU:N	2.32	0.51
3:J:825:VAL:CG1	3:J:833:GLU:HB3	2.40	0.51
3:J:1349:GLU:O	3:J:1353:VAL:HG12	2.11	0.51
5:L:121:LYS:O	5:L:124:GLU:HB2	2.11	0.51
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.74	0.51
2:C:1269:ARG:HG2	3:D:343:LEU:HD11	1.93	0.51
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.17	0.51
5:F:426:LYS:HD3	5:F:428:SER:HB2	1.93	0.51
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.92	0.51
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.93	0.51
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.41	0.51
2:I:696:ASP:O	2:I:697:LYS:HB3	2.09	0.51
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.26	0.51
3:J:68:TYR:C	3:J:92:VAL:HG23	2.34	0.51
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.25	0.51
5:L:372:ALA:O	5:L:376:LYS:HG3	2.11	0.51
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.93	0.51
2:C:62:TYR:C	2:C:64:GLY:N	2.68	0.51
2:C:106:GLU:O	2:C:109:ALA:HB2	2.10	0.51
2:C:147:SER:OG	2:C:455:SER:HB3	2.10	0.51
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.41	0.51
2:C:1006:GLU:O	2:C:1010:GLN:N	2.44	0.51
2:C:1134:GLN:O	2:C:1135:GLN:HG2	2.09	0.51
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.10	0.51
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.11	0.51
1:G:219:ARG:HA	1:G:222:THR:HB	1.92	0.51
2:I:98:VAL:C	2:I:121:GLU:HA	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.92	0.51
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.41	0.51
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.92	0.51
2:C:268:ARG:HD2	2:C:270:THR:CG2	2.40	0.51
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.11	0.51
3:D:432:LEU:HD21	3:D:489:ASN:CB	2.40	0.51
2:I:494:ASN:HB3	2:I:497:PRO:HG2	1.91	0.51
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.16	0.51
2:I:582:ASN:HB3	2:I:586:PHE:N	2.25	0.51
2:I:1174:GLU:O	2:I:1177:ARG:HG2	2.11	0.51
3:J:680:ASN:O	3:J:683:ILE:HG22	2.09	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.44	0.51
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.46	0.51
3:D:266:ASN:O	3:D:270:ARG:HB2	2.10	0.51
3:D:702:GLN:HG3	3:D:723:TYR:OH	2.09	0.51
5:F:487:MET:HA	5:F:487:MET:HE2	1.91	0.51
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.92	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.46	0.51
2:I:1012:GLU:O	2:I:1016:GLU:HG3	2.10	0.51
3:J:103:GLY:C	3:J:244:VAL:HG22	2.36	0.51
5:L:108:VAL:HG11	5:L:381:GLU:C	2.35	0.51
5:L:247:GLU:O	5:L:251:LYS:HG3	2.10	0.51
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.93	0.51
2:I:397:LEU:O	2:I:398:SER:OG	2.22	0.51
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.11	0.51
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.93	0.51
3:J:420:PRO:O	3:J:471:PRO:HD2	2.11	0.51
3:J:615:LYS:HE2	3:J:616:PRO:HD3	1.92	0.51
3:J:857:LEU:HD13	3:J:858:VAL:HG13	1.92	0.51
2:C:42:ASP:O	2:C:44:GLU:N	2.36	0.51
2:C:882:ILE:HD12	2:C:882:ILE:H	1.76	0.51
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.93	0.51
1:G:56:VAL:HG21	1:G:144:ILE:HG23	1.91	0.51
2:I:1158:LYS:HG3	2:I:1159:VAL:N	2.25	0.51
3:J:557:LYS:HA	3:J:563:LEU:HA	1.93	0.51
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.26	0.51
3:J:1319:PHE:C	3:J:1319:PHE:CD1	2.89	0.51
1:A:228:LEU:O	1:A:231:PHE:N	2.42	0.50
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.10	0.50
1:A:318:LEU:HD23	1:A:321:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:SER:HB3	2:C:7:GLU:CG	2.34	0.50
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.46	0.50
2:C:600:THR:HG22	2:C:601:ASP:N	2.26	0.50
2:C:987:GLU:O	2:C:991:LYS:HE3	2.10	0.50
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.26	0.50
3:D:147:ILE:HG13	3:D:147:ILE:O	2.11	0.50
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.50
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.43	0.50
2:I:465:ARG:O	2:I:469:VAL:HG13	2.11	0.50
2:I:561:ILE:HD11	2:I:665:ALA:HB1	1.93	0.50
4:K:59:ILE:HG23	4:K:64:LEU:HD21	1.93	0.50
5:L:124:GLU:O	5:L:128:ASN:HB2	2.11	0.50
1:A:152:TYR:CE2	1:A:154:PRO:HB3	2.46	0.50
2:C:802:VAL:CG2	2:C:1098:LEU:HD22	2.41	0.50
3:D:318:GLY:C	3:D:320:ASN:H	2.19	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:847:ASP:HB3	3:D:859:PRO:HA	1.94	0.50
3:D:1227:HIS:HA	3:D:1230:THR:CG2	2.39	0.50
5:F:572:THR:HG23	5:F:575:GLU:HG3	1.94	0.50
2:I:557:ARG:NH2	2:I:608:ALA:HA	2.26	0.50
2:I:959:ASP:O	2:I:963:GLU:HG2	2.11	0.50
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.76	0.50
3:J:1280:VAL:O	3:J:1284:ARG:N	2.37	0.50
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.92	0.50
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.74	0.50
1:A:12:ARG:H	1:A:30:PRO:HD2	1.76	0.50
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.44	0.50
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.91	0.50
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.26	0.50
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.93	0.50
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.92	0.50
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.11	0.50
3:J:825:VAL:C	3:J:826:ILE:HG13	2.36	0.50
3:D:45:ASN:O	3:D:46:TYR:HD2	1.94	0.50
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.50
5:F:142:THR:O	5:F:146:GLU:HG3	2.12	0.50
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.46	0.50
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.46	0.50
2:I:1322:SER:HB3	3:J:345:LYS:HZ1	1.77	0.50
3:J:277:ASN:HA	3:J:280:LYS:HG3	1.92	0.50
3:J:923:ILE:O	3:J:926:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:474:MET:C	5:L:476:ARG:H	2.15	0.50
3:D:793:SER:O	3:D:797:THR:HG23	2.10	0.50
5:F:585:GLU:O	5:F:589:GLN:HG3	2.11	0.50
2:I:486:THR:HG23	2:I:487:LEU:H	1.77	0.50
2:I:998:LEU:HD12	2:I:998:LEU:N	2.26	0.50
3:J:514:THR:HG21	3:J:596:LEU:HB2	1.94	0.50
5:L:234:THR:O	5:L:245:ALA:HB2	2.11	0.50
5:L:347:ILE:HB	5:L:355:ILE:HD11	1.93	0.50
2:C:93:SER:OG	2:C:126:GLU:OE1	2.26	0.50
3:D:261:ALA:HA	5:F:505:ILE:H	1.76	0.50
3:D:702:GLN:O	3:D:718:SER:N	2.37	0.50
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.41	0.50
3:D:849:LEU:CB	3:D:853:THR:HG23	2.41	0.50
1:H:51:MET:HB3	1:H:178:SER:CB	2.41	0.50
2:I:156:PHE:CZ	2:I:158:ASP:HB2	2.47	0.50
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.26	0.50
5:L:551:LEU:CD2	5:L:597:LYS:HD2	2.41	0.50
2:C:60:GLN:O	2:C:476:LYS:HE2	2.11	0.50
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.76	0.50
2:C:886:LYS:HB3	2:C:917:SER:HA	1.93	0.50
3:D:21:LYS:NZ	3:D:23:ALA:HB2	2.26	0.50
3:D:80:HIS:CB	3:D:83:VAL:HG11	2.41	0.50
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.12	0.50
3:D:849:LEU:HA	3:D:855:ASP:O	2.10	0.50
2:I:607:SER:OG	2:I:609:ILE:HG13	2.12	0.50
3:J:761:ALA:H	3:J:771:GLN:NE2	2.09	0.50
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.93	0.50
5:L:108:VAL:HG11	5:L:381:GLU:O	2.11	0.50
1:A:71:LYS:HD3	1:A:72:GLU:H	1.76	0.50
2:C:345:PRO:O	2:C:349:GLU:HG2	2.12	0.50
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.92	0.50
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.94	0.50
3:D:697:MET:SD	3:D:741:ALA:HB3	2.51	0.50
3:D:770:LEU:H	3:D:770:LEU:HD22	1.77	0.50
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.24	0.50
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.77	0.50
5:F:414:LYS:O	5:F:417:ASP:N	2.43	0.50
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.41	0.50
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.93	0.50
1:G:166:ARG:O	1:G:167:PRO:C	2.55	0.50
1:H:88:LEU:HD21	1:H:115:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:250:THR:HA	2:I:268:ARG:HA	1.94	0.50
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.93	0.50
5:L:483:LEU:HD12	5:L:483:LEU:H	1.76	0.50
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.77	0.50
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.94	0.50
1:A:274:ALA:O	1:A:275:ILE:HG13	2.12	0.50
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.93	0.50
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.47	0.50
2:C:884:VAL:HG21	2:C:1050:VAL:HB	1.93	0.50
2:C:897:PRO:HB2	2:C:898:GLU:OE1	2.12	0.50
3:D:1353:VAL:HG13	3:D:1355:ARG:HG2	1.94	0.50
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.94	0.50
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.27	0.50
5:F:606:VAL:O	5:F:609:SER:OG	2.30	0.50
1:G:47:LEU:HB3	1:G:183:ILE:HD13	1.94	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.93	0.50
2:I:494:ASN:OD1	5:L:471:LEU:HD13	2.11	0.50
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.57	0.50
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.93	0.50
1:A:250:ASP:CB	5:F:601:PRO:HB3	2.42	0.49
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.94	0.49
5:F:298:PRO:HD2	5:F:326:TRP:CD1	2.48	0.49
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.38	0.49
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.27	0.49
2:I:1129:ASN:CB	2:I:1177:ARG:HB2	2.41	0.49
2:I:1156:ARG:HB2	2:I:1156:ARG:NH1	2.23	0.49
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.21	0.49
2:I:1262:LYS:C	2:I:1264:GLN:H	2.20	0.49
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.12	0.49
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.42	0.49
3:J:905:ARG:CZ	3:J:910:ASN:HD21	2.25	0.49
2:C:303:ASP:HB3	2:C:306:THR:CG2	2.42	0.49
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.47	0.49
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.12	0.49
3:D:342:LEU:O	3:D:343:LEU:C	2.54	0.49
4:E:72:GLN:O	4:E:76:GLU:HG3	2.12	0.49
1:G:45:ARG:CD	2:I:1083:GLU:HB3	2.42	0.49
2:I:138:ILE:O	2:I:139:ASN:ND2	2.44	0.49
3:J:515:ARG:O	3:J:545:HIS:HB3	2.12	0.49
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.77	0.49
4:K:3:ARG:NE	4:K:3:ARG:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:341:LEU:CD2	5:L:344:LEU:HD23	2.42	0.49
1:A:295:LEU:HD23	1:A:299:SER:HB2	1.94	0.49
2:C:104:ILE:O	2:C:113:THR:HA	2.11	0.49
3:D:647:PRO:HG3	3:D:697:MET:CB	2.42	0.49
3:D:660:GLU:O	3:D:663:GLU:HB2	2.11	0.49
3:D:901:ARG:HA	3:D:908:ILE:HA	1.94	0.49
3:D:1250:ASP:O	3:D:1251:LYS:C	2.55	0.49
3:D:1299:GLY:HA2	3:J:1301:THR:CG2	2.42	0.49
3:D:1359:ALA:O	3:D:1363:TYR:N	2.44	0.49
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.77	0.49
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.48	0.49
3:J:156:ARG:HH12	3:J:157:GLN:HE21	1.59	0.49
3:J:825:VAL:HG22	3:J:833:GLU:H	1.78	0.49
5:L:289:LYS:HG2	5:L:293:GLU:OE1	2.13	0.49
5:L:574:GLU:N	5:L:574:GLU:OE1	2.45	0.49
3:D:292:VAL:O	3:D:296:LYS:HG3	2.12	0.49
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.94	0.49
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.95	0.49
3:J:363:LEU:HB2	3:J:450:HIS:CE1	2.48	0.49
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.41	0.49
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.94	0.49
5:L:379:MET:HG2	5:L:416:VAL:HG22	1.94	0.49
2:C:696:ASP:CB	2:C:798:GLN:HG2	2.32	0.49
2:C:1268:GLN:HE22	3:D:352:ARG:NE	2.10	0.49
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.45	0.49
2:I:26:TYR:OH	2:I:28:LEU:HD12	2.13	0.49
2:I:96:LEU:HD23	2:I:124:MET:HG3	1.93	0.49
2:I:933:VAL:HG11	2:I:945:ALA:HB2	1.94	0.49
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.11	0.49
2:C:617:ALA:HA	2:C:636:CYS:SG	2.52	0.49
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.28	0.49
3:D:161:THR:HG22	3:D:164:GLN:CB	2.41	0.49
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.95	0.49
3:D:849:LEU:H	3:D:849:LEU:HD22	1.77	0.49
3:D:1167:LYS:CD	3:D:1174:ARG:HD2	2.41	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.12	0.49
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.11	0.49
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.34	0.49
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.94	0.49
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.76	0.49
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:O	1:A:167:PRO:C	2.52	0.49
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.12	0.49
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.28	0.49
2:C:122:VAL:CG1	2:C:493:ILE:HD13	2.42	0.49
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.94	0.49
2:C:292:ILE:HG22	2:C:317:LEU:HB2	1.94	0.49
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.57	0.49
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.93	0.49
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.46	0.49
1:G:166:ARG:HD2	1:G:166:ARG:C	2.37	0.49
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.49
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.39	0.49
5:L:325:PRO:HG2	5:L:326:TRP:CD1	2.47	0.49
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.42	0.49
1:B:115:ILE:HG22	1:B:116:THR:N	2.28	0.49
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.48	0.49
2:C:891:GLY:O	2:C:892:GLU:HG3	2.13	0.49
5:F:326:TRP:O	5:F:330:LEU:HG	2.12	0.49
5:F:390:ILE:HD12	5:F:435:ILE:HG21	1.95	0.49
1:H:56:VAL:HG21	1:H:144:ILE:HD11	1.94	0.49
2:I:124:MET:HE2	2:I:493:ILE:HD11	1.93	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
2:I:619:ALA:HB1	2:I:657:THR:HA	1.94	0.49
2:I:698:PRO:HA	2:I:1231:TYR:CD1	2.48	0.49
3:J:16:GLU:HG3	3:J:17:PHE:CD2	2.45	0.49
3:J:56:LEU:HD12	3:J:56:LEU:H	1.78	0.49
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.77	0.49
1:A:59:VAL:HG21	1:A:85:LEU:HD12	1.95	0.49
1:B:108:GLY:O	1:B:133:LEU:HB2	2.12	0.49
2:C:1246:ARG:NH1	2:C:1249:GLY:HA3	2.27	0.49
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.63	0.49
2:I:60:GLN:O	2:I:476:LYS:HE2	2.12	0.49
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.49
3:J:901:ARG:HA	3:J:908:ILE:HA	1.94	0.49
5:L:262:VAL:HG11	5:L:264:LYS:HZ2	1.75	0.49
5:L:469:GLN:O	5:L:473:GLU:HB2	2.13	0.49
5:L:585:GLU:HA	5:L:588:ARG:HD2	1.95	0.49
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.12	0.49
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.95	0.49
2:C:421:SER:N	2:C:424:ASP:OD2	2.45	0.49
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:465:ARG:HA	5:F:468:ARG:CZ	2.42	0.49
2:I:560:PRO:HG3	3:J:773:PHE:CE2	2.48	0.49
2:I:848:GLU:CG	2:I:888:THR:HG22	2.43	0.49
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.13	0.49
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.39	0.49
3:J:358:GLY:N	3:J:359:PRO:HD3	2.28	0.49
3:J:517:CYS:HB2	3:J:716:GLN:OE1	2.13	0.49
5:L:487:MET:HE2	5:L:487:MET:HA	1.94	0.49
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.78	0.48
3:D:710:ASP:CG	3:D:711:GLY:H	2.20	0.48
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.43	0.48
5:F:484:ALA:C	5:F:491:GLU:HB2	2.38	0.48
5:F:503:GLU:OE1	5:F:504:PRO:HD2	2.13	0.48
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.94	0.48
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.27	0.48
1:A:77:ASP:O	1:A:80:GLU:N	2.46	0.48
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.78	0.48
1:A:234:LEU:HD12	1:B:218:ARG:NH1	2.28	0.48
2:C:70:TYR:HA	2:C:100:LEU:CD2	2.42	0.48
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.28	0.48
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.94	0.48
3:D:201:LEU:O	3:D:217:LEU:HD11	2.13	0.48
3:D:204:GLU:HB3	3:D:217:LEU:HD21	1.94	0.48
3:D:1286:LYS:HA	3:D:1289:ASN:HB2	1.95	0.48
1:G:166:ARG:N	1:G:167:PRO:HD2	2.28	0.48
2:I:243:PRO:O	2:I:246:LEU:HD12	2.13	0.48
2:I:470:ARG:HA	2:I:473:ARG:HD2	1.95	0.48
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.28	0.48
3:J:192:MET:HE2	3:J:197:GLU:OE2	2.13	0.48
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.48
3:J:554:GLU:HA	3:J:580:TRP:HZ2	1.78	0.48
3:J:848:VAL:HG11	3:J:877:VAL:HG21	1.94	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.48
1:A:82:LEU:HB3	1:A:173:VAL:HG12	1.95	0.48
1:B:63:GLY:CA	1:B:71:LYS:HE3	2.36	0.48
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.96	0.48
2:C:487:LEU:H	2:C:487:LEU:HD23	1.79	0.48
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.43	0.48
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.14	0.48
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.94	0.48
3:D:1227:HIS:CA	3:D:1230:THR:HG22	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
2:I:971:LEU:HD22	2:I:1018:TYR:HD1	1.79	0.48
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.48
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.48	0.48
3:J:615:LYS:O	3:J:619:ILE:HG22	2.13	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
5:L:283:GLN:O	5:L:287:ILE:HG13	2.14	0.48
5:L:577:GLY:HA3	5:L:583:THR:CG2	2.32	0.48
2:C:42:ASP:C	2:C:44:GLU:H	2.21	0.48
2:C:488:MET:O	2:C:490:GLN:N	2.44	0.48
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.95	0.48
2:C:1101:LEU:O	3:D:731:ARG:HD3	2.14	0.48
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.14	0.48
2:I:30:ILE:H	2:I:30:ILE:CD1	2.17	0.48
2:I:528:ARG:HD3	2:I:663:VAL:HG21	1.96	0.48
2:I:632:ASP:O	2:I:647:ARG:HB2	2.13	0.48
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.78	0.48
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.93	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	1.94	0.48
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.48	0.48
3:J:48:THR:HB	3:J:50:LYS:HG3	1.96	0.48
2:C:553:THR:O	2:C:557:ARG:HD2	2.12	0.48
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.14	0.48
2:C:615:VAL:HG11	2:C:649:GLN:O	2.13	0.48
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.48	0.48
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.93	0.48
3:D:1165:PHE:CD1	3:D:1165:PHE:N	2.81	0.48
1:G:226:GLU:O	1:G:229:GLU:HG3	2.13	0.48
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.28	0.48
2:I:158:ASP:CG	2:I:159:SER:H	2.21	0.48
2:I:646:SER:HB3	2:I:649:GLN:CG	2.44	0.48
2:I:655:VAL:N	2:I:659:GLN:OE1	2.46	0.48
2:I:850:ILE:O	2:I:850:ILE:HG22	2.13	0.48
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	2.14	0.48
2:I:1282:GLY:O	2:I:1284:ALA:N	2.47	0.48
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.78	0.48
1:A:227:GLN:CG	1:B:39:LEU:HD11	2.41	0.48
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.79	0.48
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.96	0.48
2:C:906:PHE:HE2	5:F:608:ARG:HH11	1.61	0.48
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:810:THR:HG23	3:D:811:GLU:N	2.28	0.48
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.95	0.48
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.48
1:G:231:PHE:CD1	1:G:231:PHE:O	2.66	0.48
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.96	0.48
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.48
2:C:408:SER:O	2:C:431:LYS:NZ	2.46	0.48
2:C:811:ASN:HD22	2:C:1098:LEU:C	2.21	0.48
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	0.48
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.48
3:D:83:VAL:O	3:D:91:GLU:HA	2.13	0.48
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.42	0.48
3:D:537:TYR:CZ	3:D:544:LEU:HD22	2.49	0.48
3:D:683:ILE:CD1	3:D:754:ILE:HG23	2.43	0.48
4:E:39:VAL:HG21	4:E:56:GLU:HG3	1.95	0.48
5:F:507:MET:O	5:F:519:LEU:HB3	2.14	0.48
1:G:77:ASP:O	1:G:81:ILE:HG13	2.13	0.48
1:G:142:MET:HG3	1:G:144:ILE:HG13	1.95	0.48
2:I:1192:GLU:OE2	3:J:764:ARG:NH1	2.47	0.48
3:J:478:LEU:HD13	4:K:24:ALA:HA	1.96	0.48
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.29	0.48
5:L:343:LYS:H	5:L:343:LYS:HD2	1.79	0.48
1:B:46:ILE:HD12	1:B:224:LEU:HB2	1.95	0.48
2:C:13:LYS:O	2:C:1183:ALA:N	2.45	0.48
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.47	0.48
3:D:83:VAL:HG13	3:D:92:VAL:CG1	2.44	0.48
3:D:363:LEU:HB2	3:D:450:HIS:CE1	2.49	0.48
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.48
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.42	0.48
2:I:607:SER:N	2:I:610:GLU:HB2	2.28	0.48
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.49	0.48
5:L:316:PHE:O	5:L:320:ILE:HG13	2.14	0.48
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.43	0.48
2:C:617:ALA:HB3	2:C:653:MET:CB	2.44	0.48
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.78	0.48
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.48	0.48
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.14	0.48
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.96	0.48
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.79	0.48
5:F:292:VAL:HG21	5:F:299:LYS:CG	2.44	0.48
5:F:511:ILE:CG1	5:F:512:GLY:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:LEU:HD12	1:H:13:LEU:O	2.14	0.48
2:I:369:MET:SD	2:I:370:MET:SD	3.12	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.94	0.48
2:I:897:PRO:HD3	3:J:77:ARG:HH22	1.78	0.48
3:J:744:ARG:HH11	3:J:763:PHE:HZ	1.61	0.48
3:J:1319:PHE:C	3:J:1319:PHE:HD1	2.22	0.48
5:L:130:VAL:HG23	5:L:266:PHE:HZ	1.79	0.48
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.49	0.48
1:A:315:GLY:C	1:A:316:MET:HG3	2.39	0.48
1:B:92:VAL:HG12	1:B:95:LYS:HB3	1.96	0.48
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.44	0.48
2:C:169:LYS:HD3	2:C:190:PRO:HA	1.96	0.48
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.48	0.48
3:D:215:LYS:CE	3:D:216:LYS:HG3	2.43	0.48
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	1.96	0.48
5:F:577:GLY:CA	5:F:583:THR:HG23	2.34	0.48
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.45	0.48
1:A:252:ILE:HG22	1:A:278:ILE:CD1	2.44	0.47
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.46	0.47
2:C:189:ASP:OD1	2:C:193:ASN:N	2.38	0.47
2:C:324:LYS:C	2:C:327:GLN:HE21	2.16	0.47
2:C:1142:ARG:HD3	2:C:1161:LEU:HD13	1.96	0.47
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.49	0.47
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.49	0.47
3:D:252:LEU:HD23	3:D:262:THR:HB	1.96	0.47
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.96	0.47
3:D:1162:ILE:O	3:D:1178:THR:N	2.47	0.47
3:D:1171:GLY:C	3:D:1193:TRP:HZ3	2.21	0.47
5:F:348:GLU:CG	5:F:354:THR:HA	2.44	0.47
2:I:885:GLY:HA2	2:I:917:SER:CB	2.41	0.47
2:I:976:ARG:HB2	2:I:997:TRP:CZ3	2.48	0.47
3:J:490:ILE:HA	3:J:500:ILE:CG1	2.43	0.47
3:J:647:PRO:HG3	3:J:697:MET:CA	2.44	0.47
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.47
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.30	0.47
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.40	0.47
3:D:58:CYS:SG	3:D:60:ARG:HB3	2.55	0.47
3:D:75:TYR:CD2	3:D:80:HIS:HD2	2.27	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.95	0.47
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.47	0.47
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:PRO:O	1:H:12:ARG:HG3	2.14	0.47
2:I:38:PHE:HB2	2:I:457:GLY:O	2.13	0.47
2:I:383:SER:O	2:I:387:ASN:HB2	2.14	0.47
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.97	0.47
2:I:667:LEU:HD23	2:I:704:MET:HB2	1.95	0.47
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.47	0.47
3:J:259:ARG:HD2	5:L:505:ILE:CD1	2.40	0.47
3:J:517:CYS:CA	3:J:716:GLN:HE22	2.25	0.47
3:J:1319:PHE:O	3:J:1322:ALA:HB3	2.14	0.47
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.78	0.47
1:A:12:ARG:HG2	1:A:13:LEU:H	1.80	0.47
2:C:39:ILE:HG23	2:C:39:ILE:O	2.14	0.47
2:C:519:ASN:HB3	2:C:522:SER:CB	2.44	0.47
2:C:522:SER:O	2:C:525:THR:HG22	2.13	0.47
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.14	0.47
3:D:630:ALA:O	3:D:633:ALA:HB3	2.15	0.47
3:D:710:ASP:CG	3:D:711:GLY:N	2.73	0.47
5:F:456:MET:HE1	5:F:497:VAL:HG13	1.96	0.47
1:H:67:GLU:O	1:H:78:ILE:HB	2.14	0.47
1:H:110:VAL:HG23	1:H:133:LEU:HD13	1.97	0.47
2:I:10:ARG:NH2	2:I:791:LEU:HB2	2.28	0.47
2:I:153:PRO:HB2	2:I:401:GLY:HA2	1.96	0.47
2:I:202:ARG:NH1	2:I:369:MET:HA	2.29	0.47
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.22	0.47
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.45	0.47
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.96	0.47
2:I:1142:ARG:NH1	2:I:1169:VAL:HG21	2.29	0.47
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.96	0.47
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.61	0.47
2:C:395:TYR:HB3	2:C:419:ILE:CG2	2.45	0.47
2:C:493:ILE:O	2:C:493:ILE:HG12	2.13	0.47
1:G:156:SER:CB	2:I:1059:ARG:HH22	2.26	0.47
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.39	0.47
2:I:568:ASN:HB2	2:I:571:LEU:HB2	1.95	0.47
2:I:849:GLU:HB2	2:I:851:THR:HG22	1.96	0.47
2:I:932:GLN:HB3	2:I:934:PHE:CE2	2.50	0.47
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.03	0.47
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.97	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.45	0.47
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.29	0.47
3:J:133:ARG:O	3:J:137:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.96	0.47
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.21	0.47
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.96	0.47
3:J:709:ARG:HD2	3:J:710:ASP:H	1.78	0.47
5:L:362:ASN:HA	5:L:365:MET:HB2	1.96	0.47
5:L:392:LYS:O	5:L:395:THR:HG22	2.14	0.47
5:L:558:VAL:HG23	5:L:580:PHE:HE2	1.79	0.47
2:C:1269:ARG:CG	3:D:343:LEU:HD11	2.43	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.46	0.47
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.96	0.47
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.79	0.47
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.97	0.47
2:I:670:PHE:CD1	2:I:1113:LEU:HD23	2.49	0.47
2:I:1299:ASN:O	2:I:1303:LYS:HG2	2.15	0.47
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.97	0.47
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.96	0.47
5:L:311:THR:O	5:L:341:LEU:HD21	2.14	0.47
5:L:557:LYS:HG3	5:L:561:MET:HE1	1.97	0.47
1:A:11:PRO:HD2	1:B:227:GLN:O	2.15	0.47
1:A:58:GLU:HG2	1:A:158:ARG:NH2	2.25	0.47
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.96	0.47
2:C:785:ASP:OD2	2:C:791:LEU:N	2.46	0.47
2:C:861:ALA:HB1	2:C:882:ILE:CD1	2.45	0.47
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.97	0.47
2:C:1281:TYR:OH	3:D:431:ARG:O	2.32	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.47
3:D:193:ASP:CG	3:D:196:GLN:HG2	2.39	0.47
3:D:810:THR:O	3:D:911:LYS:HE2	2.14	0.47
4:E:15:ASN:HB3	4:E:18:ASP:H	1.80	0.47
1:H:79:LEU:O	1:H:82:LEU:HB2	2.14	0.47
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.97	0.47
5:L:454:VAL:O	5:L:458:GLU:HG3	2.15	0.47
5:L:585:GLU:O	5:L:589:GLN:HG3	2.14	0.47
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.96	0.47
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.44	0.47
2:C:63:SER:C	2:C:65:ASN:H	2.21	0.47
2:C:256:GLU:OE2	2:C:261:VAL:HG22	2.14	0.47
2:C:670:PHE:CD1	2:C:1113:LEU:HD23	2.50	0.47
2:C:785:ASP:HB3	2:C:789:THR:O	2.13	0.47
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.47
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:239:LEU:HD23	3:D:239:LEU:HA	1.62	0.47
3:D:514:THR:HG21	3:D:596:LEU:HG	1.97	0.47
3:D:1327:GLU:OE2	3:D:1329:THR:HB	2.14	0.47
5:F:583:THR:O	5:F:584:ARG:HB2	2.14	0.47
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	1.97	0.47
2:I:802:VAL:CG2	2:I:1098:LEU:HD13	2.45	0.47
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.14	0.47
3:J:418:GLU:HB3	4:K:48:VAL:HG23	1.97	0.47
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.47
3:J:697:MET:HE2	3:J:698:MET:HG2	1.97	0.47
3:J:1273:ASP:HB3	3:J:1276:GLU:CD	2.40	0.47
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.27	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.83	0.47
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.95	0.47
2:C:667:LEU:HD23	2:C:704:MET:HB2	1.96	0.47
2:C:857:VAL:HG21	2:C:862:LEU:HD21	1.97	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.70	0.47
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.79	0.47
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:CB	2.44	0.47
1:G:58:GLU:CD	1:G:145:LYS:HE3	2.39	0.47
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.97	0.47
2:I:964:LEU:HD13	2:I:1021:LEU:O	2.14	0.47
3:J:658:GLU:O	3:J:661:VAL:HG22	2.14	0.47
3:J:1162:ILE:HD12	3:J:1163:VAL:H	1.80	0.47
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.97	0.47
5:L:415:ALA:O	5:L:419:PHE:N	2.48	0.47
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.97	0.47
1:A:263:THR:HG23	1:A:266:SER:H	1.78	0.47
2:C:980:VAL:HA	2:C:984:VAL:HA	1.97	0.47
2:C:1028:LYS:O	2:C:1032:LYS:HB2	2.15	0.47
2:C:1164:PHE:C	2:C:1166:ASP:H	2.23	0.47
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.78	0.47
3:D:124:ILE:HG23	3:D:189:LEU:HD21	1.96	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.23	0.47
3:D:412:LEU:HD23	3:D:416:ILE:HG12	1.96	0.47
3:D:518:VAL:HB	3:D:707:ILE:HD13	1.97	0.47
1:G:73:GLY:HA2	1:G:134:THR:HG22	1.96	0.47
2:I:337:PHE:CE2	2:I:343:HIS:CD2	3.03	0.47
3:J:481:ARG:O	4:K:6:VAL:HG11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:C	1:A:187:VAL:HG11	2.40	0.47
2:C:210:LEU:O	2:C:215:TYR:HB2	2.15	0.47
3:D:746:LEU:HG	3:D:758:PRO:HG3	1.96	0.47
3:D:870:ASP:O	3:D:874:GLU:N	2.44	0.47
2:I:519:ASN:HB3	2:I:522:SER:HB2	1.97	0.47
2:I:551:HIS:CE1	2:I:553:THR:OG1	2.68	0.47
2:I:561:ILE:O	2:I:680:LEU:HD12	2.15	0.47
2:I:596:ASP:CG	2:I:597:GLY:N	2.73	0.47
2:I:1014:LEU:O	2:I:1018:TYR:HB2	2.15	0.47
2:I:1223:ARG:HG3	3:J:635:SER:O	2.15	0.47
3:J:484:MET:HE2	3:J:484:MET:HB3	1.72	0.47
3:J:850:LYS:HB3	3:J:851:PRO:CD	2.42	0.47
1:A:310:ARG:HA	1:A:310:ARG:HE	1.79	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.97	0.46
2:C:490:GLN:HG3	5:F:472:GLN:CG	2.43	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
3:D:647:PRO:HG3	3:D:697:MET:CA	2.45	0.46
2:I:324:LYS:O	2:I:327:GLN:NE2	2.48	0.46
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.33	0.46
2:I:975:ILE:O	2:I:979:LEU:HB2	2.15	0.46
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.50	0.46
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.79	0.46
3:J:189:LEU:HB3	3:J:234:PRO:CB	2.43	0.46
3:J:691:ASP:O	3:J:695:LYS:HG2	2.15	0.46
3:J:707:ILE:H	3:J:707:ILE:HD12	1.80	0.46
5:L:288:MET:CG	5:L:299:LYS:HE2	2.45	0.46
2:C:632:ASP:O	2:C:647:ARG:HB2	2.15	0.46
2:C:746:ALA:CB	2:C:974:ARG:HE	2.28	0.46
2:C:879:GLY:HA2	2:C:920:VAL:HG12	1.97	0.46
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.46
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.97	0.46
3:D:19:ALA:H	3:D:1344:LEU:HD12	1.80	0.46
3:D:905:ARG:HH12	4:E:10:VAL:CG1	2.28	0.46
3:D:1156:LEU:HD22	3:D:1156:LEU:N	2.29	0.46
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.97	0.46
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.97	0.46
5:F:313:ASP:CG	5:F:338:HIS:HE2	2.23	0.46
1:G:166:ARG:O	1:G:168:ILE:N	2.48	0.46
1:H:201:LEU:HG	1:H:203:ILE:CD1	2.46	0.46
2:I:985:GLU:CG	2:I:988:LYS:HD2	2.46	0.46
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.97	0.46
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.28	0.46
1:A:73:GLY:C	1:A:134:THR:HG22	2.41	0.46
1:B:106:GLY:O	1:B:133:LEU:HB3	2.15	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.30	0.46
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.76	0.46
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.96	0.46
3:D:744:ARG:HG3	3:D:744:ARG:O	2.15	0.46
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.44	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.50	0.46
5:F:97:PRO:HA	5:F:100:MET:HG3	1.98	0.46
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.15	0.46
5:F:504:PRO:C	5:F:505:ILE:HD12	2.40	0.46
1:G:22:THR:OG1	1:G:23:HIS:N	2.48	0.46
2:I:817:LEU:CD1	2:I:1085:MET:HE1	2.46	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.15	0.46
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.47	0.46
3:J:233:LYS:H	3:J:236:TRP:HE3	1.63	0.46
3:J:683:ILE:HD11	3:J:754:ILE:HG21	1.98	0.46
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.46
3:J:1250:ASP:O	3:J:1251:LYS:C	2.58	0.46
3:J:1281:GLU:O	3:J:1285:VAL:HB	2.16	0.46
5:L:129:GLN:HB2	5:L:368:GLY:HA3	1.98	0.46
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.73	0.46
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.98	0.46
1:B:153:VAL:O	1:B:175:ALA:N	2.22	0.46
2:C:1252:SER:HB3	2:C:1255:THR:O	2.16	0.46
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.67	0.46
4:E:71:GLU:O	4:E:75:GLN:HG3	2.15	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.45	0.46
3:J:801:VAL:O	3:J:805:GLN:HB2	2.15	0.46
5:L:114:GLU:HG3	5:L:115:GLY:H	1.81	0.46
5:L:253:SER:O	5:L:257:LYS:HG3	2.15	0.46
5:L:346:GLN:HG2	5:L:346:GLN:O	2.14	0.46
2:C:229:ILE:CD1	2:C:334:GLU:HG2	2.46	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.45	0.46
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.80	0.46
3:D:367:GLY:HA3	3:D:448:GLN:CB	2.38	0.46
3:D:702:GLN:HA	3:D:723:TYR:CE2	2.50	0.46
3:D:848:VAL:HG13	3:D:857:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1284:ARG:NH2	3:J:1292:LEU:HD11	2.30	0.46
5:F:287:ILE:O	5:F:291:CYS:SG	2.70	0.46
2:I:582:ASN:O	2:I:585:GLY:N	2.47	0.46
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.44	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
2:I:921:PRO:HB2	2:I:924:VAL:HG22	1.97	0.46
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.51	0.46
3:J:293:ARG:O	3:J:294:ASN:C	2.57	0.46
3:J:293:ARG:O	3:J:296:LYS:N	2.49	0.46
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.13	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.15	0.46
2:C:600:THR:HG22	2:C:601:ASP:H	1.81	0.46
2:C:1247:SER:OG	2:C:1248:THR:N	2.49	0.46
3:D:484:MET:HE2	3:D:484:MET:HB3	1.70	0.46
3:D:647:PRO:CG	3:D:697:MET:HB3	2.42	0.46
3:D:847:ASP:OD1	3:D:847:ASP:N	2.42	0.46
3:D:1163:VAL:HG21	3:D:1175:LEU:HD21	1.98	0.46
5:F:461:ASN:O	5:F:465:ARG:HG2	2.15	0.46
5:F:519:LEU:HD23	5:F:519:LEU:C	2.41	0.46
1:G:51:MET:HE1	1:G:216:ALA:HA	1.98	0.46
2:I:553:THR:O	2:I:557:ARG:HD2	2.16	0.46
2:I:1023:HIS:O	2:I:1027:LYS:HG2	2.15	0.46
3:J:245:LEU:O	3:J:250:ARG:NE	2.46	0.46
3:J:848:VAL:H	3:J:858:VAL:HG22	1.81	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.26	0.46
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.53	0.46
1:A:296:GLY:H	1:A:299:SER:CB	2.20	0.46
2:C:95:PRO:CA	2:C:126:GLU:HG2	2.46	0.46
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.46	0.46
2:C:867:GLU:H	2:C:867:GLU:HG3	1.17	0.46
2:C:953:LEU:HD13	2:C:1036:ILE:HD12	1.97	0.46
2:C:1142:ARG:HH11	2:C:1161:LEU:CD1	2.28	0.46
3:D:710:ASP:OD1	3:D:711:GLY:N	2.49	0.46
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.46	0.46
1:H:95:LYS:HZ3	1:H:98:VAL:HG23	1.78	0.46
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.46
2:I:738:GLU:HA	2:I:741:MET:CE	2.46	0.46
2:I:811:ASN:N	2:I:811:ASN:OD1	2.48	0.46
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.97	0.46
2:I:1180:MET:HA	2:I:1181:PRO:HD3	1.78	0.46
2:I:1255:THR:O	2:I:1257:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.15	0.46
3:J:1157:ALA:HB3	3:J:1207:GLY:N	2.28	0.46
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.15	0.46
5:L:372:ALA:O	5:L:375:ALA:HB3	2.16	0.46
1:B:57:THR:OG1	1:B:147:GLN:HB3	2.16	0.46
2:C:91:THR:HB	2:C:138:ILE:O	2.16	0.46
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.97	0.46
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.97	0.46
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.46
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.81	0.46
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.46
3:D:1197:ASN:HB2	3:D:1212:ASP:OD2	2.16	0.46
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.80	0.46
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.46
5:F:383:ASN:O	5:F:386:LEU:HB3	2.15	0.46
2:I:106:GLU:O	2:I:109:ALA:HB2	2.16	0.46
2:I:569:ILE:C	2:I:571:LEU:H	2.23	0.46
2:I:1139:ALA:O	2:I:1143:GLU:HB2	2.16	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.97	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.16	0.46
1:B:217:ILE:HA	1:B:220:ALA:HB3	1.96	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.96	0.46
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.16	0.46
2:C:1269:ARG:HD3	3:D:343:LEU:HD21	1.96	0.46
3:D:123:ARG:NH1	3:D:1334:GLU:HG3	2.31	0.46
3:D:708:ASN:HB3	3:D:712:GLN:O	2.16	0.46
5:F:226:ALA:O	5:F:230:VAL:HG12	2.15	0.46
5:F:316:PHE:O	5:F:320:ILE:HG13	2.15	0.46
5:F:489:MET:O	5:F:491:GLU:N	2.49	0.46
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.51	0.46
1:H:217:ILE:HA	1:H:220:ALA:HB3	1.98	0.46
2:I:886:LYS:CE	2:I:916:SER:HB3	2.46	0.46
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.98	0.46
3:J:267:ASP:OD1	3:J:271:ARG:NH2	2.49	0.46
5:L:138:PRO:HD2	5:L:353:LEU:HD11	1.98	0.46
5:L:288:MET:O	5:L:292:VAL:HG23	2.16	0.46
2:C:131:THR:HG22	2:C:132:ASP:H	1.81	0.46
2:C:730:SER:O	2:C:753:LEU:HB2	2.15	0.46
2:C:890:LYS:NZ	2:C:891:GLY:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:ARG:HD2	2:C:989:LEU:CD2	2.46	0.46
3:D:58:CYS:SG	3:D:59:ALA:N	2.89	0.46
3:D:137:ARG:CG	3:D:142:GLU:HB2	2.45	0.46
3:D:744:ARG:O	3:D:759:ILE:HB	2.15	0.46
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.46
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.46
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.46
2:I:290:GLU:HG2	2:I:319:LEU:HD12	1.97	0.46
3:J:452:LEU:HD11	3:J:625:MET:HB2	1.98	0.46
3:J:491:LEU:HD22	3:J:496:GLY:O	2.16	0.46
3:J:514:THR:HG21	3:J:596:LEU:CG	2.46	0.46
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.41	0.46
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.13	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.51	0.46
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.16	0.46
1:B:38:THR:HG23	1:B:39:LEU:N	2.32	0.45
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.51	0.45
2:C:744:GLY:O	2:C:746:ALA:N	2.48	0.45
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.80	0.45
2:C:811:ASN:N	2:C:811:ASN:OD1	2.48	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.50	0.45
3:D:45:ASN:O	3:D:46:TYR:HB3	2.15	0.45
3:D:102:MET:HE2	3:D:244:VAL:O	2.16	0.45
3:D:627:THR:HG23	3:D:628:GLY:N	2.31	0.45
3:D:860:ARG:HH11	3:D:860:ARG:CB	2.26	0.45
3:D:1347:LEU:O	3:D:1348:LYS:C	2.59	0.45
5:F:222:ALA:O	5:F:226:ALA:N	2.45	0.45
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.41	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.45	0.45
2:I:91:THR:HB	2:I:138:ILE:O	2.16	0.45
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.49	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.80	0.45
2:I:1296:ASP:OD2	2:I:1321:GLU:N	2.49	0.45
3:J:93:THR:HG22	3:J:94:GLN:H	1.80	0.45
3:J:385:LEU:HA	3:J:385:LEU:HD23	1.73	0.45
3:J:474:LEU:HB2	4:K:28:ARG:NH1	2.31	0.45
3:J:805:GLN:HE22	3:J:1348:LYS:HD3	1.80	0.45
3:J:844:THR:HG23	3:J:864:LEU:HD21	1.98	0.45
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.68	0.45
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.31	0.45
1:A:321:TRP:CD2	1:A:322:PRO:HB3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:HB3	1:B:141:SER:O	2.15	0.45
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.75	0.45
2:C:960:LEU:HD11	2:C:1028:LYS:HE2	1.97	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.46	0.45
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.65	0.45
3:D:423:LEU:HB3	3:D:466:MET:HE1	1.98	0.45
3:D:521:LYS:HB3	3:D:541:LEU:O	2.16	0.45
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.97	0.45
2:I:175:ARG:HD3	2:I:183:TRP:CE3	2.52	0.45
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.48	0.45
2:I:1212:LEU:HD11	2:I:1227:VAL:HG11	1.98	0.45
2:I:1292:THR:HG22	2:I:1293:VAL:N	2.31	0.45
3:J:267:ASP:HA	3:J:270:ARG:NH2	2.28	0.45
3:J:1298:VAL:O	3:J:1298:VAL:HG13	2.16	0.45
3:J:1327:GLU:OE1	3:J:1330:ARG:HB2	2.17	0.45
1:A:189:ALA:HB1	1:A:191:ARG:NH2	2.31	0.45
2:C:30:ILE:H	2:C:30:ILE:HD12	1.82	0.45
2:C:83:GLN:O	2:C:87:ILE:HG13	2.17	0.45
2:C:210:LEU:HB2	2:C:220:ILE:HD11	1.97	0.45
2:C:455:SER:HA	2:C:459:MET:HE2	1.97	0.45
2:C:744:GLY:C	2:C:746:ALA:N	2.71	0.45
2:C:800:MET:HG3	2:C:1096:ILE:CD1	2.46	0.45
2:C:883:LEU:HB3	2:C:1052:VAL:HG21	1.99	0.45
3:D:58:CYS:SG	3:D:60:ARG:N	2.87	0.45
3:D:210:SER:OG	3:D:213:LYS:HD2	2.16	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
5:F:95:THR:O	5:F:96:ASP:C	2.59	0.45
5:F:99:ARG:HD3	5:F:99:ARG:HA	1.72	0.45
5:F:290:LEU:O	5:F:333:VAL:HG11	2.16	0.45
5:F:386:LEU:O	5:F:390:ILE:HG13	2.17	0.45
2:I:486:THR:HG23	2:I:487:LEU:N	2.31	0.45
2:I:1196:LYS:O	2:I:1200:LYS:HG3	2.17	0.45
5:L:557:LYS:HG3	5:L:561:MET:CE	2.46	0.45
1:A:47:LEU:O	1:A:180:VAL:HG21	2.17	0.45
2:C:15:PHE:CD2	2:C:1190:ALA:HB2	2.51	0.45
2:C:1307:ASN:O	2:C:1311:GLY:N	2.50	0.45
3:D:113:HIS:C	3:D:113:HIS:ND1	2.74	0.45
3:D:247:PRO:HA	3:D:250:ARG:CZ	2.47	0.45
3:D:255:LEU:HD13	3:D:255:LEU:HA	1.82	0.45
3:D:298:MET:SD	5:F:402:LEU:HB3	2.57	0.45
3:D:805:GLN:C	3:D:807:LEU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:15:ASN:C	4:E:17:PHE:H	2.24	0.45
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.81	0.45
2:I:95:PRO:HB3	2:I:123:TYR:CE1	2.51	0.45
2:I:119:GLU:CG	2:I:489:PRO:HD2	2.43	0.45
2:I:814:ASP:OD1	2:I:814:ASP:N	2.49	0.45
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.99	0.45
5:L:310:GLU:O	5:L:344:LEU:HD21	2.16	0.45
2:C:87:ILE:HG13	2:C:87:ILE:H	1.51	0.45
2:C:117:ILE:H	2:C:117:ILE:HG12	1.59	0.45
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.81	0.45
2:C:826:ASP:O	2:C:829:THR:HB	2.16	0.45
2:C:1117:LEU:HD21	2:C:1182:ILE:HD12	1.99	0.45
2:C:1230:MET:HG2	2:C:1232:MET:HG3	1.99	0.45
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.98	0.45
3:D:311:ARG:NH2	3:D:1329:THR:HG21	2.32	0.45
3:D:490:ILE:HA	3:D:500:ILE:HG13	1.98	0.45
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.95	0.45
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.82	0.45
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.98	0.45
2:I:974:ARG:HD3	2:I:1010:GLN:HE21	1.82	0.45
3:J:193:ASP:HB3	3:J:196:GLN:HG2	1.98	0.45
3:J:398:LYS:O	3:J:402:GLU:HB2	2.16	0.45
3:J:532:GLU:HB2	3:J:535:ARG:NH2	2.30	0.45
3:J:811:GLU:O	3:J:895:CYS:HA	2.16	0.45
3:J:861:ASN:HD22	3:J:883:ARG:HH11	1.63	0.45
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.51	0.45
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.97	0.45
1:A:237:VAL:O	1:B:13:LEU:HA	2.17	0.45
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.47	0.45
2:C:738:GLU:HA	2:C:741:MET:HE2	1.98	0.45
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.99	0.45
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.16	0.45
2:C:1207:SER:C	2:C:1209:GLN:N	2.73	0.45
3:D:405:GLU:O	3:D:408:VAL:HG22	2.17	0.45
3:D:1350:ASN:OD1	3:D:1355:ARG:HD2	2.17	0.45
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.50	0.45
2:I:361:SER:O	2:I:364:VAL:HB	2.16	0.45
2:I:526:HIS:O	2:I:529:ARG:HB2	2.17	0.45
2:I:738:GLU:HA	2:I:741:MET:HE2	1.97	0.45
3:J:73:GLY:O	3:J:76:LYS:HG3	2.17	0.45
5:L:565:ILE:HG22	5:L:566:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.52	0.45
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.50	0.45
2:C:615:VAL:HG13	2:C:651:ASP:N	2.29	0.45
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.80	0.45
3:D:98:ARG:O	3:D:247:PRO:HD2	2.17	0.45
3:D:276:ASN:O	3:D:280:LYS:HG2	2.17	0.45
3:D:491:LEU:HD23	3:D:491:LEU:HA	1.72	0.45
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.42	0.45
5:F:96:ASP:O	5:F:99:ARG:N	2.42	0.45
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.98	0.45
2:I:898:GLU:CB	5:L:540:LEU:HD22	2.46	0.45
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.17	0.45
2:I:1306:LYS:HE2	5:L:535:ALA:HA	1.97	0.45
3:J:451:PRO:HD2	3:J:625:MET:SD	2.57	0.45
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.17	0.45
5:L:583:THR:HG22	5:L:584:ARG:N	2.32	0.45
2:C:239:MET:N	2:C:285:ILE:O	2.48	0.45
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.32	0.45
3:D:47:ARG:NH1	5:F:500:ILE:HD11	2.31	0.45
3:D:327:LEU:HA	3:D:327:LEU:HD23	1.74	0.45
3:D:678:ARG:HD2	3:D:678:ARG:C	2.42	0.45
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.82	0.45
1:G:51:MET:HA	1:G:52:PRO:HD3	1.80	0.45
1:G:150:ARG:NH1	1:H:7:GLU:O	2.42	0.45
2:I:976:ARG:O	2:I:980:VAL:HG23	2.17	0.45
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.98	0.45
2:I:1340:GLU:HG2	3:J:21:LYS:HB2	1.98	0.45
3:J:35:PHE:HE1	3:J:101:ARG:HH11	1.64	0.45
3:J:474:LEU:CD2	4:K:28:ARG:HG2	2.47	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.31	0.45
1:A:31:LEU:HD12	1:A:201:LEU:HB2	1.99	0.45
1:A:60:GLU:HG3	1:A:169:GLY:O	2.17	0.45
1:A:90:VAL:O	1:A:210:THR:HG21	2.17	0.45
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.99	0.45
1:A:312:LEU:HD12	1:A:312:LEU:H	1.81	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.17	0.45
2:C:796:LEU:HD12	2:C:796:LEU:N	2.30	0.45
2:C:871:VAL:O	2:C:944:ARG:NH1	2.50	0.45
2:C:1146:GLN:HG2	2:C:1160:ASP:OD1	2.16	0.45
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.44	0.45
5:F:100:MET:HE2	5:F:100:MET:HB3	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:LEU:HD22	1:H:171:LEU:HD11	1.99	0.45
2:I:272:ARG:HD3	2:I:273:HIS:CD2	2.52	0.45
2:I:682:GLY:O	2:I:686:GLN:HB2	2.17	0.45
3:J:193:ASP:HB3	3:J:196:GLN:CG	2.46	0.45
3:J:510:LEU:HD12	3:J:628:GLY:HA2	1.99	0.45
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.97	0.45
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.98	0.45
1:A:282:VAL:HG22	1:A:316:MET:SD	2.56	0.45
2:C:353:VAL:O	2:C:355:PRO:HD3	2.17	0.45
2:C:688:GLN:OE1	2:C:1237:HIS:CE1	2.69	0.45
2:C:1262:LYS:C	2:C:1264:GLN:H	2.25	0.45
2:C:1276:TRP:HA	2:C:1279:GLU:OE1	2.17	0.45
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.31	0.45
3:D:256:ASP:C	3:D:258:GLY:H	2.25	0.45
3:D:478:LEU:HG	4:E:47:THR:HG23	1.98	0.45
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.45
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.86	0.45
1:G:50:SER:HG	1:H:35:PHE:HE1	1.64	0.45
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.40	0.45
2:I:618:GLN:OE1	3:J:769:VAL:HB	2.16	0.45
2:I:658:GLN:O	2:I:661:VAL:HG22	2.17	0.45
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.99	0.45
2:I:1287:LEU:HD23	2:I:1288:GLN:N	2.32	0.45
3:J:128:LEU:HD23	3:J:192:MET:CE	2.47	0.45
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.41	0.45
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.17	0.45
2:C:106:GLU:HG3	2:C:107:ARG:N	2.32	0.44
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.17	0.44
2:C:202:ARG:NH1	2:C:368:ARG:HH22	2.14	0.44
2:C:253:PHE:C	2:C:265:LYS:HB2	2.43	0.44
2:C:865:LEU:HD23	2:C:871:VAL:HA	1.99	0.44
3:D:427:PRO:HB2	3:D:429:LEU:CD2	2.47	0.44
3:D:853:THR:HG22	3:D:854:ALA:N	2.29	0.44
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.32	0.44
1:G:14:VAL:HG13	1:G:27:THR:HB	1.98	0.44
2:I:106:GLU:HG3	2:I:107:ARG:N	2.31	0.44
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
2:I:674:ASP:O	3:J:772:TYR:OH	2.33	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.71	0.44
3:J:48:THR:C	3:J:50:LYS:N	2.75	0.44
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:419:HIS:C	3:J:419:HIS:CD2	2.96	0.44
3:J:1149:ARG:HH21	3:J:1153:PRO:HG2	1.80	0.44
5:L:292:VAL:HG21	5:L:299:LYS:CG	2.47	0.44
1:A:285:THR:OG1	1:A:286:GLU:N	2.50	0.44
2:C:18:ARG:HG2	2:C:1188:ASP:OD1	2.17	0.44
2:C:557:ARG:HB3	2:C:587:LEU:HD13	2.00	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.81	0.44
2:C:814:ASP:OD1	2:C:814:ASP:N	2.50	0.44
2:C:950:GLU:O	2:C:953:LEU:HB3	2.16	0.44
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.83	0.44
3:D:343:LEU:HD13	3:D:344:GLY:N	2.33	0.44
3:D:357:VAL:HB	3:D:358:GLY:H	1.67	0.44
3:D:412:LEU:O	3:D:415:VAL:HG22	2.17	0.44
3:D:518:VAL:N	3:D:716:GLN:HE22	2.15	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HG3	1.99	0.44
3:D:1146:GLU:HG2	3:D:1148:ARG:NH2	2.33	0.44
5:F:572:THR:O	5:F:576:VAL:HG23	2.18	0.44
1:H:217:ILE:O	1:H:218:ARG:C	2.60	0.44
2:I:670:PHE:CE1	2:I:1184:THR:HG21	2.52	0.44
2:I:945:ALA:O	2:I:949:GLU:HB2	2.17	0.44
2:I:981:ALA:HB1	2:I:1007:LYS:HZ3	1.81	0.44
3:J:845:ALA:HB3	3:J:846:GLU:HG2	1.99	0.44
3:J:1291:GLU:HG2	3:J:1297:LYS:NZ	2.32	0.44
5:L:362:ASN:HA	5:L:365:MET:CB	2.46	0.44
1:A:66:HIS:HD1	1:A:66:HIS:C	2.24	0.44
1:A:285:THR:O	1:A:289:LEU:HG	2.18	0.44
1:B:6:THR:OG1	1:B:7:GLU:N	2.50	0.44
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.80	0.44
2:C:858:GLY:O	2:C:862:LEU:HG	2.18	0.44
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.00	0.44
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.17	0.44
3:D:45:ASN:O	3:D:46:TYR:CD2	2.69	0.44
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.98	0.44
3:D:416:ILE:HA	3:D:416:ILE:HD12	1.72	0.44
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.98	0.44
5:F:130:VAL:HA	5:F:133:SER:HB2	1.98	0.44
1:G:200:LYS:HB2	1:G:200:LYS:HE2	1.60	0.44
1:H:34:GLY:O	1:H:38:THR:HG22	2.18	0.44
2:I:153:PRO:HB2	2:I:401:GLY:CA	2.48	0.44
2:I:269:ILE:H	2:I:269:ILE:HD12	1.81	0.44
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.86	0.44
5:L:137:TYR:CD2	5:L:273:MET:HE2	2.52	0.44
2:C:202:ARG:HH11	2:C:369:MET:HB2	1.83	0.44
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.52	0.44
2:C:1082:ILE:H	2:C:1082:ILE:CD1	2.29	0.44
2:C:1160:ASP:CG	2:C:1161:LEU:HA	2.41	0.44
3:D:56:LEU:H	3:D:56:LEU:HD12	1.82	0.44
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.47	0.44
3:D:291:ILE:CD1	5:F:409:ASN:HB3	2.47	0.44
3:D:1227:HIS:C	3:D:1230:THR:HG22	2.43	0.44
3:D:1283:SER:O	3:D:1286:LYS:N	2.50	0.44
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.52	0.44
2:I:812:PHE:N	2:I:815:SER:OG	2.50	0.44
2:I:1210:ILE:HG22	2:I:1211:ARG:N	2.32	0.44
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.32	0.44
3:J:327:LEU:HD23	3:J:327:LEU:HA	1.65	0.44
3:J:490:ILE:HA	3:J:500:ILE:HG13	2.00	0.44
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.69	0.44
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	1.98	0.44
3:J:844:THR:OG1	3:J:860:ARG:O	2.14	0.44
3:J:1219:ASP:O	3:J:1222:ARG:N	2.50	0.44
5:L:511:ILE:CG1	5:L:512:GLY:H	2.30	0.44
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.68	0.44
1:A:219:ARG:O	1:A:223:ILE:HG13	2.17	0.44
2:C:5:TYR:CD2	2:C:778:GLU:HB2	2.53	0.44
2:C:616:ILE:HG22	2:C:617:ALA:O	2.18	0.44
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.53	0.44
2:C:895:LEU:HD11	2:C:900:LYS:HG3	1.99	0.44
3:D:26:SER:OG	3:D:28:ASP:N	2.50	0.44
3:D:53:ARG:HA	3:D:54:ASP:HA	1.72	0.44
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.66	0.44
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.83	0.44
3:D:469:HIS:O	3:D:471:PRO:HD3	2.18	0.44
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.80	0.44
2:I:178:PRO:HB3	2:I:395:TYR:CE2	2.53	0.44
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.98	0.44
3:J:510:LEU:HD22	3:J:601:ILE:CD1	2.48	0.44
3:J:736:GLN:O	3:J:739:GLN:N	2.44	0.44
5:L:139:GLU:CG	5:L:351:THR:HA	2.46	0.44
5:L:363:ARG:O	5:L:367:ILE:HG13	2.17	0.44
5:L:476:ARG:HD2	5:L:477:GLU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:O	1:B:195:ARG:N	2.50	0.44
2:C:708:VAL:CG1	2:C:794:LEU:HD22	2.47	0.44
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.82	0.44
2:C:898:GLU:HB3	5:F:544:THR:HG21	1.99	0.44
3:D:94:GLN:HB2	3:D:96:LYS:HB2	1.99	0.44
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.44
3:D:827:GLU:CB	3:D:832:LYS:HD2	2.48	0.44
4:E:62:GLN:O	4:E:66:VAL:HG23	2.16	0.44
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
5:F:561:MET:HA	5:F:567:MET:HE1	1.99	0.44
1:G:14:VAL:HG22	1:G:15:ASP:N	2.33	0.44
1:G:75:GLN:HA	2:I:729:ALA:H	1.81	0.44
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.25	0.44
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.99	0.44
1:H:224:LEU:O	1:H:228:LEU:HG	2.17	0.44
2:I:617:ALA:HB3	2:I:653:MET:CB	2.48	0.44
2:I:705:GLU:CD	2:I:705:GLU:H	2.25	0.44
3:J:761:ALA:N	3:J:771:GLN:HE22	2.15	0.44
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.50	0.44
5:L:105:MET:HE2	5:L:384:LEU:HB2	1.99	0.44
1:B:191:ARG:O	1:B:191:ARG:HG2	2.15	0.44
2:C:866:ASP:OD2	2:C:869:GLY:N	2.51	0.44
2:C:903:ARG:NE	2:C:910:ALA:HB2	2.32	0.44
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.18	0.44
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.44
3:D:442:ILE:HD13	3:D:442:ILE:HA	1.81	0.44
3:D:466:MET:HE2	3:D:466:MET:HB3	1.78	0.44
2:I:157:PHE:CD1	2:I:174:ALA:HB2	2.53	0.44
2:I:1122:LYS:NZ	2:I:1178:LYS:O	2.41	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.99	0.44
2:I:1223:ARG:HD3	3:J:637:ALA:HA	1.98	0.44
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.81	0.44
3:J:161:THR:H	3:J:164:GLN:HB2	1.83	0.44
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.44
3:J:805:GLN:CD	3:J:1348:LYS:HD3	2.43	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44
1:B:228:LEU:C	1:B:230:ALA:H	2.25	0.44
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.99	0.44
2:C:494:ASN:HB3	2:C:497:PRO:CG	2.48	0.44
2:C:960:LEU:O	2:C:963:GLU:HB2	2.18	0.44
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.50	0.44
3:D:279:LEU:HD11	3:D:296:LYS:HG2	2.00	0.44
3:D:532:GLU:O	3:D:536:LEU:HB2	2.17	0.44
3:D:660:GLU:O	3:D:664:ILE:HG12	2.18	0.44
3:D:849:LEU:HB2	3:D:853:THR:HG23	1.99	0.44
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.33	0.44
5:F:390:ILE:O	5:F:393:LYS:HB2	2.18	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.99	0.44
5:F:466:ILE:HG21	5:F:486:ARG:HG3	1.99	0.44
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.81	0.44
2:I:130:MET:HE3	2:I:136:PHE:CE2	2.53	0.44
2:I:614:TYR:CD1	2:I:652:TYR:CE1	3.06	0.44
2:I:800:MET:HE3	2:I:800:MET:HB3	1.55	0.44
2:I:870:ILE:CG2	2:I:944:ARG:HD3	2.47	0.44
2:I:1132:LEU:HD13	2:I:1177:ARG:HD2	2.00	0.44
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.82	0.44
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.82	0.44
3:J:442:ILE:HD13	3:J:442:ILE:HA	1.80	0.44
3:J:596:LEU:HD11	3:J:604:MET:CE	2.45	0.44
3:J:697:MET:HE1	3:J:737:ILE:CG2	2.47	0.44
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.44
5:L:114:GLU:HG3	5:L:115:GLY:N	2.32	0.44
5:L:297:MET:HA	5:L:326:TRP:HB3	2.00	0.44
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.48	0.44
1:A:317:ARG:O	1:A:318:LEU:HD13	2.18	0.44
1:B:54:CYS:O	1:B:90:VAL:HB	2.18	0.44
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.44
2:C:484:LEU:HB2	2:C:485:ASP:H	1.62	0.44
3:D:169:LEU:HD23	3:D:169:LEU:HA	1.82	0.44
3:D:172:PHE:HB3	3:D:175:GLU:OE2	2.17	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
3:D:847:ASP:CA	3:D:860:ARG:H	2.31	0.44
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.18	0.44
2:I:867:GLU:H	2:I:867:GLU:HG3	1.61	0.44
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.48	0.44
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.44
3:J:59:ALA:HA	3:J:63:GLY:O	2.18	0.44
3:J:238:ILE:HD13	3:J:238:ILE:HA	1.74	0.44
3:J:416:ILE:HA	3:J:416:ILE:HD12	1.70	0.44
5:L:226:ALA:O	5:L:230:VAL:HG12	2.18	0.44
5:L:311:THR:HG21	5:L:348:GLU:CD	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:575:GLU:O	5:L:579:GLN:HG2	2.17	0.44
1:A:295:LEU:CD2	1:A:300:LEU:HB2	2.48	0.43
1:A:319:GLU:HA	1:A:319:GLU:OE2	2.18	0.43
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.43
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.48	0.43
2:C:198:ILE:O	2:C:201:ARG:HB2	2.18	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
3:D:678:ARG:HD3	3:D:682:VAL:CG2	2.48	0.43
3:D:707:ILE:HD11	3:D:716:GLN:CG	2.46	0.43
3:D:772:TYR:O	3:D:775:SER:N	2.51	0.43
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.00	0.43
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.33	0.43
1:H:84:ASN:ND2	1:H:129:VAL:O	2.50	0.43
1:H:86:LYS:HG2	1:H:173:VAL:CG1	2.48	0.43
1:H:115:ILE:HG22	1:H:116:THR:N	2.33	0.43
2:I:600:THR:CG2	2:I:602:GLU:HG2	2.41	0.43
2:I:971:LEU:O	2:I:1014:LEU:HD23	2.18	0.43
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.48	0.43
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.91	0.43
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.99	0.43
3:J:298:MET:SD	5:L:406:GLN:HG3	2.58	0.43
3:J:525:MET:O	3:J:548:VAL:HG13	2.18	0.43
3:J:858:VAL:HG11	3:J:872:LEU:HD21	2.00	0.43
4:K:39:VAL:HG21	4:K:56:GLU:HG3	2.00	0.43
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.00	0.43
1:B:57:THR:O	1:B:173:VAL:N	2.47	0.43
2:C:817:LEU:HD11	2:C:1085:MET:HE1	1.99	0.43
2:C:1308:ILE:HD12	2:C:1308:ILE:HG23	1.72	0.43
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.43
3:D:61:ILE:HB	3:D:62:PHE:CD2	2.53	0.43
3:D:316:ILE:HA	3:D:323:PRO:HA	2.00	0.43
3:D:660:GLU:HB3	3:D:685:ILE:CD1	2.23	0.43
3:D:799:ARG:HD2	3:D:1146:GLU:OE1	2.17	0.43
3:D:846:GLU:HA	3:D:860:ARG:HD3	2.00	0.43
3:D:919:ALA:CB	3:D:1255:VAL:HG21	2.47	0.43
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.42	0.43
5:F:316:PHE:CZ	5:F:334:SER:HA	2.52	0.43
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.99	0.43
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.26	0.43
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.53	0.43
2:I:466:VAL:O	2:I:469:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:987:GLU:HG2	2:I:991:LYS:HE3	2.00	0.43
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	2.01	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.53	0.43
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.99	0.43
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.17	0.43
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.43
5:L:148:TYR:O	5:L:151:VAL:N	2.41	0.43
5:L:166:VAL:HG23	5:L:258:GLN:HA	2.00	0.43
5:L:276:MET:O	5:L:280:VAL:HG23	2.18	0.43
5:L:316:PHE:HZ	5:L:334:SER:CA	2.22	0.43
5:L:412:LEU:CD1	5:L:435:ILE:HD11	2.42	0.43
5:L:561:MET:HB2	5:L:561:MET:HE3	1.61	0.43
2:C:15:PHE:HA	2:C:1155:VAL:HG11	2.01	0.43
2:C:218:GLU:HG3	2:C:299:LYS:HA	2.00	0.43
2:C:490:GLN:HG3	5:F:472:GLN:HG3	1.99	0.43
2:C:761:GLN:O	2:C:762:ASN:HB2	2.16	0.43
3:D:80:HIS:ND1	3:D:80:HIS:N	2.66	0.43
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.43
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.00	0.43
5:F:472:GLN:CD	5:F:472:GLN:C	2.85	0.43
1:G:75:GLN:C	2:I:729:ALA:HB2	2.43	0.43
1:H:125:LYS:HB3	1:H:125:LYS:HE2	1.77	0.43
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.34	0.43
2:I:882:ILE:HG13	2:I:919:ARG:NH1	2.33	0.43
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.52	0.43
3:J:69:GLU:HG3	3:J:76:LYS:HG2	2.00	0.43
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.15	0.43
5:L:292:VAL:HG21	5:L:299:LYS:HG3	2.00	0.43
2:C:569:ILE:C	2:C:571:LEU:H	2.25	0.43
2:C:599:VAL:HG21	2:C:623:LEU:HD13	2.00	0.43
2:C:902:LEU:HD12	5:F:607:LEU:HD23	2.01	0.43
2:C:985:GLU:O	2:C:989:LEU:N	2.42	0.43
2:C:987:GLU:HG2	2:C:991:LYS:CE	2.46	0.43
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.32	0.43
3:D:395:LYS:HG2	5:F:536:THR:HG21	2.01	0.43
3:D:452:LEU:HD23	3:D:452:LEU:HA	1.84	0.43
3:D:1171:GLY:O	3:D:1193:TRP:HZ3	2.02	0.43
5:F:137:TYR:CD2	5:F:273:MET:HE2	2.54	0.43
2:I:184:LEU:HD12	2:I:184:LEU:HA	1.64	0.43
2:I:377:THR:HG22	2:I:379:GLU:OE2	2.19	0.43
2:I:600:THR:HG22	2:I:601:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:972:PHE:HD2	2:I:975:ILE:HD12	1.84	0.43
2:I:1083:GLU:H	2:I:1083:GLU:HG3	1.58	0.43
2:I:1164:PHE:O	2:I:1166:ASP:N	2.51	0.43
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.00	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.48	0.43
3:J:500:ILE:HG22	3:J:500:ILE:O	2.18	0.43
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.54	0.43
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.00	0.43
3:J:905:ARG:HH11	4:K:16:ARG:HB2	1.83	0.43
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.01	0.43
4:K:19:LEU:CD1	4:K:54:ILE:HG21	2.48	0.43
5:L:576:VAL:O	5:L:580:PHE:HB2	2.19	0.43
1:A:227:GLN:OE1	1:A:227:GLN:HA	2.17	0.43
1:B:152:TYR:CD1	1:B:176:CYS:HA	2.53	0.43
2:C:318:SER:O	2:C:322:LEU:HG	2.19	0.43
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
2:C:1110:GLY:O	2:C:1114:GLU:HB2	2.19	0.43
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.19	0.43
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.49	0.43
3:D:193:ASP:HB3	3:D:196:GLN:CG	2.48	0.43
3:D:363:LEU:O	3:D:363:LEU:HG	2.17	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.31	0.43
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:CG2	2.48	0.43
5:F:561:MET:HB2	5:F:561:MET:HE3	1.88	0.43
5:F:573:LEU:HD13	5:F:588:ARG:CZ	2.48	0.43
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.34	0.43
3:J:519:ASN:CG	3:J:709:ARG:HD3	2.43	0.43
3:J:899:TYR:CE1	3:J:1251:LYS:HD2	2.52	0.43
5:L:213:ASP:HB2	5:L:216:LEU:HB3	1.99	0.43
2:C:30:ILE:HD12	2:C:30:ILE:N	2.34	0.43
2:C:202:ARG:HH12	2:C:368:ARG:HH22	1.66	0.43
2:C:403:MET:HE3	2:C:403:MET:HB3	1.71	0.43
2:C:800:MET:HE3	2:C:800:MET:HB3	1.47	0.43
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.19	0.43
2:C:1268:GLN:HE22	3:D:352:ARG:CD	2.31	0.43
2:C:1282:GLY:HA3	4:E:17:PHE:HE1	1.82	0.43
3:D:262:THR:OG1	3:D:263:SER:N	2.52	0.43
3:D:556:GLU:C	3:D:558:ASP:H	2.27	0.43
3:D:848:VAL:HG13	3:D:857:LEU:HD13	2.00	0.43
3:D:1355:ARG:NH2	3:D:1369:ARG:HH12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:227:GLN:HG3	5:F:252:LEU:HA	2.00	0.43
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.29	0.43
2:I:107:ARG:HA	2:I:108:GLU:HA	1.71	0.43
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.19	0.43
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.41	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.71	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.19	0.43
3:J:768:ASN:HD21	3:J:770:LEU:HD23	1.84	0.43
3:J:853:THR:C	3:J:855:ASP:H	2.25	0.43
3:J:1371:ARG:O	3:J:1371:ARG:HG2	2.16	0.43
5:L:449:THR:OG1	5:L:503:GLU:OE1	2.36	0.43
5:L:519:LEU:C	5:L:519:LEU:HD23	2.44	0.43
2:C:211:ARG:HA	2:C:215:TYR:O	2.18	0.43
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.43
3:D:348:ASP:O	3:D:349:TYR:C	2.60	0.43
3:D:516:ASP:HA	3:D:545:HIS:HB2	2.00	0.43
3:D:588:PRO:HB2	3:D:590:SER:OG	2.19	0.43
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.00	0.43
2:I:1204:LEU:HB3	2:I:1205:PRO:HD2	2.00	0.43
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.01	0.43
4:K:13:ILE:HD11	4:K:54:ILE:HG23	2.01	0.43
5:L:414:LYS:HD3	5:L:434:TRP:CZ3	2.51	0.43
1:A:78:ILE:HA	1:A:81:ILE:HG13	2.00	0.43
1:A:270:LEU:HD22	1:A:275:ILE:HG21	2.00	0.43
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.99	0.43
2:C:600:THR:HG21	2:C:602:GLU:HG2	2.00	0.43
2:C:738:GLU:HA	2:C:741:MET:CE	2.48	0.43
2:C:739:ASP:OD1	2:C:739:ASP:N	2.45	0.43
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.49	0.43
3:D:825:VAL:HG22	3:D:833:GLU:N	2.32	0.43
3:D:1175:LEU:HD12	3:D:1175:LEU:HA	1.86	0.43
3:D:1184:ASP:N	3:D:1185:PRO:HD3	2.33	0.43
3:D:1279:GLN:NE2	3:D:1317:GLU:OE2	2.52	0.43
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.34	0.43
1:H:219:ARG:HA	1:H:222:THR:HB	2.01	0.43
2:I:170:VAL:CG2	2:I:172:TYR:CZ	2.99	0.43
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.83	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:CD2	2.47	0.43
3:J:19:ALA:H	3:J:1344:LEU:HD12	1.84	0.43
3:J:75:TYR:OH	3:J:86:GLU:OE2	2.35	0.43
3:J:528:THR:HG22	3:J:532:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:592:VAL:HA	3:J:596:LEU:HD21	2.01	0.43
5:L:414:LYS:O	5:L:417:ASP:N	2.51	0.43
1:A:66:HIS:O	1:A:66:HIS:ND1	2.49	0.43
2:C:95:PRO:HA	2:C:126:GLU:HA	2.01	0.43
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.54	0.43
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.86	0.43
3:D:278:ARG:O	3:D:282:LEU:HG	2.19	0.43
3:D:303:VAL:O	3:D:306:LEU:HB3	2.19	0.43
3:D:797:THR:HG22	3:D:924:GLY:HA3	2.00	0.43
5:F:139:GLU:HG2	5:F:351:THR:HA	2.01	0.43
5:F:467:SER:O	5:F:471:LEU:N	2.52	0.43
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.99	0.43
1:G:107:ILE:HG12	1:G:135:ASP:O	2.19	0.43
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.33	0.43
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.43
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.00	0.43
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.51	0.43
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.19	0.43
2:I:1305:TYR:CG	5:L:531:PRO:HB2	2.53	0.43
3:J:223:LEU:O	3:J:226:ALA:HB3	2.18	0.43
3:J:654:ILE:O	3:J:658:GLU:HB2	2.18	0.43
5:L:96:ASP:OD2	5:L:98:VAL:HG13	2.19	0.43
5:L:141:ILE:HD13	5:L:256:PHE:CD1	2.54	0.43
5:L:227:GLN:HG3	5:L:252:LEU:HA	2.00	0.43
5:L:250:LEU:O	5:L:254:GLU:HG2	2.19	0.43
5:L:343:LYS:HA	5:L:346:GLN:HB3	2.01	0.43
5:L:397:ARG:HB3	5:L:443:ILE:HD13	2.00	0.43
1:A:300:LEU:HD13	1:A:304:LYS:HE2	2.00	0.43
2:C:250:THR:HA	2:C:268:ARG:HA	2.01	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.01	0.43
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.76	0.43
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.43	0.43
3:D:309:ASN:OD1	3:D:314:ARG:HA	2.18	0.43
3:D:681:LYS:O	3:D:685:ILE:HG23	2.19	0.43
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.43
3:D:762:ASN:OD1	3:D:765:GLU:HG3	2.19	0.43
5:F:537:THR:C	5:F:539:SER:N	2.72	0.43
1:H:65:LEU:CD2	1:H:171:LEU:HD21	2.47	0.43
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.54	0.43
2:I:125:GLY:CA	2:I:499:SER:HB2	2.45	0.43
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:854:ILE:HD11	2:I:885:GLY:HA3	2.00	0.43
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.01	0.43
3:J:404:GLU:HG2	3:J:409:TRP:CZ2	2.54	0.43
3:J:545:HIS:CD2	3:J:719:PHE:HE1	2.37	0.43
5:L:312:SER:OG	5:L:313:ASP:N	2.52	0.43
5:L:504:PRO:C	5:L:505:ILE:HD12	2.44	0.43
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.60	0.42
2:C:38:PHE:HB2	2:C:457:GLY:O	2.19	0.42
2:C:69:GLN:HG2	2:C:101:ARG:O	2.19	0.42
2:C:819:SER:HB3	2:C:1085:MET:SD	2.59	0.42
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.20	0.42
3:D:84:ILE:H	3:D:84:ILE:HG13	1.67	0.42
3:D:847:ASP:CB	3:D:860:ARG:H	2.32	0.42
3:D:872:LEU:HD22	3:D:877:VAL:HG11	2.01	0.42
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	2.00	0.42
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	2.01	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
3:D:1199:PHE:HB2	3:D:1202:GLU:CB	2.46	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.19	0.42
3:J:825:VAL:HG11	3:J:833:GLU:HB3	2.00	0.42
3:J:1167:LYS:O	3:J:1168:GLU:HG2	2.18	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.54	0.42
5:L:134:VAL:HG22	5:L:273:MET:HE1	2.00	0.42
5:L:513:ASP:C	5:L:515:GLU:H	2.27	0.42
1:B:48:LEU:CD2	3:D:535:ARG:HG3	2.48	0.42
1:B:134:THR:HG23	1:B:135:ASP:N	2.34	0.42
3:D:198:CYS:HA	3:D:221:ILE:CD1	2.49	0.42
3:D:427:PRO:O	3:D:429:LEU:HD22	2.19	0.42
3:D:604:MET:HE3	3:D:604:MET:HB2	1.82	0.42
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.42
3:D:1252:HIS:O	3:D:1255:VAL:HG22	2.20	0.42
1:G:18:GLN:HG3	1:G:24:ALA:HB2	2.02	0.42
1:G:31:LEU:HA	1:G:31:LEU:HD23	1.67	0.42
1:H:33:ARG:HD3	1:H:197:ASP:OD2	2.18	0.42
2:I:47:TYR:OH	2:I:398:SER:HB2	2.19	0.42
2:I:734:ILE:O	2:I:748:ILE:HB	2.18	0.42
2:I:870:ILE:HG22	2:I:944:ARG:HH11	1.81	0.42
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.42
3:J:521:LYS:NZ	3:J:540:GLY:O	2.51	0.42
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.54	0.42
3:J:641:ILE:HD13	3:J:644:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:742:GLY:O	3:J:762:ASN:HB3	2.19	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
3:J:912:GLY:HA2	3:J:1363:TYR:CD1	2.53	0.42
5:L:357:GLN:HA	5:L:360:ASP:HB2	2.01	0.42
1:A:164:ASP:C	1:A:166:ARG:H	2.26	0.42
1:A:261:GLU:CD	2:C:859:GLU:H	2.27	0.42
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.84	0.42
2:C:301:TYR:CE2	2:C:333:ILE:HA	2.53	0.42
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.54	0.42
2:C:1002:LEU:HD23	2:C:1003:THR:O	2.19	0.42
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.59	0.42
3:D:140:TYR:O	3:D:297:ARG:NH1	2.52	0.42
3:D:519:ASN:HA	3:D:523:GLU:OE1	2.19	0.42
3:D:817:HIS:CE1	3:D:860:ARG:NH2	2.87	0.42
3:D:1142:ALA:O	3:D:1143:ASP:C	2.61	0.42
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.49	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.55	0.42
4:E:49:ILE:O	4:E:53:GLU:HG3	2.19	0.42
5:F:98:VAL:O	5:F:102:MET:HB2	2.18	0.42
5:F:486:ARG:HG2	5:F:486:ARG:NH1	2.34	0.42
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.42
1:G:82:LEU:HD13	1:G:173:VAL:HG12	2.01	0.42
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.34	0.42
1:H:178:SER:HA	1:H:179:PRO:HD3	1.76	0.42
2:I:17:LYS:HZ3	2:I:17:LYS:HG3	1.18	0.42
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.02	0.42
3:J:271:ARG:HE	3:J:271:ARG:HB2	1.40	0.42
3:J:382:TYR:CE1	3:J:398:LYS:HA	2.53	0.42
3:J:810:THR:HG22	3:J:894:VAL:H	1.84	0.42
3:J:1175:LEU:HA	3:J:1175:LEU:HD12	1.84	0.42
5:L:100:MET:HE2	5:L:100:MET:HB3	1.96	0.42
5:L:280:VAL:HG21	5:L:358:VAL:HG11	2.01	0.42
5:L:338:HIS:HA	5:L:341:LEU:HB2	2.00	0.42
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.54	0.42
1:A:297:LYS:O	1:A:301:THR:OG1	2.14	0.42
1:B:87:GLY:O	1:B:128:HIS:NE2	2.52	0.42
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.80	0.42
2:C:972:PHE:HB3	2:C:994:ARG:HH21	1.81	0.42
3:D:98:ARG:O	3:D:248:ASP:HB2	2.19	0.42
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.40	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1183:SER:CB	3:D:1185:PRO:HD3	2.50	0.42
3:D:1301:THR:CG2	3:J:1301:THR:HG23	2.50	0.42
1:G:41:ASN:CG	2:I:1218:GLY:HA3	2.44	0.42
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.60	0.42
2:I:671:LEU:HD23	2:I:1186:VAL:HG11	2.02	0.42
2:I:719:LYS:N	2:I:751:TYR:OH	2.52	0.42
2:I:976:ARG:CD	2:I:989:LEU:HD23	2.41	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA3	2.00	0.42
3:J:26:SER:O	3:J:30:ILE:HG13	2.19	0.42
3:J:168:ALA:O	3:J:172:PHE:HD2	2.03	0.42
3:J:809:VAL:HG12	3:J:911:LYS:HA	2.00	0.42
8:J:2004:4C6:O	8:J:2004:4C6:H19	2.19	0.42
5:L:220:LYS:O	5:L:223:GLU:HB3	2.20	0.42
1:A:82:LEU:HB3	1:A:173:VAL:CG1	2.50	0.42
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.78	0.42
1:B:154:PRO:HD2	1:B:157:THR:OG1	2.20	0.42
2:C:614:TYR:CE1	2:C:652:TYR:HE1	2.37	0.42
3:D:42:GLU:HG2	3:D:52:GLU:HG2	2.00	0.42
3:D:253:VAL:HG21	5:F:523:ILE:HG21	2.01	0.42
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.54	0.42
3:D:811:GLU:O	3:D:895:CYS:HA	2.20	0.42
3:D:872:LEU:O	3:D:877:VAL:HG12	2.19	0.42
1:G:222:THR:O	1:G:226:GLU:HB2	2.19	0.42
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.19	0.42
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.42
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.19	0.42
2:I:845:LEU:H	2:I:845:LEU:HG	1.49	0.42
2:I:1106:ARG:HB3	2:I:1108:ASN:ND2	2.34	0.42
2:I:1217:THR:C	2:I:1219:GLU:H	2.27	0.42
3:J:255:LEU:HA	3:J:255:LEU:HD13	1.85	0.42
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.53	0.42
3:J:735:ALA:O	3:J:738:ARG:HB3	2.19	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.35	0.42
3:J:894:VAL:HG22	3:J:1258:ARG:HH11	1.85	0.42
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.52	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.34	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.20	0.42
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.99	0.42
1:A:150:ARG:HH11	1:B:6:THR:N	2.18	0.42
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.01	0.42
1:B:196:THR:HG22	1:B:197:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:VAL:C	2:C:121:GLU:HA	2.44	0.42
2:C:138:ILE:HG22	2:C:139:ASN:N	2.35	0.42
2:C:168:GLY:O	2:C:170:VAL:N	2.34	0.42
2:C:202:ARG:HH11	2:C:369:MET:CB	2.31	0.42
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.34	0.42
2:C:885:GLY:HA2	2:C:917:SER:HB3	2.02	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.20	0.42
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.83	0.42
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.54	0.42
5:F:105:MET:HE2	5:F:384:LEU:HB2	2.01	0.42
1:G:224:LEU:HD22	1:H:228:LEU:CD1	2.49	0.42
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.71	0.42
2:I:147:SER:HB2	2:I:529:ARG:O	2.20	0.42
2:I:812:PHE:HZ	3:J:503:SER:CB	2.32	0.42
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.42
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.50	0.42
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.55	0.42
3:J:400:MET:HE2	3:J:400:MET:HB3	1.87	0.42
3:J:598:LYS:C	3:J:601:ILE:HG22	2.45	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HD3	2.01	0.42
3:J:885:VAL:H	3:J:885:VAL:HG22	1.49	0.42
1:A:34:GLY:C	1:A:36:GLY:N	2.75	0.42
1:A:61:ILE:HG22	1:A:62:ASP:N	2.34	0.42
1:A:182:ARG:O	1:A:183:ILE:HD12	2.20	0.42
2:C:317:LEU:HD11	2:C:333:ILE:HG21	2.02	0.42
2:C:960:LEU:HD13	2:C:960:LEU:HA	1.75	0.42
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	2.19	0.42
3:D:641:ILE:HD13	3:D:644:MET:CE	2.49	0.42
3:D:689:ALA:O	3:D:692:ARG:HB2	2.19	0.42
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.01	0.42
1:H:48:LEU:HG	1:H:183:ILE:HD11	2.01	0.42
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.91	0.42
2:I:23:ASP:OD1	2:I:23:ASP:N	2.38	0.42
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.87	0.42
2:I:672:GLU:H	2:I:672:GLU:HG3	1.27	0.42
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.49	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.20	0.42
3:J:495:ASN:C	3:J:497:GLU:H	2.27	0.42
5:L:112:THR:O	5:L:116:GLU:HG3	2.19	0.42
5:L:399:LEU:HG	5:L:403:ASP:HB3	2.02	0.42
2:C:39:ILE:O	2:C:40:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HB3	2:C:90:VAL:HG23	2.01	0.42
2:C:150:HIS:CD2	2:C:150:HIS:N	2.87	0.42
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.49	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.30	0.42
2:C:1222:GLU:C	2:C:1223:ARG:HG3	2.44	0.42
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.42
3:D:372:MET:O	3:D:376:LEU:HD12	2.20	0.42
5:F:111:LEU:HA	5:F:111:LEU:HD23	1.77	0.42
5:F:117:ILE:HA	5:F:120:ALA:HB3	2.00	0.42
5:F:253:SER:O	5:F:257:LYS:HG3	2.20	0.42
2:I:210:LEU:HB2	2:I:220:ILE:HD11	2.02	0.42
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.32	0.42
2:I:697:LYS:HA	2:I:795:ALA:HB2	2.02	0.42
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.50	0.42
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
2:I:830:THR:HG23	2:I:832:HIS:NE2	2.35	0.42
2:I:856:ASN:CB	5:L:613:ASP:HA	2.50	0.42
2:I:943:LYS:O	2:I:947:GLU:HG3	2.20	0.42
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.50	0.42
3:J:521:LYS:HD2	3:J:541:LEU:O	2.18	0.42
3:J:1227:HIS:C	3:J:1230:THR:HG22	2.45	0.42
5:L:292:VAL:HA	5:L:297:MET:O	2.19	0.42
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.51	0.42
1:B:217:ILE:O	1:B:218:ARG:C	2.60	0.42
2:C:48:GLY:H	2:C:51:ALA:HB3	1.84	0.42
2:C:397:LEU:O	2:C:398:SER:OG	2.29	0.42
2:C:615:VAL:HG22	2:C:650:VAL:HA	2.01	0.42
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.02	0.42
3:D:63:GLY:HA3	3:D:98:ARG:HG3	2.01	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.02	0.42
3:D:718:SER:OG	3:D:720:ASN:HB3	2.20	0.42
3:D:903:LEU:HB3	3:D:905:ARG:N	2.35	0.42
5:F:414:LYS:HD3	5:F:434:TRP:CZ3	2.55	0.42
5:F:448:ARG:HE	5:F:448:ARG:HB3	1.70	0.42
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.70	0.42
5:F:499:LYS:HA	5:F:502:LYS:HE2	2.00	0.42
1:G:40:GLY:HA2	1:G:201:LEU:HD21	2.02	0.42
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.02	0.42
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.54	0.42
2:I:421:SER:H	2:I:424:ASP:HB2	1.85	0.42
2:I:971:LEU:HG	2:I:1014:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:422:LEU:O	3:J:468:VAL:HA	2.19	0.42
3:J:423:LEU:HB3	3:J:466:MET:CE	2.50	0.42
3:J:701:LEU:HD12	3:J:723:TYR:HD2	1.85	0.42
3:J:835:LEU:HG	3:J:839:VAL:CG2	2.49	0.42
3:J:857:LEU:HD12	3:J:858:VAL:H	1.84	0.42
3:J:885:VAL:HG12	3:J:894:VAL:CG1	2.50	0.42
3:J:1173:ARG:HH21	3:J:1196:LEU:HD21	1.85	0.42
5:L:470:MET:HE3	5:L:478:PRO:HB3	2.02	0.42
1:A:46:ILE:CG2	1:A:223:ILE:HD12	2.50	0.42
2:C:622:ASN:O	2:C:630:VAL:HB	2.20	0.42
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.34	0.42
3:D:823:THR:HA	3:D:835:LEU:HD13	2.02	0.42
3:D:915:ILE:HA	3:D:918:ILE:HG23	2.01	0.42
3:D:1162:ILE:HD12	3:D:1163:VAL:H	1.85	0.42
1:G:115:ILE:HG22	1:G:116:THR:N	2.35	0.42
1:H:47:LEU:O	1:H:180:VAL:HG21	2.20	0.42
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.90	0.42
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.42
2:I:836:LEU:HD21	2:I:921:PRO:HD3	2.01	0.42
2:I:1134:GLN:NE2	2:I:1136:GLN:OE1	2.53	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.50	0.42
3:J:54:ASP:HB3	3:J:60:ARG:HH11	1.85	0.42
3:J:116:PHE:O	3:J:123:ARG:HB2	2.20	0.42
3:J:537:TYR:CE2	3:J:544:LEU:HD22	2.54	0.42
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.42
4:K:54:ILE:HA	4:K:59:ILE:O	2.20	0.42
5:L:418:LYS:HD2	5:L:434:TRP:CH2	2.55	0.42
1:A:231:PHE:HE1	1:B:28:LEU:HD23	1.85	0.41
2:C:6:THR:HG21	2:C:782:VAL:HG23	2.01	0.41
2:C:202:ARG:NH1	2:C:369:MET:HB2	2.35	0.41
2:C:685:MET:HE3	2:C:685:MET:HB2	1.70	0.41
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.50	0.41
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.28	0.41
3:D:151:MET:HE2	3:D:151:MET:HB3	2.00	0.41
3:D:358:GLY:N	3:D:359:PRO:HD3	2.35	0.41
3:D:581:MET:HE2	3:D:581:MET:HB3	1.88	0.41
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	2.33	0.41
1:H:10:LYS:HA	1:H:11:PRO:HD3	1.82	0.41
2:I:62:TYR:O	2:I:64:GLY:N	2.53	0.41
2:I:170:VAL:HG21	2:I:172:TYR:OH	2.19	0.41
2:I:525:THR:HG21	2:I:687:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:898:GLU:HB3	5:L:540:LEU:CD2	2.45	0.41
2:I:1121:ALA:HB2	2:I:1182:ILE:CD1	2.49	0.41
2:I:1276:TRP:HA	2:I:1279:GLU:OE1	2.19	0.41
3:J:88:CYS:O	3:J:90:VAL:N	2.53	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.73	0.41
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.50	0.41
4:K:21:LEU:HA	4:K:21:LEU:HD12	1.66	0.41
5:L:117:ILE:HG23	5:L:421:TYR:CE1	2.55	0.41
1:A:27:THR:O	1:A:28:LEU:HD12	2.20	0.41
1:A:98:VAL:HG22	1:A:100:LEU:HD12	2.02	0.41
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.87	0.41
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.86	0.41
2:C:494:ASN:HB3	2:C:497:PRO:CD	2.50	0.41
2:C:632:ASP:HB2	2:C:633:LEU:HD23	2.02	0.41
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.41
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.02	0.41
2:C:1192:GLU:O	2:C:1195:ILE:HB	2.20	0.41
2:C:1281:TYR:CD2	3:D:431:ARG:HB2	2.55	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.19	0.41
3:D:712:GLN:H	3:D:712:GLN:HG2	1.51	0.41
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.49	0.41
5:F:376:LYS:HZ3	5:F:417:ASP:CG	2.28	0.41
5:F:470:MET:O	5:F:478:PRO:HD3	2.20	0.41
1:H:73:GLY:HA2	1:H:134:THR:CG2	2.36	0.41
2:I:202:ARG:H	2:I:202:ARG:HG3	1.73	0.41
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.55	0.41
2:I:698:PRO:HA	2:I:1231:TYR:CE1	2.54	0.41
2:I:718:ALA:HB2	2:I:783:LEU:HD23	2.01	0.41
2:I:820:GLU:N	2:I:1080:ASN:O	2.53	0.41
2:I:920:VAL:HG13	2:I:921:PRO:HD2	2.01	0.41
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.60	0.41
3:J:85:CYS:SG	3:J:86:GLU:N	2.93	0.41
3:J:491:LEU:HD23	3:J:498:PRO:HA	2.00	0.41
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.02	0.41
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.85	0.41
5:L:165:PHE:HE1	5:L:259:PHE:CD2	2.37	0.41
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.02	0.41
1:A:8:PHE:HE1	1:A:32:GLU:OE1	2.04	0.41
1:A:18:GLN:HA	1:A:24:ALA:CB	2.49	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:671:LEU:HD23	2:C:1186:VAL:CG1	2.50	0.41
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.70	0.41
3:D:278:ARG:O	3:D:278:ARG:HG2	2.20	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:D:461:PHE:C	3:D:463:GLY:H	2.27	0.41
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.83	0.41
3:D:788:LEU:C	3:D:790:THR:N	2.79	0.41
3:D:820:ILE:HD11	3:D:822:MET:HE2	2.02	0.41
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.41
5:F:320:ILE:O	5:F:327:SER:HB3	2.21	0.41
1:G:44:ARG:HG3	1:G:183:ILE:CG2	2.45	0.41
1:G:189:ALA:HB1	1:G:191:ARG:NH2	2.35	0.41
2:I:15:PHE:CE1	2:I:1194:GLU:HB3	2.56	0.41
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.72	0.41
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.84	0.41
2:I:429:MET:HE2	2:I:429:MET:HB3	1.94	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41
2:I:971:LEU:HD11	2:I:1014:LEU:O	2.19	0.41
3:J:515:ARG:NH2	3:J:717:VAL:HG23	2.34	0.41
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.02	0.41
3:J:1162:ILE:HD12	3:J:1163:VAL:N	2.35	0.41
5:L:271:ASN:O	5:L:275:VAL:HG23	2.20	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.19	0.41
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.83	0.41
2:C:12:ARG:NE	2:C:793:GLU:OE1	2.39	0.41
2:C:658:GLN:O	2:C:660:VAL:N	2.54	0.41
2:C:896:THR:HB	2:C:897:PRO:HD2	2.02	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.84	0.41
3:D:646:ILE:H	3:D:646:ILE:HG12	1.58	0.41
3:D:701:LEU:HD12	3:D:723:TYR:CD2	2.51	0.41
3:D:723:TYR:CE1	3:D:727:ASP:HB2	2.55	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.54	0.41
5:F:344:LEU:O	5:F:355:ILE:HD11	2.19	0.41
1:G:190:ALA:HA	1:G:200:LYS:HE2	2.02	0.41
2:I:550:VAL:CG1	3:J:777:HIS:HA	2.50	0.41
2:I:571:LEU:HA	2:I:571:LEU:HD23	1.62	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.65	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.02	0.41
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.33	0.41
3:J:796:LEU:HD12	3:J:796:LEU:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.73	0.41
5:L:157:ARG:HB3	5:L:160:ASP:OD2	2.19	0.41
5:L:381:GLU:O	5:L:384:LEU:HG	2.20	0.41
1:A:22:THR:O	1:A:207:THR:N	2.37	0.41
1:A:92:VAL:HG11	1:A:98:VAL:HG11	2.03	0.41
1:B:51:MET:HB3	1:B:178:SER:HB2	2.01	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HG2	2.02	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.20	0.41
2:C:848:GLU:CG	2:C:888:THR:HG22	2.50	0.41
2:C:850:ILE:HG22	2:C:850:ILE:O	2.21	0.41
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.02	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.02	0.41
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.55	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.02	0.41
3:D:654:ILE:O	3:D:658:GLU:N	2.49	0.41
3:D:832:LYS:NZ	3:D:1243:LEU:HD12	2.35	0.41
5:F:124:GLU:O	5:F:128:ASN:HB2	2.21	0.41
5:F:388:ILE:O	5:F:392:LYS:HG3	2.21	0.41
1:G:102:LEU:HD23	1:G:115:ILE:CG1	2.45	0.41
1:H:134:THR:HG23	1:H:135:ASP:N	2.34	0.41
2:I:49:LEU:HB2	2:I:73:TYR:CZ	2.56	0.41
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.55	0.41
2:I:836:LEU:HD11	2:I:1054:LEU:HD22	2.02	0.41
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.21	0.41
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.41
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.36	0.41
3:J:116:PHE:O	3:J:124:ILE:HG13	2.20	0.41
3:J:130:MET:HE2	3:J:135:ILE:HG12	2.02	0.41
3:J:138:VAL:HG21	3:J:145:VAL:HB	2.02	0.41
3:J:616:PRO:HA	3:J:619:ILE:HG22	2.03	0.41
3:J:825:VAL:HG13	3:J:833:GLU:HB3	2.02	0.41
4:K:44:ASP:HB2	4:K:49:ILE:HG13	2.01	0.41
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.03	0.41
1:A:54:CYS:HB3	1:A:148:ARG:HD3	2.02	0.41
1:A:56:VAL:CG2	1:A:144:ILE:HG23	2.51	0.41
1:A:295:LEU:HD22	1:A:300:LEU:HB2	2.02	0.41
1:A:316:MET:HB2	1:A:316:MET:HE3	1.54	0.41
1:B:98:VAL:HG11	1:B:121:VAL:HG22	2.03	0.41
1:B:108:GLY:HA2	1:B:109:PRO:HD3	1.83	0.41
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.02	0.41
2:C:626:GLU:HB2	2:C:628:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:921:PRO:HB2	2:C:924:VAL:HG22	2.03	0.41
3:D:368:LEU:CD2	3:D:373:ALA:HB2	2.48	0.41
3:D:377:PHE:O	3:D:378:LYS:C	2.64	0.41
5:F:281:ARG:HH11	5:F:281:ARG:HD2	1.71	0.41
5:F:583:THR:HG22	5:F:584:ARG:N	2.35	0.41
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.78	0.41
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.20	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.03	0.41
2:I:209:ILE:HD13	2:I:209:ILE:HG21	1.84	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:O	2.19	0.41
2:I:1111:GLN:HB2	2:I:1230:MET:HE2	2.01	0.41
3:J:133:ARG:HD2	3:J:133:ARG:HA	1.86	0.41
3:J:678:ARG:O	3:J:682:VAL:HG23	2.20	0.41
3:J:860:ARG:HD2	3:J:860:ARG:HA	1.89	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.94	0.41
1:A:18:GLN:HA	1:A:24:ALA:HB2	2.03	0.41
1:A:260:LEU:HB2	1:A:262:LEU:HG	2.02	0.41
1:B:15:ASP:O	1:B:27:THR:HG23	2.21	0.41
2:C:136:PHE:HE2	2:C:456:VAL:HG11	1.85	0.41
2:C:297:VAL:HG12	2:C:315:MET:O	2.20	0.41
2:C:421:SER:H	2:C:424:ASP:CB	2.33	0.41
2:C:906:PHE:HE2	5:F:608:ARG:NH1	2.19	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.36	0.41
3:D:205:LEU:HD13	3:D:205:LEU:C	2.46	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41
3:D:1178:THR:HA	3:D:1179:PRO:HD3	1.75	0.41
3:D:1266:ILE:HD12	3:D:1274:PHE:N	2.36	0.41
5:F:310:GLU:O	5:F:344:LEU:HD21	2.21	0.41
1:G:49:SER:HB3	2:I:1083:GLU:OE2	2.21	0.41
1:H:203:ILE:HD12	1:H:203:ILE:N	2.36	0.41
2:I:385:PHE:CE2	2:I:390:PHE:HE2	2.38	0.41
2:I:511:LEU:HD23	2:I:511:LEU:HA	1.77	0.41
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.50	0.41
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.19	0.41
2:I:1323:PHE:CE1	2:I:1327:LEU:HD11	2.56	0.41
3:J:395:LYS:CG	5:L:536:THR:HG21	2.45	0.41
3:J:903:LEU:CD2	3:J:909:ILE:HD12	2.51	0.41
5:L:383:ASN:C	5:L:385:ARG:N	2.78	0.41
5:L:607:LEU:O	5:L:610:PHE:HB2	2.21	0.41
1:A:102:LEU:O	1:A:141:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG23	1:A:174:ASP:O	2.21	0.41
1:A:216:ALA:O	1:A:218:ARG:N	2.54	0.41
1:A:321:TRP:CE2	1:A:322:PRO:HB3	2.56	0.41
2:C:59:ILE:HD13	2:C:59:ILE:HG21	1.75	0.41
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.56	0.41
2:C:594:VAL:HG22	2:C:599:VAL:HG22	2.03	0.41
2:C:1281:TYR:CD2	2:C:1281:TYR:N	2.88	0.41
2:C:1288:GLN:O	2:C:1292:THR:HB	2.20	0.41
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.83	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.55	0.41
3:D:555:TYR:HB3	3:D:563:LEU:HD23	2.02	0.41
3:D:736:GLN:O	3:D:737:ILE:C	2.63	0.41
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.36	0.41
5:F:474:MET:O	5:F:476:ARG:N	2.48	0.41
1:G:31:LEU:HB2	1:G:199:ASP:O	2.21	0.41
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.56	0.41
2:I:95:PRO:HB3	2:I:123:TYR:HE1	1.85	0.41
2:I:211:ARG:NE	2:I:354:ASP:OD2	2.35	0.41
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.56	0.41
2:I:487:LEU:H	2:I:487:LEU:HD23	1.85	0.41
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.35	0.41
2:I:1124:ILE:HG21	2:I:1180:MET:HE3	2.02	0.41
2:I:1164:PHE:C	2:I:1166:ASP:H	2.29	0.41
2:I:1274:GLU:HG3	3:J:428:THR:OG1	2.19	0.41
3:J:335:GLN:CB	3:J:336:GLY:HA3	2.51	0.41
3:J:360:TYR:CD1	3:J:360:TYR:C	2.98	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
5:L:499:LYS:HE3	5:L:499:LYS:HB2	1.75	0.41
1:A:155:ALA:H	1:A:174:ASP:HA	1.86	0.41
1:A:208:ASN:OD1	1:A:208:ASN:N	2.53	0.41
1:A:318:LEU:HD22	1:A:318:LEU:N	2.36	0.41
1:B:192:VAL:O	1:B:194:GLN:N	2.53	0.41
2:C:62:TYR:HE1	2:C:476:LYS:O	2.03	0.41
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.56	0.41
2:C:420:LEU:HA	2:C:420:LEU:HD23	1.76	0.41
2:C:757:THR:O	2:C:765:ILE:HG23	2.21	0.41
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.51	0.41
2:C:1164:PHE:C	2:C:1166:ASP:N	2.79	0.41
2:C:1250:SER:HB3	2:C:1259:LEU:O	2.21	0.41
3:D:601:ILE:HG21	3:D:601:ILE:HD13	1.78	0.41
3:D:625:MET:HE2	3:D:625:MET:HB3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:840:LEU:HD12	3:D:864:LEU:O	2.20	0.41
3:D:925:GLU:C	3:D:927:GLY:N	2.79	0.41
5:F:483:LEU:HD12	5:F:483:LEU:N	2.34	0.41
1:G:39:LEU:CD2	1:H:224:LEU:HD11	2.51	0.41
1:G:178:SER:HA	1:G:179:PRO:HD3	1.91	0.41
1:H:100:LEU:HD11	1:H:121:VAL:CG2	2.50	0.41
2:I:161:LYS:HA	2:I:170:VAL:HA	2.03	0.41
2:I:207:THR:HG21	2:I:351:LEU:HG	2.02	0.41
2:I:315:MET:HE3	2:I:315:MET:HB2	1.81	0.41
2:I:337:PHE:CD1	2:I:337:PHE:C	2.97	0.41
2:I:519:ASN:HB3	2:I:522:SER:CB	2.51	0.41
2:I:590:PRO:HG3	2:I:605:TYR:CE1	2.55	0.41
2:I:1207:SER:C	2:I:1209:GLN:H	2.27	0.41
3:J:156:ARG:NH1	3:J:157:GLN:NE2	2.69	0.41
3:J:294:ASN:O	3:J:298:MET:HG3	2.21	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.76	0.41
3:J:357:VAL:HB	3:J:358:GLY:H	1.75	0.41
3:J:504:GLN:HG3	3:J:505:ASP:H	1.86	0.41
3:J:527:LEU:HB3	3:J:532:GLU:CG	2.51	0.41
3:J:722:ILE:HD11	3:J:740:LEU:HD23	2.01	0.41
3:J:805:GLN:HB3	3:J:806:ASP:H	1.73	0.41
3:J:842:ARG:HB3	3:J:882:VAL:HG11	2.02	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:CG	2.51	0.41
3:J:1372:ARG:HE	3:J:1372:ARG:HB2	1.64	0.41
4:K:15:ASN:O	4:K:16:ARG:HB3	2.21	0.41
5:L:96:ASP:O	5:L:98:VAL:N	2.54	0.41
5:L:138:PRO:HB2	5:L:351:THR:O	2.20	0.41
5:L:166:VAL:HG23	5:L:258:GLN:O	2.21	0.41
5:L:227:GLN:CG	5:L:252:LEU:HA	2.50	0.41
5:L:262:VAL:O	5:L:263:PRO:C	2.63	0.41
5:L:291:CYS:HB3	5:L:297:MET:SD	2.61	0.41
5:L:573:LEU:CD1	5:L:588:ARG:HE	2.33	0.41
1:A:107:ILE:H	1:A:107:ILE:HG13	1.71	0.41
1:A:134:THR:HG21	2:C:727:VAL:O	2.21	0.41
1:A:165:GLU:OE1	1:A:172:LEU:HD21	2.21	0.41
1:B:38:THR:HG23	1:B:39:LEU:H	1.85	0.41
1:B:48:LEU:CD1	1:B:183:ILE:HD11	2.50	0.41
2:C:22:LEU:HD22	2:C:23:ASP:N	2.36	0.41
2:C:369:MET:O	2:C:372:PRO:HD3	2.21	0.41
2:C:666:SER:OG	2:C:704:MET:HG3	2.21	0.41
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:256:ASP:C	3:D:258:GLY:N	2.78	0.41
3:D:307:LEU:HD23	3:D:307:LEU:HA	1.81	0.41
3:D:339:ARG:O	3:D:340:GLN:HG2	2.20	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.21	0.41
5:F:465:ARG:HB3	5:F:468:ARG:HH12	1.86	0.41
1:G:134:THR:HG23	1:G:135:ASP:N	2.36	0.41
1:H:51:MET:HE1	1:H:220:ALA:HA	2.03	0.41
2:I:211:ARG:NH2	2:I:351:LEU:HD22	2.36	0.41
2:I:405:PHE:CE2	2:I:409:LEU:HD12	2.56	0.41
2:I:974:ARG:HD2	2:I:1014:LEU:CD2	2.51	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.95	0.41
3:J:64:PRO:O	3:J:95:THR:OG1	2.33	0.41
3:J:234:PRO:HD2	3:J:235:GLU:OE2	2.21	0.41
3:J:369:PRO:HB3	3:J:444:GLY:O	2.20	0.41
3:J:440:VAL:O	3:J:442:ILE:HG12	2.21	0.41
5:L:463:LEU:HD23	5:L:463:LEU:HA	1.73	0.41
1:B:133:LEU:HD11	1:B:140:ILE:HG21	2.03	0.40
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.03	0.40
2:C:455:SER:O	2:C:456:VAL:C	2.64	0.40
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.36	0.40
2:C:1303:LYS:HA	2:C:1303:LYS:HD3	1.78	0.40
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.36	0.40
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.52	0.40
3:D:277:ASN:HA	3:D:280:LYS:HG3	2.03	0.40
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.03	0.40
3:D:664:ILE:HG22	3:D:678:ARG:HG2	2.02	0.40
3:D:1345:ARG:CG	3:D:1370:MET:HE1	2.43	0.40
1:G:26:VAL:HG22	1:G:203:ILE:HB	2.04	0.40
1:H:6:THR:O	1:H:6:THR:HG22	2.21	0.40
2:I:197:ARG:HH12	2:I:203:LYS:HB2	1.86	0.40
2:I:402:ARG:HG2	2:I:416:GLY:H	1.86	0.40
2:I:559:CYS:CB	2:I:662:SER:HB3	2.50	0.40
2:I:663:VAL:H	2:I:663:VAL:HG22	1.51	0.40
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.03	0.40
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.96	0.40
3:J:481:ARG:O	3:J:485:MET:HB2	2.20	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	0.40
5:L:409:ASN:O	5:L:413:MET:HG3	2.22	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
1:A:83:LEU:HB3	2:C:694:ARG:NH2	2.36	0.40
2:C:62:TYR:CE1	2:C:476:LYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:GLU:H	2:C:121:GLU:HG3	1.57	0.40
2:C:271:ALA:O	2:C:275:ARG:HG3	2.21	0.40
2:C:530:ILE:O	2:C:572:ILE:O	2.40	0.40
2:C:620:ASN:O	2:C:620:ASN:CG	2.64	0.40
2:C:1146:GLN:O	2:C:1150:ASP:OD2	2.39	0.40
2:C:1320:PRO:HB3	3:D:345:LYS:HZ3	1.86	0.40
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.03	0.40
3:D:318:GLY:C	3:D:320:ASN:N	2.78	0.40
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.40
3:D:489:ASN:HA	3:D:904:ALA:HB1	2.03	0.40
3:D:920:ALA:O	3:D:921:GLN:C	2.64	0.40
3:D:1327:GLU:HG2	3:D:1328:THR:N	2.35	0.40
3:D:1357:ILE:O	3:D:1362:GLY:HA3	2.21	0.40
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.90	0.40
5:F:599:ARG:O	5:F:604:SER:HB2	2.21	0.40
1:G:45:ARG:CG	1:H:38:THR:HB	2.36	0.40
1:G:75:GLN:HG3	1:G:76:GLU:OE2	2.21	0.40
1:H:86:LYS:HD2	1:H:174:ASP:HB2	2.03	0.40
2:I:85:CYS:SG	2:I:92:TYR:HA	2.61	0.40
2:I:136:PHE:CE1	2:I:506:PHE:HE2	2.40	0.40
2:I:228:VAL:HG13	2:I:239:MET:HE3	2.04	0.40
2:I:564:PRO:HG2	2:I:568:ASN:O	2.20	0.40
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.86	0.40
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.77	0.40
3:J:1233:ILE:HG22	3:J:1234:VAL:N	2.36	0.40
5:L:164:GLY:O	5:L:260:ARG:HB2	2.20	0.40
2:C:9:LYS:O	2:C:1175:ASN:ND2	2.53	0.40
2:C:63:SER:C	2:C:65:ASN:N	2.79	0.40
2:C:72:SER:O	2:C:98:VAL:HG13	2.21	0.40
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.56	0.40
2:C:616:ILE:HG13	2:C:652:TYR:HB2	2.03	0.40
2:C:656:SER:OG	2:C:658:GLN:HB2	2.21	0.40
2:C:1064:ASP:OD1	2:C:1239:VAL:HG12	2.22	0.40
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	2.03	0.40
2:C:1281:TYR:OH	3:D:434:ILE:O	2.39	0.40
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.86	0.40
3:D:57:PHE:CD2	3:D:57:PHE:N	2.88	0.40
3:D:1353:VAL:O	3:D:1353:VAL:HG22	2.22	0.40
5:F:584:ARG:HD2	5:F:584:ARG:HA	1.74	0.40
1:G:76:GLU:CD	1:G:132:HIS:H	2.28	0.40
1:H:100:LEU:HB3	1:H:115:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:ARG:HD2	3:J:581:MET:HE1	2.03	0.40
1:H:205:MET:HE1	1:H:217:ILE:HG13	2.03	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.03	0.40
2:I:517:GLN:NE2	2:I:759:SER:HA	2.37	0.40
2:I:579:ALA:O	2:I:580:GLN:HG3	2.21	0.40
2:I:606:LEU:HD23	2:I:611:GLU:HA	2.04	0.40
2:I:726:TYR:CZ	2:I:728:ASP:HB2	2.56	0.40
2:I:920:VAL:HA	2:I:921:PRO:HD3	1.92	0.40
3:J:401:VAL:HA	3:J:408:VAL:HG11	2.02	0.40
3:J:511:TYR:HE1	3:J:724:MET:CG	2.33	0.40
3:J:511:TYR:CE1	3:J:724:MET:HG2	2.53	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.40
5:L:568:ASN:ND2	5:L:568:ASN:H	2.19	0.40
1:B:19:VAL:O	1:B:23:HIS:HB3	2.21	0.40
2:C:10:ARG:HD3	2:C:1181:PRO:CG	2.46	0.40
2:C:596:ASP:CG	2:C:597:GLY:H	2.19	0.40
2:C:838:CYS:HB2	2:C:918:LEU:HB3	2.03	0.40
2:C:1120:ALA:C	2:C:1123:GLY:H	2.29	0.40
3:D:45:ASN:O	3:D:46:TYR:CB	2.70	0.40
3:D:1372:ARG:HE	3:D:1372:ARG:HB2	1.73	0.40
5:F:316:PHE:CE1	5:F:337:VAL:HB	2.57	0.40
5:F:426:LYS:HE2	5:F:428:SER:OG	2.22	0.40
5:F:551:LEU:HD11	5:F:598:LEU:HD21	2.02	0.40
1:G:74:VAL:HG21	1:G:81:ILE:HD11	2.04	0.40
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.84	0.40
1:H:88:LEU:HD21	1:H:115:ILE:CD1	2.51	0.40
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.85	0.40
2:I:197:ARG:HH22	2:I:203:LYS:HE2	1.86	0.40
2:I:337:PHE:CE2	2:I:343:HIS:HD2	2.40	0.40
2:I:964:LEU:HD21	2:I:1022:LYS:HD2	2.03	0.40
3:J:41:PRO:HA	3:J:56:LEU:HD11	2.02	0.40
3:J:268:LEU:HD22	3:J:306:LEU:HA	2.03	0.40
3:J:452:LEU:HD23	3:J:452:LEU:HA	1.81	0.40
3:J:722:ILE:HG21	3:J:722:ILE:HD13	1.79	0.40
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	2.04	0.40
4:K:22:VAL:HG13	4:K:64:LEU:CD1	2.51	0.40
5:L:431:ALA:O	5:L:434:TRP:N	2.55	0.40
1:A:67:GLU:H	1:A:67:GLU:HG2	1.46	0.40
2:C:107:ARG:HA	2:C:108:GLU:HA	1.52	0.40
2:C:133:ASN:ND2	2:C:713:GLY:HA3	2.37	0.40
2:C:161:LYS:HA	2:C:170:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:PRO:HA	2:C:492:MET:HE3	2.04	0.40
2:C:723:VAL:HG12	2:C:724:VAL:N	2.37	0.40
2:C:901:LEU:HD12	2:C:901:LEU:O	2.21	0.40
3:D:34:SER:OG	3:D:103:GLY:HA2	2.21	0.40
3:D:121:PRO:HD2	3:D:123:ARG:HH21	1.86	0.40
3:D:647:PRO:HD3	3:D:697:MET:HB3	2.04	0.40
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.66	0.40
3:D:925:GLU:C	3:D:927:GLY:H	2.29	0.40
5:F:437:GLN:HG3	5:F:438:ALA:N	2.35	0.40
5:F:547:VAL:HG13	5:F:598:LEU:CD2	2.46	0.40
1:G:155:ALA:HA	1:G:158:ARG:HG3	2.03	0.40
1:G:219:ARG:HE	1:G:219:ARG:HB2	1.68	0.40
1:G:224:LEU:HD23	1:G:224:LEU:O	2.22	0.40
1:H:155:ALA:HB2	1:H:174:ASP:N	2.36	0.40
2:I:810:TYR:HB3	2:I:817:LEU:HD23	2.03	0.40
2:I:960:LEU:C	2:I:1025:PHE:HE2	2.29	0.40
2:I:979:LEU:HD23	2:I:989:LEU:CD2	2.52	0.40
2:I:989:LEU:HD13	2:I:1000:LEU:HD13	2.04	0.40
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.46	0.40
3:J:804:ALA:O	3:J:806:ASP:N	2.54	0.40
3:J:1262:ARG:HH11	3:J:1262:ARG:HD3	1.73	0.40
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.87	0.40
5:L:219:GLU:O	5:L:222:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	317/329 (96%)	243 (77%)	48 (15%)	26 (8%)	0 8
1	B	213/329 (65%)	193 (91%)	15 (7%)	5 (2%)	5 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	225/329 (68%)	195 (87%)	21 (9%)	9 (4%)	2	20
1	H	212/329 (64%)	193 (91%)	15 (7%)	4 (2%)	6	33
2	C	1338/1342 (100%)	1210 (90%)	111 (8%)	17 (1%)	9	39
2	I	1338/1342 (100%)	1207 (90%)	112 (8%)	19 (1%)	9	38
3	D	1157/1407 (82%)	1031 (89%)	101 (9%)	25 (2%)	5	30
3	J	1146/1407 (81%)	1032 (90%)	92 (8%)	22 (2%)	6	33
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	5	29
4	K	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	9	39
5	F	462/613 (75%)	424 (92%)	30 (6%)	8 (2%)	7	35
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	35
All	All	7035/8222 (86%)	6307 (90%)	582 (8%)	146 (2%)	5	31

All (146) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
5	F	490	PRO
5	F	566	ASP
5	F	584	ARG
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	426	ALA
3	J	710	ASP
3	J	850	LYS
3	J	1169	THR
3	J	1294	ALA
5	L	490	PRO
5	L	569	THR
5	L	584	ARG
1	A	14	VAL
1	A	104	LYS
1	A	162	GLU
1	A	167	PRO
1	A	177	TYR
1	A	179	PRO
1	A	242	VAL
1	A	319	GLU
2	C	121	GLU
2	C	747	GLY
2	C	897	PRO
2	C	1059	ARG
2	C	1153	ALA
2	C	1165	SER
3	D	10	ALA
3	D	13	LYS
3	D	49	PHE
3	D	417	ARG

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Mol	Chain	Res	Type
3	D	745	GLY
3	D	805	GLN
3	D	850	LYS
5	F	569	THR
1	G	9	LEU
1	G	14	VAL
1	G	196	THR
1	H	138	ALA
2	I	44	GLU
3	J	334	LYS
3	J	335	GLN
3	J	342	LEU
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
4	K	33	GLY
5	L	395	THR
5	L	475	GLY
5	L	566	ASP
1	A	52	PRO
1	A	196	THR
1	A	216	ALA
2	C	983	GLY
2	C	1154	ASP
3	D	46	TYR
3	D	806	ASP
3	D	1274	PHE
5	F	602	SER
1	G	62	ASP
1	H	193	GLU
2	I	983	GLY
2	I	1059	ARG
2	I	1165	SER
3	J	49	PHE
3	J	417	ARG
1	A	164	ASP
1	A	324	ALA
1	B	13	LEU
1	B	14	VAL
1	B	20	SER
2	C	63	SER
3	D	1297	LYS

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Mol	Chain	Res	Type
3	D	1344	LEU
1	H	134	THR
2	I	201	ARG
3	J	46	TYR
5	L	96	ASP
1	A	124	VAL
1	A	275	ILE
2	C	1151	LEU
3	D	454	CYS
5	F	96	ASP
5	F	395	THR
1	G	22	THR
1	H	20	SER
2	I	160	ASP
3	J	1180	VAL
3	J	1297	LYS
1	A	115	ILE
1	A	315	GLY
1	B	136	GLU
3	D	1180	VAL
1	G	232	VAL
2	I	892	GLU
3	J	314	ARG
3	J	712	GLN
3	D	89	GLY
3	D	831	VAL
5	F	475	GLY
2	C	1317	PRO
3	D	357	VAL
3	J	826	ILE
1	A	293	PRO
2	I	1186	VAL
3	J	89	GLY
5	L	97	PRO
3	D	828	GLY
4	E	86	ILE
2	I	1202	GLY
3	J	357	VAL
3	J	586	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	226 (81%)	52 (19%)	1	10
1	B	186/286 (65%)	162 (87%)	24 (13%)	4	22
1	G	193/286 (68%)	168 (87%)	25 (13%)	4	21
1	H	183/286 (64%)	163 (89%)	20 (11%)	6	27
2	C	1155/1157 (100%)	1018 (88%)	137 (12%)	5	24
2	I	1154/1157 (100%)	1026 (89%)	128 (11%)	6	27
3	D	964/1168 (82%)	847 (88%)	117 (12%)	5	24
3	J	962/1168 (82%)	851 (88%)	111 (12%)	5	25
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	27
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	33
5	F	417/540 (77%)	368 (88%)	49 (12%)	5	25
5	L	418/540 (77%)	363 (87%)	55 (13%)	4	21
All	All	6049/7024 (86%)	5317 (88%)	732 (12%)	5	24

All (732) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	9	LEU
1	A	19	VAL
1	A	23	HIS
1	A	25	LYS
1	A	26	VAL
1	A	64	VAL
1	A	67	GLU
1	A	70	THR
1	A	71	LYS
1	A	74	VAL
1	A	75	GLN
1	A	77	ASP

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Mol	Chain	Res	Type
1	A	79	LEU
1	A	81	ILE
1	A	83	LEU
1	A	98	VAL
1	A	102	LEU
1	A	110	VAL
1	A	116	THR
1	A	121	VAL
1	A	137	ASN
1	A	140	ILE
1	A	156	SER
1	A	159	ILE
1	A	164	ASP
1	A	165	GLU
1	A	172	LEU
1	A	180	VAL
1	A	182	ARG
1	A	186	ASN
1	A	192	VAL
1	A	211	ILE
1	A	227	GLN
1	A	231	PHE
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	252	ILE
1	A	262	LEU
1	A	269	CYS
1	A	276	HIS
1	A	282	VAL
1	A	284	ARG
1	A	295	LEU
1	A	300	LEU
1	A	306	VAL
1	A	307	LEU
1	A	316	MET
1	A	318	LEU
1	A	319	GLU
1	B	13	LEU
1	B	14	VAL
1	B	16	ILE
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	27	THR
1	B	58	GLU
1	B	60	GLU
1	B	62	ASP
1	B	64	VAL
1	B	65	LEU
1	B	79	LEU
1	B	80	GLU
1	B	92	VAL
1	B	95	LYS
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
1	B	232	VAL
1	B	233	ASP
2	C	11	ILE
2	C	17	LYS
2	C	21	VAL
2	C	22	LEU
2	C	23	ASP
2	C	46	GLN
2	C	55	SER
2	C	56	VAL
2	C	82	VAL
2	C	86	GLN
2	C	91	THR
2	C	103	VAL
2	C	107	ARG
2	C	108	GLU
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	131	THR
2	C	135	THR
2	C	138	ILE

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Mol	Chain	Res	Type
2	C	170	VAL
2	C	208	ILE
2	C	219	GLN
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	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	451	ARG
2	C	456	VAL
2	C	481	LEU
2	C	484	LEU
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	510	GLN
2	C	518	ASN
2	C	521	LEU
2	C	530	ILE
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	563	THR
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	625	GLU
2	C	633	LEU
2	C	635	THR
2	C	637	ARG
2	C	660	VAL
2	C	663	VAL

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Mol	Chain	Res	Type
2	C	672	GLU
2	C	680	LEU
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	750	ILE
2	C	757	THR
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	782	VAL
2	C	791	LEU
2	C	800	MET
2	C	808	ASN
2	C	823	VAL
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	918	LEU
2	C	951	MET
2	C	979	LEU
2	C	980	VAL
2	C	984	VAL
2	C	1002	LEU
2	C	1014	LEU
2	C	1037	THR
2	C	1050	VAL
2	C	1054	LEU
2	C	1073	LYS
2	C	1076	ILE
2	C	1078	LYS
2	C	1082	ILE
2	C	1098	LEU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1141	LEU

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Mol	Chain	Res	Type
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	1162	SER
2	C	1163	THR
2	C	1164	PHE
2	C	1180	MET
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1225	VAL
2	C	1227	VAL
2	C	1233	LEU
2	C	1238	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1255	THR
2	C	1265	PHE
2	C	1281	TYR
2	C	1287	LEU
2	C	1289	GLU
2	C	1291	LEU
2	C	1299	ASN
2	C	1313	HIS
2	C	1326	LEU
2	C	1327	LEU
2	C	1331	ARG
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	13	LYS
3	D	18	ASP
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	78	LEU
3	D	79	LYS
3	D	80	HIS
3	D	83	VAL

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Mol	Chain	Res	Type
3	D	84	ILE
3	D	92	VAL
3	D	95	THR
3	D	97	VAL
3	D	98	ARG
3	D	159	ILE
3	D	162	GLU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	218	THR
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	280	LYS
3	D	283	LEU
3	D	292	VAL
3	D	324	LEU
3	D	330	MET
3	D	343	LEU
3	D	346	ARG
3	D	357	VAL
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	415	VAL
3	D	416	ILE
3	D	421	VAL
3	D	423	LEU
3	D	429	LEU
3	D	490	ILE
3	D	513	MET
3	D	532	GLU
3	D	536	LEU
3	D	544	LEU
3	D	545	HIS
3	D	563	LEU
3	D	567	THR

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Mol	Chain	Res	Type
3	D	568	SER
3	D	569	LEU
3	D	573	THR
3	D	592	VAL
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	683	ILE
3	D	685	ILE
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	797	THR
3	D	799	ARG
3	D	801	VAL
3	D	826	ILE
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	867	GLN
3	D	890	THR
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	913	GLU
3	D	918	ILE
3	D	1135	THR
3	D	1146	GLU

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Mol	Chain	Res	Type
3	D	1155	ILE
3	D	1156	LEU
3	D	1163	VAL
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1196	LEU
3	D	1202	GLU
3	D	1221	LEU
3	D	1233	ILE
3	D	1251	LYS
3	D	1255	VAL
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1280	VAL
3	D	1283	SER
3	D	1332	LEU
3	D	1343	GLU
3	D	1361	THR
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	6	VAL
4	E	13	ILE
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	114	GLU
5	F	130	VAL
5	F	154	GLU
5	F	230	VAL
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU

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Mol	Chain	Res	Type
5	F	338	HIS
5	F	399	LEU
5	F	400	GLN
5	F	421	TYR
5	F	449	THR
5	F	450	ILE
5	F	469	GLN
5	F	470	MET
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	490	PRO
5	F	491	GLU
5	F	492	ASP
5	F	494	ILE
5	F	511	ILE
5	F	514	ASP
5	F	516	ASP
5	F	529	GLU
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	573	LEU
5	F	578	LYS
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	12	ARG
1	G	16	ILE
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL

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Mol	Chain	Res	Type
1	G	50	SER
1	G	64	VAL
1	G	70	THR
1	G	71	LYS
1	G	79	LEU
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	139	SER
1	G	158	ARG
1	G	163	GLU
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	211	ILE
1	G	218	ARG
1	H	16	ILE
1	H	18	GLN
1	H	27	THR
1	H	38	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	95	LYS
1	H	107	ILE
1	H	124	VAL
1	H	133	LEU
1	H	146	VAL
1	H	171	LEU
1	H	176	CYS
1	H	183	ILE
1	H	196	THR
2	I	3	TYR
2	I	4	SER

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Mol	Chain	Res	Type
2	I	11	ILE
2	I	17	LYS
2	I	21	VAL
2	I	22	LEU
2	I	23	ASP
2	I	30	ILE
2	I	46	GLN
2	I	60	GLN
2	I	86	GLN
2	I	91	THR
2	I	103	VAL
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	119	GLU
2	I	121	GLU
2	I	131	THR
2	I	138	ILE
2	I	156	PHE
2	I	170	VAL
2	I	199	ASP
2	I	208	ILE
2	I	219	GLN
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	306	THR
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	369	MET
2	I	400	VAL
2	I	419	ILE
2	I	423	ASP
2	I	445	ILE
2	I	451	ARG
2	I	453	ILE
2	I	456	VAL
2	I	484	LEU
2	I	490	GLN

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Mol	Chain	Res	Type
2	I	492	MET
2	I	493	ILE
2	I	516	ASP
2	I	518	ASN
2	I	521	LEU
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	550	VAL
2	I	553	THR
2	I	558	VAL
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	625	GLU
2	I	630	VAL
2	I	633	LEU
2	I	635	THR
2	I	637	ARG
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	757	THR
2	I	765	ILE
2	I	772	SER
2	I	773	LEU
2	I	782	VAL
2	I	800	MET
2	I	808	ASN
2	I	890	LYS
2	I	892	GLU
2	I	918	LEU

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Mol	Chain	Res	Type
2	I	951	MET
2	I	967	LEU
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1037	THR
2	I	1050	VAL
2	I	1073	LYS
2	I	1076	ILE
2	I	1078	LYS
2	I	1082	ILE
2	I	1114	GLU
2	I	1117	LEU
2	I	1134	GLN
2	I	1136	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	1172	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1206	THR
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	1253	LEU
2	I	1287	LEU
2	I	1289	GLU
2	I	1291	LEU
2	I	1299	ASN
2	I	1313	HIS
2	I	1325	VAL
2	I	1326	LEU
2	I	1327	LEU
2	I	1331	ARG
2	I	1342	GLU

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Mol	Chain	Res	Type
3	J	20	ILE
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	78	LEU
3	J	79	LYS
3	J	92	VAL
3	J	93	THR
3	J	95	THR
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	217	LEU
3	J	218	THR
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	259	ARG
3	J	280	LYS
3	J	283	LEU
3	J	292	VAL
3	J	324	LEU
3	J	330	MET
3	J	342	LEU
3	J	343	LEU
3	J	345	LYS
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	394	ILE
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	490	ILE
3	J	506	VAL
3	J	510	LEU

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Mol	Chain	Res	Type
3	J	513	MET
3	J	532	GLU
3	J	536	LEU
3	J	544	LEU
3	J	545	HIS
3	J	563	LEU
3	J	568	SER
3	J	569	LEU
3	J	573	THR
3	J	594	GLN
3	J	605	LEU
3	J	615	LYS
3	J	639	VAL
3	J	641	ILE
3	J	646	ILE
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	826	ILE
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	885	VAL
3	J	897	HIS
3	J	898	CYS
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN

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Mol	Chain	Res	Type
3	J	918	ILE
3	J	1146	GLU
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1196	LEU
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1261	LEU
3	J	1266	ILE
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1290	ARG
3	J	1292	LEU
3	J	1293	GLU
3	J	1319	PHE
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
3	J	1355	ARG
3	J	1366	HIS
4	K	3	ARG
4	K	5	THR
4	K	6	VAL
4	K	13	ILE
4	K	28	ARG
4	K	39	VAL
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	130	VAL
5	L	154	GLU
5	L	230	VAL
5	L	233	ASP
5	L	277	MET
5	L	297	MET

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Mol	Chain	Res	Type
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	338	HIS
5	L	395	THR
5	L	399	LEU
5	L	421	TYR
5	L	449	THR
5	L	450	ILE
5	L	469	GLN
5	L	470	MET
5	L	471	LEU
5	L	472	GLN
5	L	476	ARG
5	L	479	THR
5	L	482	GLU
5	L	486	ARG
5	L	488	LEU
5	L	490	PRO
5	L	491	GLU
5	L	492	ASP
5	L	494	ILE
5	L	500	ILE
5	L	511	ILE
5	L	516	ASP
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	572	THR
5	L	573	LEU
5	L	575	GLU
5	L	578	LYS
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS

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Mol	Chain	Res	Type
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	268	ASN
1	B	117	HIS
2	C	46	GLN
2	C	120	GLN
2	C	133	ASN
2	C	139	ASN
2	C	343	HIS
2	C	406	ASN
2	C	510	GLN
2	C	604	HIS
2	C	628	HIS
2	C	799	ASN
2	C	1023	HIS
2	C	1116	HIS
2	C	1136	GLN
2	C	1209	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1268	GLN
2	C	1314	GLN
3	D	200	GLN
3	D	435	GLN
3	D	450	HIS
3	D	594	GLN
3	D	702	GLN
3	D	716	GLN
3	D	861	ASN
4	E	62	GLN
5	F	129	GLN
5	F	246	GLN
5	F	301	ASN
5	F	383	ASN
5	F	446	GLN

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Mol	Chain	Res	Type
5	F	455	HIS
5	F	579	GLN
5	F	600	HIS
1	H	132	HIS
2	I	139	ASN
2	I	165	HIS
2	I	314	ASN
2	I	343	HIS
2	I	510	GLN
2	I	513	GLN
2	I	620	ASN
2	I	628	HIS
2	I	688	GLN
2	I	725	GLN
2	I	752	ASN
2	I	932	GLN
2	I	1023	HIS
2	I	1038	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1220	GLN
2	I	1237	HIS
2	I	1299	ASN
2	I	1314	GLN
3	J	157	GLN
3	J	200	GLN
3	J	206	ASN
3	J	320	ASN
3	J	430	HIS
3	J	450	HIS
3	J	465	GLN
3	J	477	GLN
3	J	489	ASN
3	J	560	ASN
3	J	594	GLN
3	J	702	GLN
3	J	716	GLN
3	J	771	GLN
3	J	817	HIS
3	J	861	ASN

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Mol	Chain	Res	Type
3	J	910	ASN
3	J	1259	GLN
3	J	1279	GLN
3	J	1366	HIS
4	K	15	ASN
4	K	61	ASN
4	K	62	GLN
5	L	294	GLN
5	L	357	GLN
5	L	406	GLN
5	L	446	GLN
5	L	469	GLN
5	L	568	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	4C6	D	2004	-	32,34,34	0.99	1 (3%)	42,51,51	1.84	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	4C6	J	2004	-	32,34,34	0.72	0	42,51,51	1.04	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	4C6	D	2004	-	-	4/15/45/45	0/4/4/4
8	4C6	J	2004	-	-	2/15/45/45	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C6	S-N	-4.41	1.60	1.64

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2004	4C6	C5-C2-S	11.11	135.50	127.23
8	J	2004	4C6	C7-C21-C	-3.00	85.26	88.05
8	J	2004	4C6	C7-C1-N	2.62	135.43	129.88
8	D	2004	4C6	C7-C1-N	2.08	134.28	129.88
8	J	2004	4C6	C1-C-C21	2.07	89.98	88.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

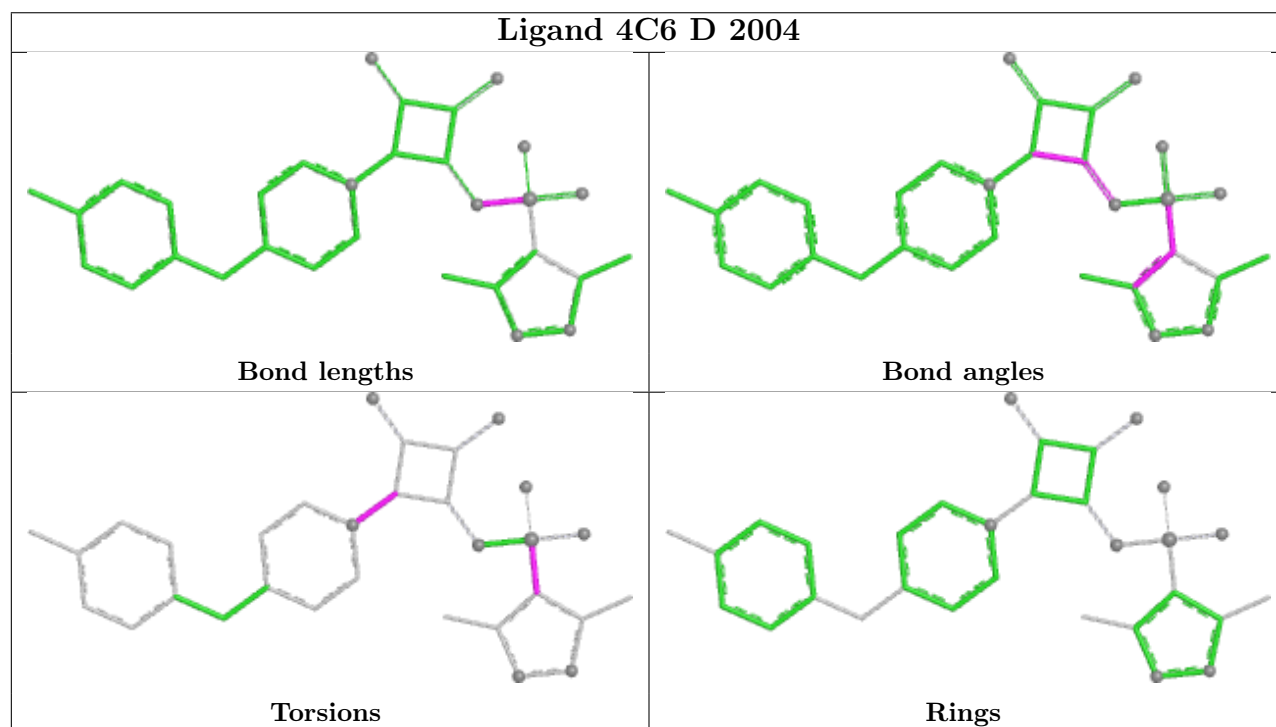
Mol	Chain	Res	Type	Atoms
8	D	2004	4C6	C3-C2-S-O2
8	D	2004	4C6	C3-C2-S-O3
8	D	2004	4C6	C5-C2-S-O3
8	J	2004	4C6	C3-C2-S-O3
8	J	2004	4C6	C3-C2-S-O2
8	D	2004	4C6	C21-C7-N2-C8

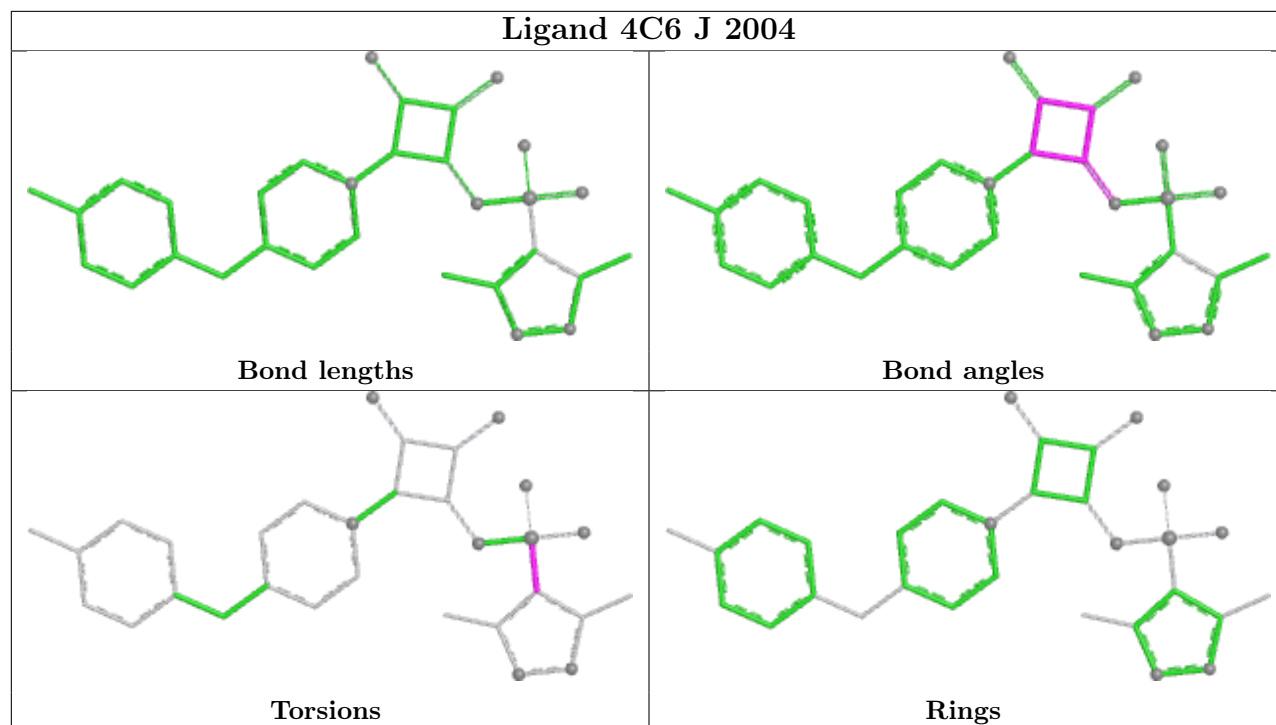
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.77	0 100 100	105, 138, 176, 185	0
1	B	217/329 (65%)	-0.63	0 100 100	114, 172, 192, 198	0
1	G	227/329 (68%)	-0.69	0 100 100	138, 159, 175, 192	0
1	H	216/329 (65%)	-0.65	0 100 100	130, 174, 192, 201	0
2	C	1340/1342 (99%)	-0.73	0 100 100	88, 126, 202, 228	0
2	I	1340/1342 (99%)	-0.73	0 100 100	108, 154, 212, 314	0
3	D	1163/1407 (82%)	-0.74	0 100 100	90, 119, 164, 197	0
3	J	1152/1407 (81%)	-0.71	1 (0%) 92 85	103, 137, 181, 211	0
4	E	89/91 (97%)	-0.77	0 100 100	129, 159, 178, 184	0
4	K	79/91 (86%)	-0.58	0 100 100	186, 221, 249, 254	0
5	F	468/613 (76%)	-0.66	0 100 100	113, 159, 233, 249	0
5	L	469/613 (76%)	-0.71	0 100 100	127, 168, 244, 260	0
All	All	7079/8222 (86%)	-0.71	1 (0%) 100 100	88, 143, 205, 314	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1215	GLU	2.4

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

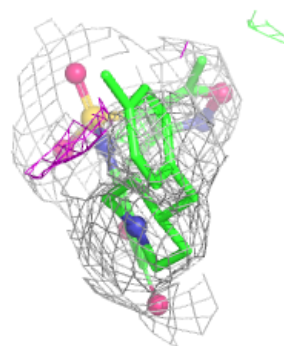
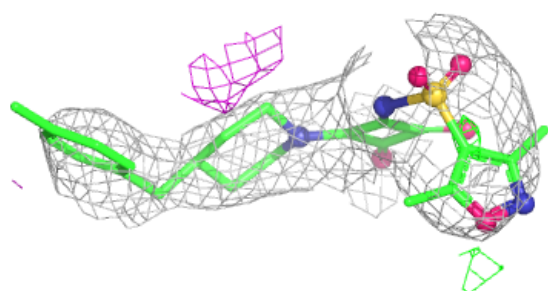
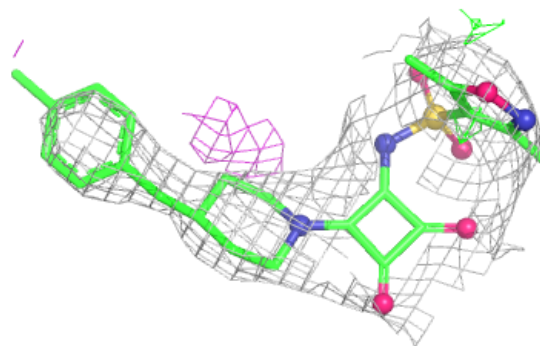
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1401	1/1	0.57	0.21	127,127,127,127	0
6	MG	I	1401	1/1	0.63	0.20	127,127,127,127	0
6	MG	D	2001	1/1	0.80	0.15	127,127,127,127	0
6	MG	J	2001	1/1	0.85	0.15	127,127,127,127	0
8	4C6	J	2004	31/31	0.97	0.11	127,127,128,141	0
8	4C6	D	2004	31/31	0.98	0.16	127,127,127,127	0
7	ZN	J	2002	1/1	0.98	0.06	190,190,190,190	0
7	ZN	D	2002	1/1	0.99	0.10	164,164,164,164	0
7	ZN	D	2003	1/1	1.00	0.04	127,127,127,127	0
7	ZN	J	2003	1/1	1.00	0.03	127,127,127,127	0

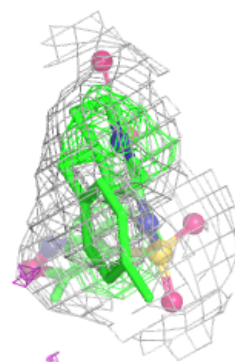
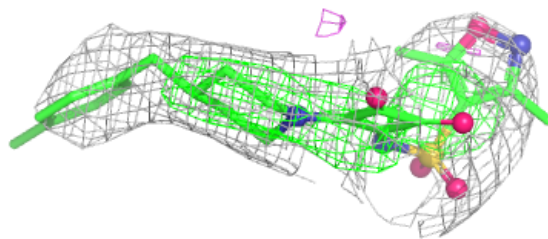
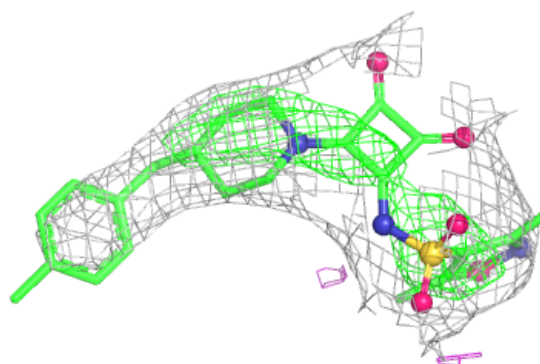
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4C6 J 2004:

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

**Electron density around 4C6 D 2004:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.