



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 8U9X / pdb_00008u9x
Title : STRUCTURAL BASIS OF TRANSCRIPTION: RNA POLYMERASE II
SUBSTRATE BINDING AND METAL COORDINATION AT 3.0 Å OF
T834P MUTANT USING A FREE-ELECTRON LASER
Authors : Arjunan, P.; Calero, G.; Kaplan, C.D.
Deposited on : 2023-09-20
Resolution : 3.05 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

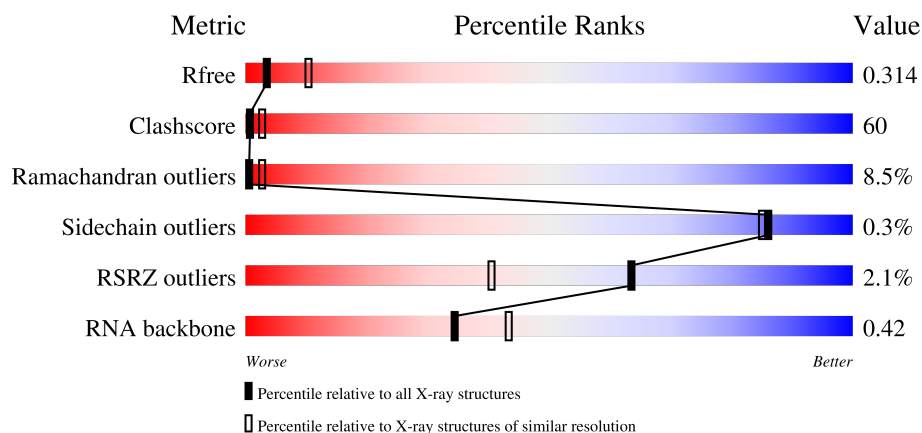
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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	1733	 2% 20% 54% 7% 19%
2	B	1224	 20% 61% 6% 13%
3	C	318	 29% 52% 16%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	T	13	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ZN	L	101	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 30893 atoms, of which 8 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0	0
			10987	6934	1918	2073	62			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	PRO	THR	conflict	UNP P04050

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1060	Total	C	N	O	S	0	0	0
			8424	5346	1475	1549	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	162	Total	C	N	O	S	0	0	0
			1287	799	224	262	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	208	Total	C	N	O	S	0	0	0
			1713	1089	303	312	9			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	117	Total	C	N	O	S	0	0	0
			951	605	158	184	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			526	336	90	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	43	Total	C	N	O	S	0	0	0
			343	211	69	59	4			

- Molecule 13 is a RNA chain called MOL_ID: 13.

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

- Molecule 14 is a DNA chain called MOL_ID: 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	13	Total	C	N	O	P	0	0	0
			260	124	44	79	13			

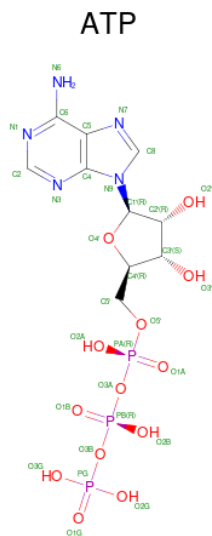
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

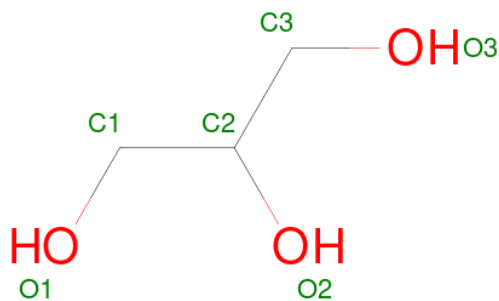
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Mn	0	0
			2	2		
16	B	1	Total	Mn	0	0
			1	1		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 18 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	E	1	Total	C	H	O	0	0
			14	3	8	3		

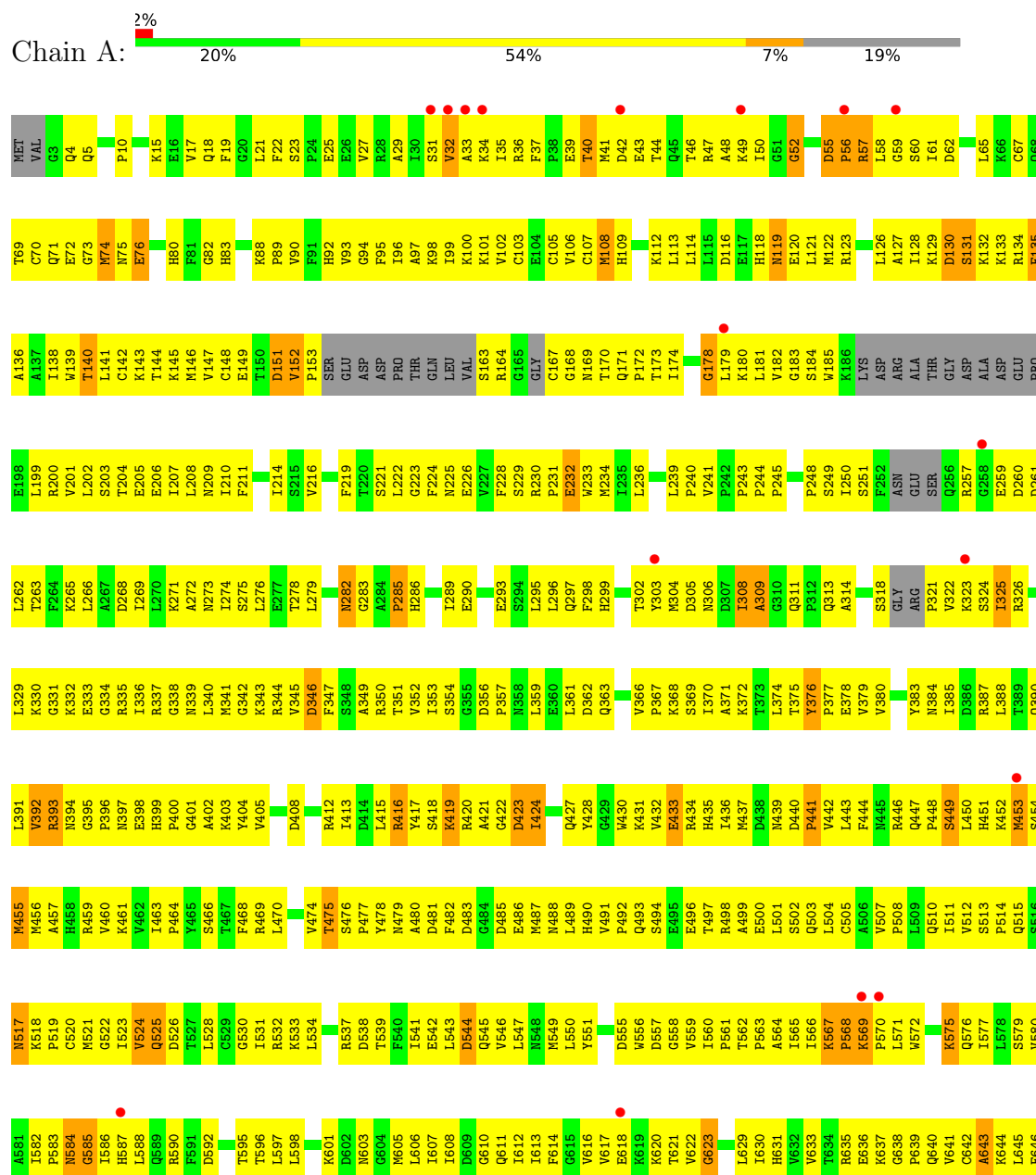
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	46	Total 46	O 46	0	0
19	B	38	Total 38	O 38	0	0
19	C	6	Total 6	O 6	0	0
19	D	5	Total 5	O 5	0	0
19	E	7	Total 7	O 7	0	0
19	F	3	Total 3	O 3	0	0
19	G	4	Total 4	O 4	0	0
19	H	3	Total 3	O 3	0	0
19	J	2	Total 2	O 2	0	0
19	K	5	Total 5	O 5	0	0
19	L	2	Total 2	O 2	0	0
19	R	1	Total 1	O 1	0	0
19	T	2	Total 2	O 2	0	0

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.

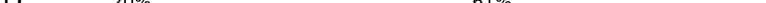
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

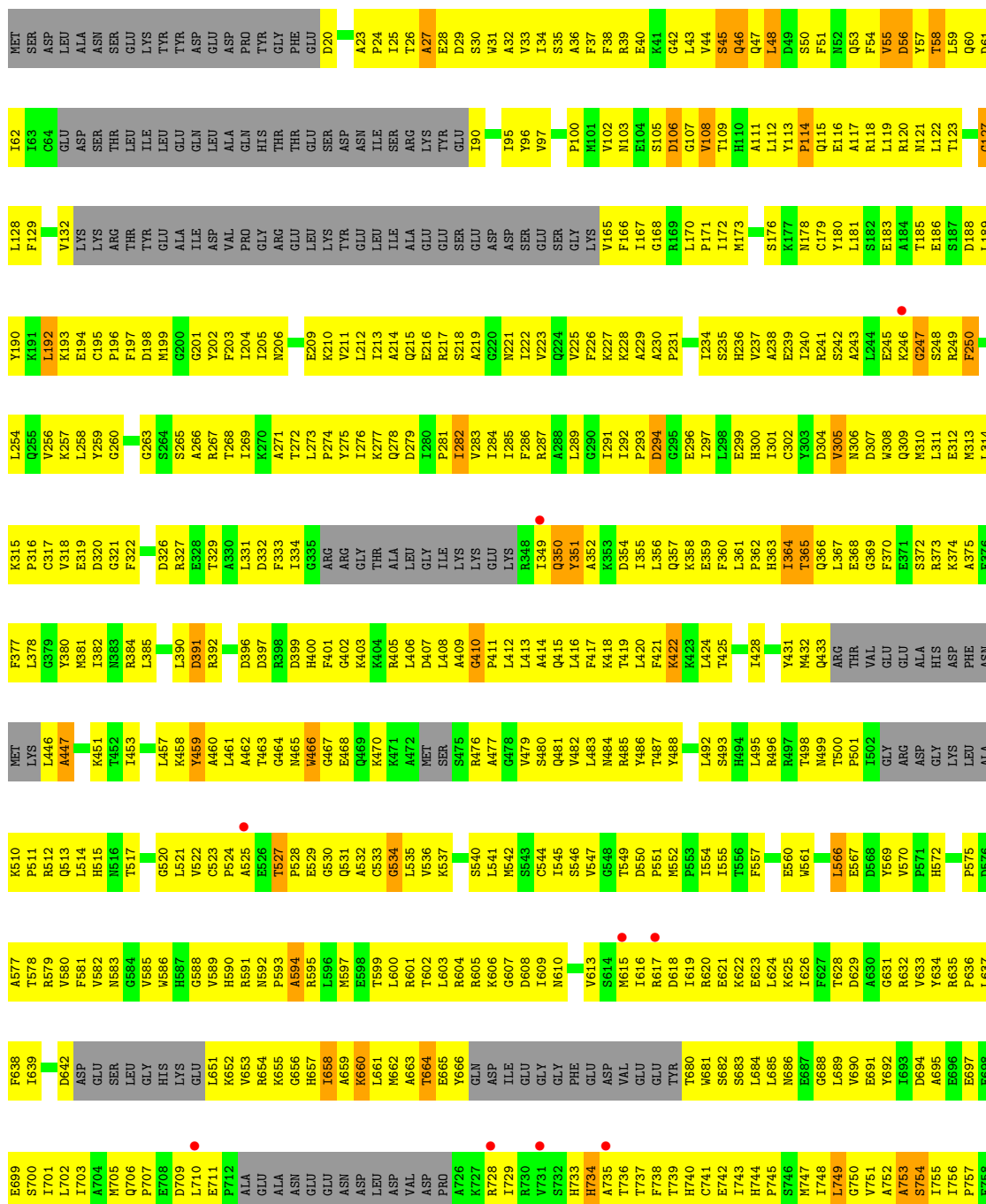


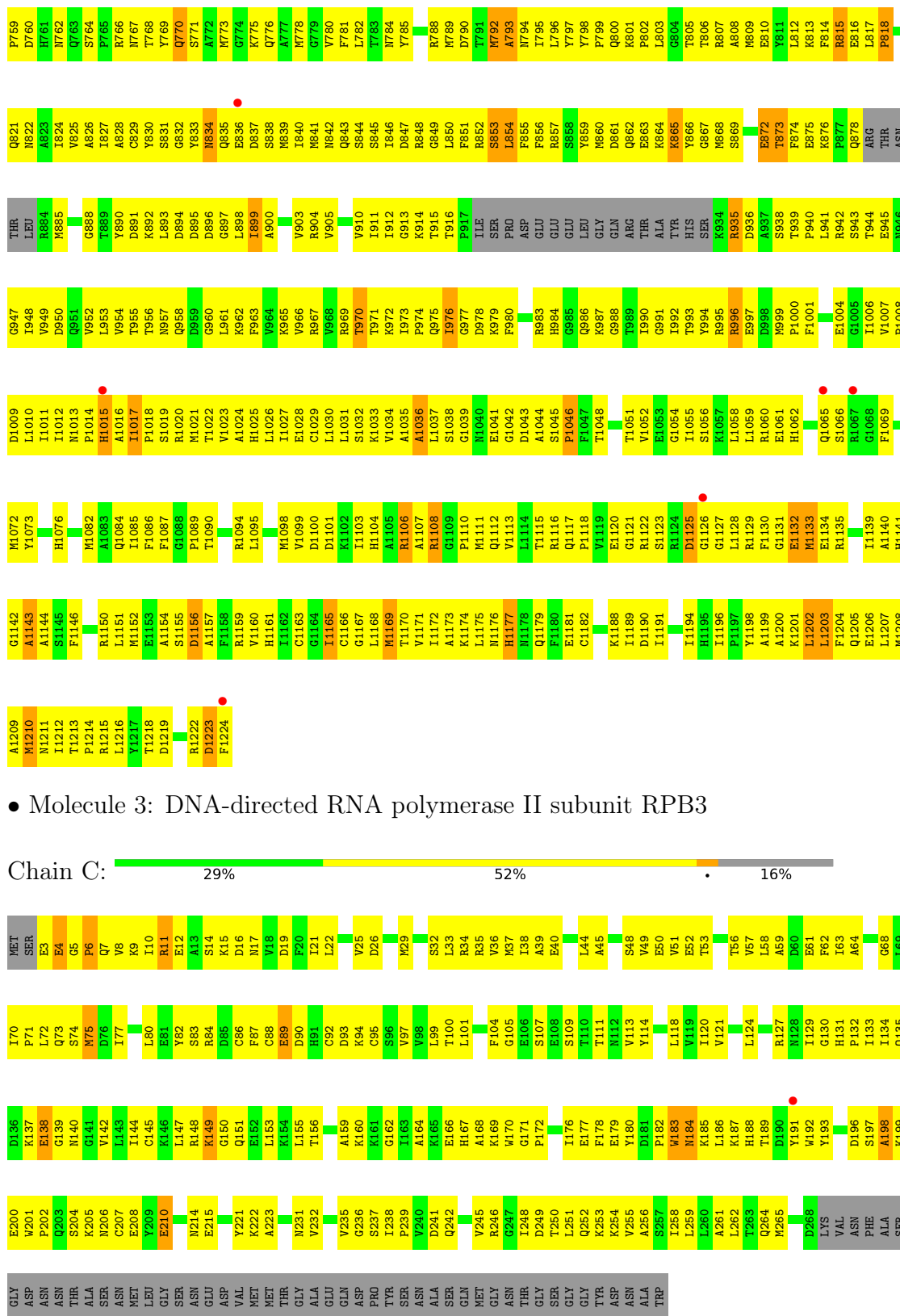
PRO	THR	LYS	S1425	S1361	V1299	S1229	P1156	K1092	V1031	I964	D900	1837	1775	L710	G647
THR	ASP	ASP	E1426	Y1362	K1300	S1229	ASP	K1093	L1032	Q965	L901	Q836	A776	L710	M648
TYR	GLU	PRO	N1427	V1363	E1301	D1233	ARG	V1094	Q1033	N966	L902	R839	F777	R711	M649
SER	LEU	ARG	V1428	P1302	P1302	L1236	SER	S1095	E1034	A967	N903	R840	G778	R711	Q650
PRO	MET	SER	I1429	Y1365	W1303	L1237	T1161	S1096	Y1035	T970	D905	L841	F779	E715	K651
THR	PHE	GLY	V1430	R1366	W1304	I1238	G1097	G1097	R1036	F971	N906	K843	W780	D716	V652
SER	SER	PRO	G1431	H1367	V1305	R1239	V1162	V1098	L1037	H972	T907	R844	W781	W718	V653
PRO	PRO	LEU	L1306	S1368	E1306	V1242	I1163	P1099	T1038	N973	L908	R845	W782	W717	M654
ALA	LEU	ALA	L1307	A1369	L1308	V1243	I1170	R1100	K1039	P978	L909	L846	W783	W719	F655
TYR	VAL	TYR	T1308	T1370	T1308	L1101	K1101	L1101	F1042	S979	D909	E847	W784	W719	W656
SER	ASP	SER	P1435	L1371	D1309	E1172	E1103	E1103	D1043	D980	P910	R848	W785	W721	L657
PRO	SER	THR	G1437	D1372	G1310	H1372	H1S	L1104	R848	L849	S911	L848	H786	L722	L658
THR	GLY	GLY	T1438	D1373	V1311	P80	PHE	L1105	V1044	L961	L912	M849	F787	L722	H659
SER	SER	SER	V1374	N1312	N1312	LVS	SER	L1106	V1045	L981	L913	W850	S788	W725	M660
PRO	ASN	ASN	G1439	V1375	SER	SER	SER	M1106	L1046	N982	E914	H851	K789	E724	G661
ASP	ASP	ASP	A1440	M1375	S1314	LEU	LEU	V1107	S1047	I983	S915	W852	D790	A725	F662
TYR	ALA	ALA	D1442	T1376	E1315	LEU	LEU	A1108	L1047	N984	S915	D853	W793	W726	S663
SER	MET	GLY	V1443	Q1377	ASP	ALA	ASP	A1109	N1048	D985	G916	N854	S793	D727	T664
PRO	ALA	ALA	M1444	Q1378	M1317	GLU	GLU	K1109	I1049	I986	T919	R857	P794	K728	G665
THR	GLY	GLY	L1445	L1381	THR	THR	GLU	N1110	E1050	V987	L920	R864	E795	A729	L666
SER	GLY	GLY	D1446	V1319	GLU	GLU	ALA	M1111	A1051	L988	G921	N858	S796	G730	G667
PRO	PHE	THR	E1447	T1385	GLU	ALA	GLU	S1115	Q1052	L988	G921	N858	S796	G730	G667
SER	THR	THR	GLY	R1386	GLU	ALA	GLU	L1116	F1053	G989	D922	S859	K797	R731	D668
TYR	ALA	ALA	L1450	R1387	SER	GLN	SER	L1117	L1054	V990	L923	L860	G798	L732	T669
SER	TYR	TYR	V1451	G1388	ASP	ASP	PHE	T1118	R1055	K991	K924	C861	F799	A733	I670
PRO	GLY	GLY	K1452	F1389	P1324	M1259	ASP	Y1119	S1056	D982	L925	N862	W800	A733	A671
THR	GLY	GLY	M1453	M1390	T1325	K1261	Q1187	L1120	V1058	N996	V927	R864	E795	W735	D672
ASP	ASP	ASP	P1455	R1391	I1327	E1255	Q1188	E1121	H1059	L997	L929	Q865	S796	W736	G673
SER	TYR	TYR	GLU	S1392	Y1328	I1263	Q1189	P1122	G1061	L998	L929	R866	K797	L737	G674
GLY	GLY	GLY	GLN	M1393	N1265	L1192	W1191	G1123	E1062	V999	E932	Y868	D739	K738	T675
GLY	GLY	GLY	ILE	T1394	N1266	L1193	L1193	G1124	M1063	L1000	Y933	C869	R808	L740	R677
PRO	ALA	ALA	ILE	G1395	M1267	R1194	R1194	A1126	M1063	L1001	K934	E870	L808	N741	E678
THR	THR	THR	THR	L1396	L1268	E1196	E1196	D1127	V1066	N1004	V937	C872	D810	W742	I679
SER	GLY	SER	GLY	L1397	E1269	E1197	E1197	Q1128	G1065	E1005	E938	D873	Q811	W743	T680
PRO	PRO	PRO	ILE	M1398	N1270	L1197	L1197	Q1129	L1067	I1006	D939	N873	E812	Q745	E681
SER	PHE	PHE	GLY	R1399	I1271	D1198	D1198	E1130	A1068	I1007	D940	D874	F813	W746	T682
TYR	ASP	GLY	ASP	G1400	M1336	A1201	A1201	A1131	A1069	I1007	R940	A875	F814	W747	T683
SER	ALA	ALA	GLY	S1401	E1337	K1202	K1202	K1132	Q1070	Q1008	F941	A876	F815	A748	A684
PRO	TYR	TYR	GLN	F1402	V1338	G1275	G1275	L1133	M1009	N1009	F942	R877	H816	K748	E686
THR	GLY	GLY	ASP	E1403	L1339	E1276	K1205	T1134	I1072	Q1011	L943	L878	A817	K752	K687
SER	GLY	GLY	GLY	E1404	G1340	E1277	D1206	R1135	G1073	E879	Y946	K880	M818	G753	K688
PRO	ALA	ALA	VAL	T1405	I1341	N1278	L1207	S1136	E1074	D1012	F947	C881	G819	W754	V690
SER	THR	THR	THR	W1406	E1342	I1279	L1207	A1137	P1075	D1013	V948	S882	G820	F755	L691
PRO	SER	SER	PRO	E1407	A1343	V1282	T1208	L1138	A1076	A1014	V948	L883	R821	W756	D692
PRO	PRO	PRO	PRO	L1408	R1344	V1283	M1209	E1139	T1077	V1015	D949	L883	E822	K756	L692
THR	GLY	GLY	THR	F1410	R1345	M1284	G1210	H1140	Q1078	L1016	G950	L883	E822	K756	V693
SER	PHE	PHE	ASN	E1411	A1346	M1284	T1141	H1141	M1079	L1017	E951	L886	L824	W757	T694
GLY	GLY	GLY	GLY	L1412	A1347	D1213	G1213	T1142	T1080	F1018	A952	C887	L825	W761	K695
VAL	SER	VAL	SER	G1413	L1348	R1215	R1215	L1143	L1081	F1018	N953	C888	R826	S762	E696
TYR	GLY	SER	GLY	A1414	Y1349	R1289	E1216	L1143	M1082	L1021	N954	S889	T827	A763	A697
SER	SER	SER	LEU	E1351	K1350	K1290	V1146	T1083	T1083	L1022	P955	D890	A828	K766	Q698
PRO	PRO	PRO	VAL	L1418	D1419	P1291	T1147	F1084	R1023	R1023	L956	A891	W829	G766	A699
THR	GLY	GLY	ASN	D1420	F1293	P1292	T1219	H1085	S1024	S1024	P957	K830	V829	Q767	N700
PHE	PHE	PHE	ALA	C1421	S1294	K1221	F1220	F1086	R1025	R1025	V958	F893	K831	Q767	L701
SER	SER	SER	ASP	D1422	T1295	K1221	F1220	F1086	L1026	L1026	N959	R896	T831	W770	L702
PRO	LEU	PRO	LEU	G1423	T1296	K1221	F1220	F1086	A1027	A1027	P960	R896	E833	E771	T703
THR	THR	THR	ASP	D1359	E1297	F1225	F1225	V1089	R1028	R1028	R961	R897	P834	G772	T703
TYR	SER	SER	ASP	V1424	W1298	W1228	W1228	S1091	S1091	R1030	P963	W899	K773	R774	K705

	ASN	SER	PRO
	GLU	TYR	THR
	ASN	SER	SER
	GLU	PRO	PRO
	ASN	THR	SER
	SER	PRO	SER
	ARG	PRO	PRO
		TYR	THR
		SER	SER
		PRO	PRO
		THR	THR
		SER	SER
		GLY	THR
		TYR	THR
		SER	SER
		PRO	PRO
		GLY	THR
		ALA	ALA
		TYR	THR
		SER	SER
		PRO	PRO
		LYS	ALA
		GLN	TYR
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		GLU	PRO
		GLN	THR
		LYS	THR
		HIS	PRO

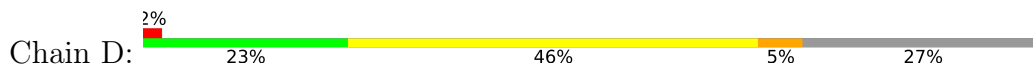
- Molecule 2: DNA-directed RNA polymerase subunit beta

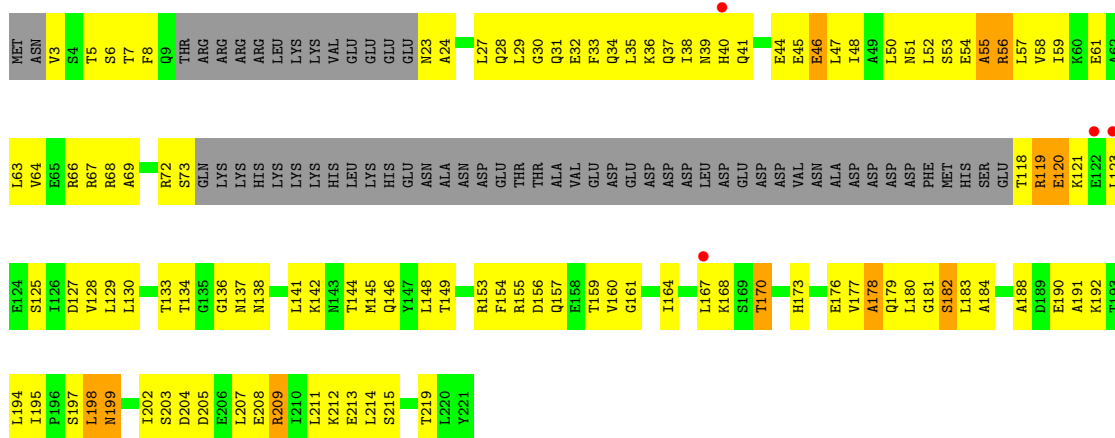
Chain B:  20% 61% 6% 13%



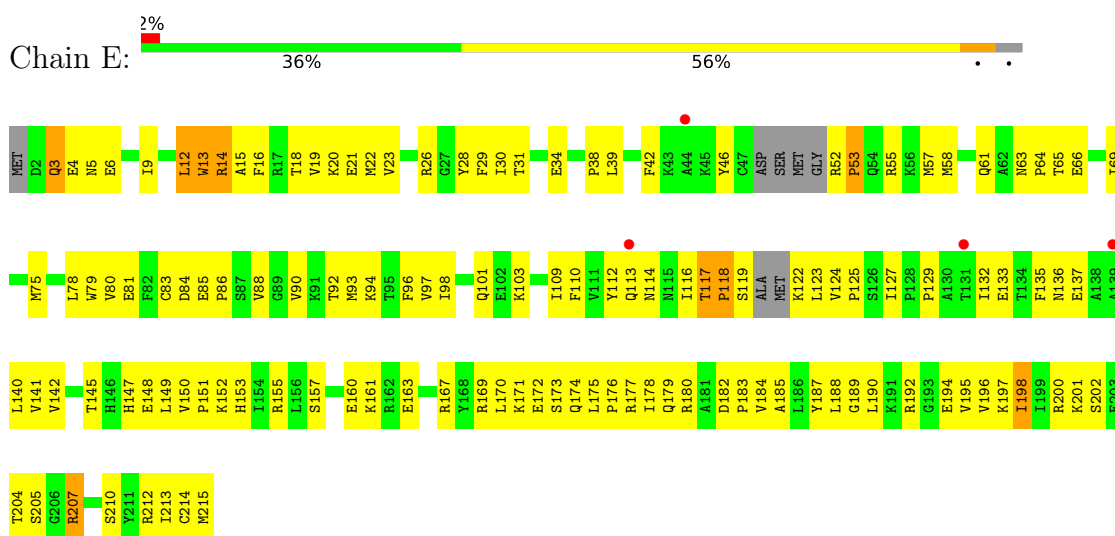


- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

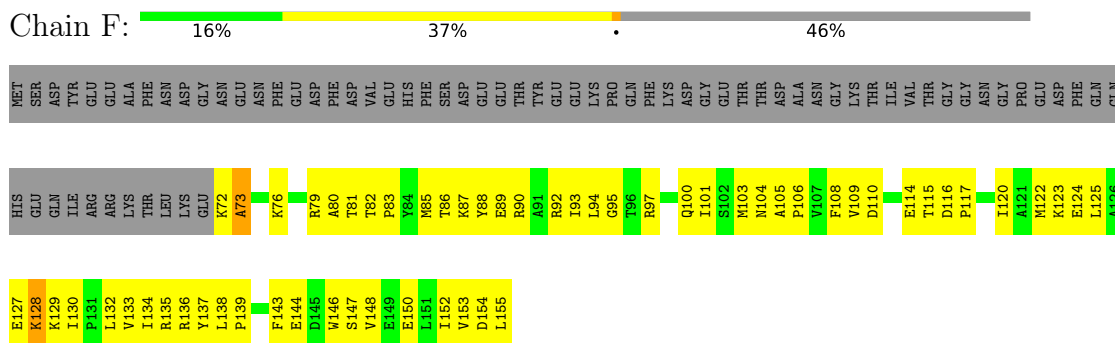




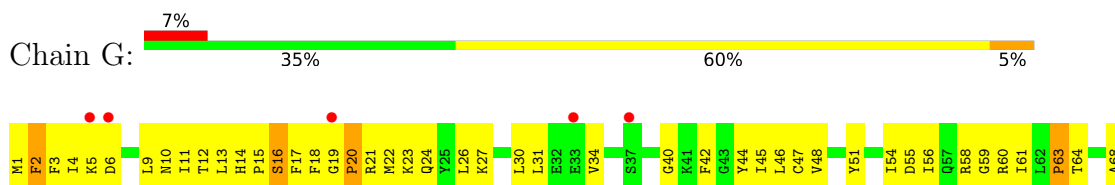
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

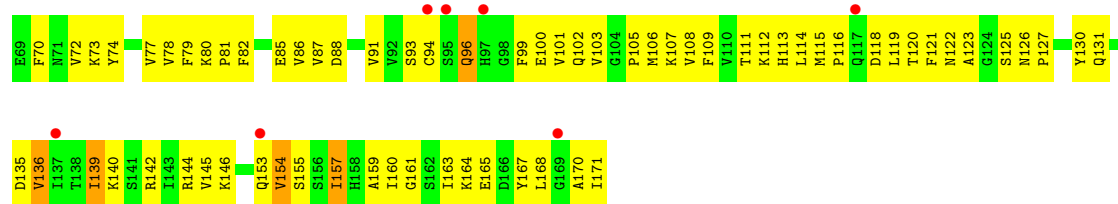


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

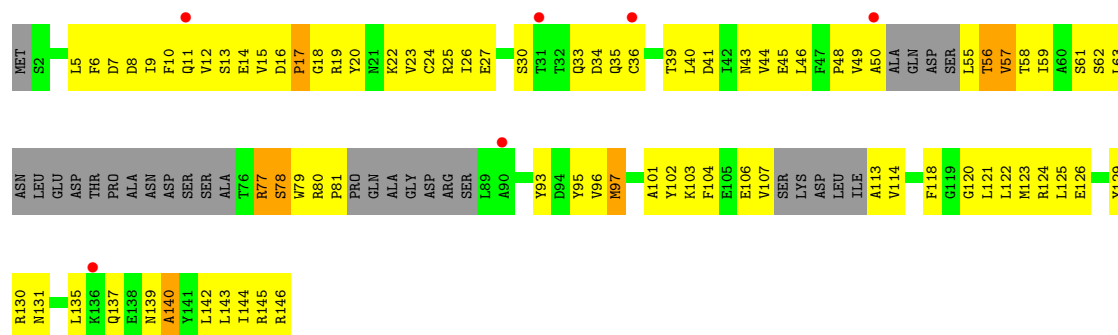


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

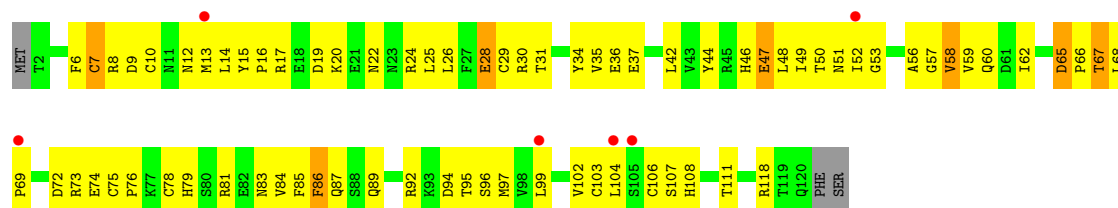




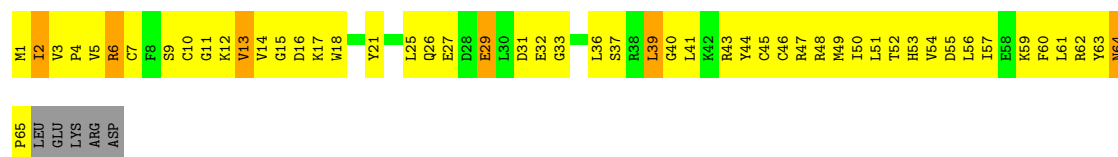
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

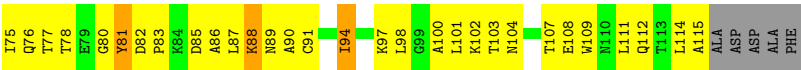


• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

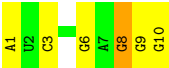
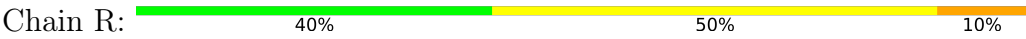




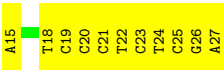
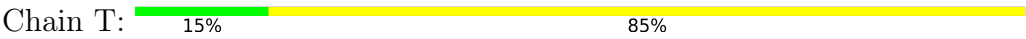
● Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



● Molecule 13: MOL_ID: 13



● Molecule 14: MOL_ID: 14



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.17Å 392.60Å 280.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.05 18.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (18.00-3.05) 99.2 (18.00-3.05)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.283 , 0.307 0.293 , 0.314	Depositor DCC
R_{free} test set	7379 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.073 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.078 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30893	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: MN, ZN, ATP, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	1/11181 (0.0%)	0.97	12/15114 (0.1%)
2	B	0.55	0/8589	0.87	6/11581 (0.1%)
3	C	0.56	0/2133	0.87	3/2891 (0.1%)
4	D	0.44	0/1296	0.74	1/1741 (0.1%)
5	E	0.89	0/1747	1.27	2/2349 (0.1%)
6	F	0.66	0/691	0.94	0/933
7	G	1.04	0/1368	1.32	1/1844 (0.1%)
8	H	0.48	0/965	0.72	0/1302
9	I	0.47	0/989	0.75	1/1331 (0.1%)
10	J	0.52	0/535	0.83	1/720 (0.1%)
11	K	0.51	0/938	0.75	0/1267
12	L	0.84	0/345	1.01	0/457
13	R	0.35	0/244	0.55	0/380
14	T	0.61	0/289	0.75	0/442
All	All	0.64	1/31310 (0.0%)	0.94	27/42352 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	N-CA	5.01	1.50	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	MET	N-CA-C	-10.79	100.11	113.28
1	A	295	LEU	N-CA-C	-7.04	105.22	113.88
1	A	1081	LEU	N-CA-C	-6.92	103.12	112.26
1	A	1080	THR	CA-CB-OG1	-6.79	99.42	109.60
10	J	39	LEU	N-CA-C	-6.72	103.00	113.02
2	B	834	ASN	N-CA-C	-6.69	105.44	112.93
1	A	271	LYS	N-CA-C	-6.53	104.95	113.12
2	B	1121	GLY	N-CA-C	6.49	120.22	111.72
1	A	55	ASP	CB-CA-C	-6.44	104.65	110.71
4	D	209	ARG	N-CA-C	-6.34	104.29	111.07
1	A	675	THR	CA-C-N	-6.12	110.78	120.63
1	A	675	THR	C-N-CA	-6.12	110.78	120.63
3	C	11	ARG	N-CA-C	-6.09	101.76	111.02
2	B	374	LYS	N-CA-C	-6.06	104.23	111.69
5	E	14	ARG	N-CA-C	-5.90	104.54	110.97
2	B	899	ILE	N-CA-C	-5.87	100.02	108.42
3	C	183	TRP	N-CA-C	-5.67	101.25	109.59
2	B	192	LEU	N-CA-C	-5.64	106.44	113.15
5	E	13	TRP	N-CA-C	-5.50	104.92	111.69
3	C	210	GLU	N-CA-C	-5.50	101.78	109.69
2	B	127	GLY	N-CA-C	5.47	118.98	111.54
1	A	1083	THR	N-CA-C	-5.35	106.76	113.72
1	A	950	GLY	N-CA-C	-5.32	105.72	114.76
1	A	1205	LYS	N-CA-C	-5.14	107.00	113.28
9	I	72	ASP	N-CA-C	-5.07	105.82	112.41
7	G	96	GLN	N-CA-C	-5.06	107.66	113.88
1	A	1216	ILE	N-CA-C	-5.00	105.62	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	PRO	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10987	0	11060	1499	0
2	B	8424	0	8455	1150	0
3	C	2095	0	2052	244	0
4	D	1287	0	1296	159	0
5	E	1713	0	1739	196	0
6	F	679	0	701	93	0
7	G	1340	0	1357	183	0
8	H	951	0	926	135	0
9	I	971	0	930	117	0
10	J	526	0	533	95	0
11	K	920	0	929	113	0
12	L	343	0	364	70	0
13	R	217	0	109	15	0
14	T	260	0	147	20	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	2	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
17	B	31	0	12	3	0
18	E	6	8	8	2	0
19	A	46	0	0	0	0
19	B	38	0	0	1	0
19	C	6	0	0	0	0
19	D	5	0	0	0	0
19	E	7	0	0	0	0
19	F	3	0	0	0	0
19	G	4	0	0	0	0
19	H	3	0	0	1	0
19	J	2	0	0	0	0
19	K	5	0	0	0	0
19	L	2	0	0	0	0
19	R	1	0	0	0	0
19	T	2	0	0	0	0
All	All	30885	8	30618	3681	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 60.

All (3681) 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)
12:L:48:CYS:SG	12:L:51:CYS:HB2	1.92	1.09
12:L:48:CYS:SG	12:L:51:CYS:CB	2.41	1.09
2:B:1082:MET:HA	3:C:189:THR:HA	1.38	1.05
12:L:30:ILE:HG22	12:L:31:CYS:H	1.23	1.04
2:B:963:PHE:HE2	2:B:965:LYS:HE2	1.22	1.03
2:B:496:ARG:HD3	2:B:751:VAL:HG21	1.44	0.99
2:B:1100:ASP:OD1	11:K:1:MET:HB3	1.62	0.99
12:L:48:CYS:HG	15:L:101:ZN:ZN	0.65	0.98
1:A:575:LYS:HE3	8:H:120:GLY:HA3	1.46	0.96
1:A:666:ILE:HD12	1:A:667:GLY:N	1.83	0.94
1:A:1343:ALA:HB1	5:E:149:LEU:HD12	1.47	0.94
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.50	0.94
1:A:1343:ALA:O	5:E:149:LEU:HD13	1.69	0.93
2:B:963:PHE:CE2	2:B:965:LYS:HE2	2.04	0.91
2:B:837:ASP:OD1	2:B:1016:ALA:HB2	1.70	0.91
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.06	0.91
1:A:511:ILE:HD13	1:A:521:MET:HE3	1.52	0.91
2:B:876:LYS:HE3	2:B:893:LEU:HB2	1.52	0.91
1:A:1356:ILE:HD12	1:A:1368:MET:HE3	1.53	0.90
1:A:88:LYS:HD3	1:A:205:GLU:OE2	1.72	0.89
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.54	0.89
2:B:39:ARG:HH22	2:B:665:GLU:HG3	1.37	0.89
9:I:85:PHE:HB2	9:I:99:LEU:HD21	1.54	0.89
4:D:40:HIS:NE2	7:G:73:LYS:HE2	1.89	0.88
8:H:56:THR:HG22	8:H:57:VAL:H	1.39	0.87
7:G:13:LEU:HD13	7:G:26:LEU:HD21	1.57	0.87
13:R:6:G:H1	14:T:23:DC:H42	1.21	0.86
1:A:1263:ILE:O	1:A:1263:ILE:HG22	1.75	0.86
2:B:1106:ARG:NH1	2:B:1126:GLY:HA2	1.90	0.86
4:D:67:ARG:HG2	4:D:67:ARG:HH11	1.40	0.86
1:A:789:LYS:HE3	9:I:67:THR:HB	1.55	0.86
3:C:242:GLN:HB3	3:C:246:ARG:NH2	1.91	0.86
2:B:496:ARG:HD3	2:B:751:VAL:CG2	2.06	0.85
1:A:335:ARG:NH2	2:B:1115:THR:HG22	1.91	0.85
2:B:1112:GLN:HG3	2:B:1113:VAL:H	1.42	0.85
2:B:247:GLY:HA2	2:B:418:LYS:HZ2	1.43	0.84
2:B:1106:ARG:HD2	2:B:1126:GLY:C	2.03	0.84
1:A:595:THR:HG22	1:A:603:ASN:HB2	1.58	0.84
1:A:808:LEU:H	1:A:808:LEU:HD12	1.43	0.84
10:J:16:ASP:OD2	10:J:17:LYS:HG3	1.76	0.84
2:B:911:ILE:HG21	2:B:966:VAL:HG21	1.59	0.83
1:A:738:LYS:HD3	1:A:739:ASP:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:HG3	2:B:836:GLU:OE2	1.79	0.83
12:L:30:ILE:HG22	12:L:31:CYS:N	1.93	0.83
1:A:666:ILE:HD12	1:A:666:ILE:C	2.03	0.83
1:A:461:LYS:O	1:A:463:ILE:HG23	1.79	0.83
1:A:1390:ASN:OD1	1:A:1402:PHE:HB3	1.78	0.83
1:A:695:LYS:HA	1:A:698:GLN:HG2	1.60	0.83
2:B:841:MET:HE1	2:B:990:ILE:HD11	1.59	0.82
7:G:1:MET:HE2	7:G:79:PHE:CD2	2.14	0.82
5:E:55:ARG:CZ	5:E:113:GLN:HE22	1.92	0.82
1:A:757:ASN:O	1:A:761:MET:HG3	1.80	0.82
7:G:1:MET:HG3	7:G:2:PHE:N	1.95	0.81
2:B:247:GLY:HA2	2:B:418:LYS:NZ	1.93	0.81
1:A:346:ASP:HB3	1:A:347:PHE:HD1	1.44	0.81
2:B:619:ILE:HD13	9:I:65:ASP:CG	2.06	0.81
12:L:46:VAL:O	12:L:47:ARG:HG2	1.79	0.81
1:A:524:VAL:HG22	1:A:525:GLN:H	1.46	0.81
12:L:55:ILE:HG23	12:L:56:LEU:H	1.46	0.80
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.63	0.80
7:G:1:MET:HG3	7:G:2:PHE:H	1.46	0.80
2:B:228:LYS:HG3	2:B:229:ALA:H	1.46	0.80
1:A:1343:ALA:HB1	5:E:149:LEU:CD1	2.11	0.80
2:B:1171:VAL:HG12	2:B:1182:CYS:HB2	1.63	0.80
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.64	0.80
1:A:449:SER:O	2:B:1133:MET:HG3	1.80	0.79
9:I:17:ARG:NH2	9:I:20:LYS:HE3	1.97	0.79
1:A:32:VAL:HG23	1:A:33:ALA:H	1.47	0.79
1:A:353:ILE:HG21	1:A:487:MET:HB2	1.63	0.79
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.13	0.79
1:A:1005:GLU:HG2	1:A:1009:ASN:ND2	1.98	0.79
4:D:66:ARG:HG3	7:G:51:TYR:HD2	1.48	0.79
2:B:635:ARG:HH21	2:B:637:LEU:HD13	1.45	0.79
8:H:135:LEU:CD1	8:H:137:GLN:HE21	1.95	0.79
1:A:41:MET:HB2	1:A:49:LYS:HA	1.65	0.78
1:A:567:LYS:C	1:A:569:LYS:H	1.90	0.78
2:B:181:LEU:HD11	2:B:189:LEU:HD23	1.64	0.78
2:B:839:MET:SD	2:B:1010:LEU:HD11	2.23	0.78
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	1.84	0.77
5:E:55:ARG:NH2	5:E:113:GLN:HE22	1.81	0.77
2:B:1017:ILE:HG13	2:B:1018:PRO:HD3	1.66	0.77
2:B:464:GLY:O	2:B:479:VAL:HG12	1.85	0.77
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:ILE:HD12	1:A:1368:MET:CE	2.14	0.77
1:A:1443:VAL:HG23	7:G:61:ILE:HB	1.67	0.77
3:C:235:VAL:HG11	10:J:6:ARG:HH21	1.49	0.77
2:B:635:ARG:HH22	2:B:742:GLU:CD	1.91	0.77
1:A:450:LEU:HD11	1:A:1074:GLU:HG2	1.66	0.76
2:B:1207:LEU:HD22	2:B:1212:ILE:HD11	1.67	0.76
8:H:11:GLN:HG2	8:H:12:VAL:H	1.49	0.76
1:A:434:ARG:NH1	1:A:437:MET:HE2	1.99	0.76
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.00	0.76
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.67	0.76
2:B:853:SER:HB3	2:B:972:LYS:HB2	1.67	0.76
8:H:97:MET:HG3	8:H:118:PHE:CE2	2.19	0.76
1:A:601:LYS:CB	1:A:603:ASN:HD21	1.99	0.76
1:A:457:ALA:O	1:A:507:VAL:HG23	1.86	0.76
1:A:525:GLN:NE2	2:B:836:GLU:CD	2.43	0.75
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.67	0.75
1:A:896:ARG:HD3	1:A:1030:ARG:HD2	1.67	0.75
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.11	0.75
2:B:1179:GLN:HG3	2:B:1188:LYS:HZ1	1.51	0.75
4:D:40:HIS:HB2	7:G:6:ASP:OD2	1.85	0.75
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.68	0.75
1:A:899:VAL:HG22	1:A:1029:ARG:HE	1.51	0.75
2:B:396:ASP:HB3	2:B:403:LYS:NZ	2.01	0.75
4:D:59:ILE:H	4:D:59:ILE:HD12	1.51	0.75
1:A:1313:LEU:O	1:A:1315:GLU:N	2.20	0.74
2:B:39:ARG:HH22	2:B:665:GLU:CG	1.99	0.74
2:B:210:LYS:HA	2:B:482:VAL:HA	1.68	0.74
1:A:335:ARG:HH21	2:B:1115:THR:HG22	1.51	0.74
1:A:666:ILE:CG2	2:B:1026:LEU:HB3	2.17	0.74
1:A:907:THR:HG22	1:A:908:LEU:H	1.52	0.74
3:C:37:MET:HE2	3:C:176:ILE:HD13	1.69	0.74
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.17	0.74
2:B:542:MET:HG3	2:B:747:MET:HE2	1.67	0.74
2:B:637:LEU:HD21	2:B:703:ILE:HG12	1.70	0.74
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.22	0.74
1:A:4:GLN:HB3	2:B:1159:ARG:HH21	1.52	0.74
1:A:341:MET:CE	1:A:1429:ILE:HD11	2.18	0.74
1:A:404:TYR:CA	1:A:415:LEU:CD1	2.65	0.74
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.18	0.74
9:I:8:ARG:HG2	9:I:34:TYR:CE2	2.22	0.74
9:I:22:ASN:HD22	9:I:24:ARG:HD2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.87	0.74
1:A:1424:VAL:HG21	2:B:1139:ILE:HD13	1.68	0.74
2:B:824:ILE:HG22	2:B:1009:ASP:CG	2.12	0.74
7:G:9:LEU:HD21	7:G:11:ILE:HD11	1.69	0.74
7:G:80:LYS:HD3	7:G:82:PHE:CE1	2.21	0.74
1:A:542:GLU:O	1:A:546:VAL:HG23	1.86	0.74
1:A:851:HIS:O	1:A:1060:PRO:HB3	1.87	0.74
2:B:684:LEU:O	2:B:690:VAL:HG22	1.87	0.74
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.67	0.74
1:A:415:LEU:HD12	1:A:415:LEU:H	1.53	0.74
2:B:663:ALA:O	2:B:666:TYR:HB2	1.88	0.74
6:F:76:LYS:HD2	6:F:79:ARG:NH2	2.03	0.74
7:G:112:LYS:HD2	7:G:113:HIS:CE1	2.23	0.74
1:A:403:LYS:O	1:A:404:TYR:CD1	2.40	0.74
1:A:560:ILE:HG23	8:H:79:TRP:HB3	1.70	0.74
1:A:754:SER:H	1:A:757:ASN:HD22	1.36	0.74
2:B:283:VAL:CG2	2:B:321:GLY:HA3	2.18	0.74
8:H:36:CYS:HB2	8:H:126:GLU:O	1.87	0.74
8:H:93:TYR:CE1	8:H:143:LEU:HD22	2.23	0.74
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.23	0.73
2:B:1125:ASP:O	2:B:1125:ASP:OD2	2.06	0.73
4:D:8:PHE:HD2	4:D:38:ILE:HD12	1.52	0.73
1:A:960:ILE:HG13	1:A:1021:LEU:HD21	1.70	0.73
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.51	0.73
2:B:1152:MET:HE1	2:B:1157:ALA:HA	1.69	0.73
3:C:121:VAL:HG23	3:C:121:VAL:O	1.87	0.73
4:D:211:LEU:HD13	4:D:214:LEU:HD22	1.71	0.73
7:G:13:LEU:HD13	7:G:26:LEU:CD2	2.18	0.73
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.70	0.73
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.24	0.73
5:E:55:ARG:CD	5:E:113:GLN:OE1	2.36	0.73
9:I:35:VAL:HG12	9:I:36:GLU:N	2.03	0.73
1:A:55:ASP:HB2	1:A:59:GLY:O	1.89	0.73
2:B:706:GLN:NE2	2:B:707:PRO:HD2	2.03	0.73
2:B:752:ALA:O	2:B:755:ILE:HG12	1.88	0.73
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.18	0.73
4:D:37:GLN:NE2	4:D:47:LEU:CD1	2.51	0.73
1:A:351:THR:HG23	1:A:352:VAL:O	1.87	0.73
1:A:637:LYS:O	1:A:641:VAL:HG21	1.88	0.73
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.70	0.73
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:ASN:O	2:B:467:GLY:N	2.22	0.73
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.53	0.73
1:A:483:ASP:OD1	1:A:483:ASP:O	2.06	0.73
1:A:1148:ILE:HG13	9:I:49:ILE:HB	1.71	0.73
2:B:805:THR:HG22	2:B:1042:GLY:O	1.89	0.73
2:B:824:ILE:HD11	10:J:44:TYR:CE2	2.23	0.73
2:B:977:GLY:H	2:B:990:ILE:HB	1.53	0.73
3:C:48:SER:HB3	12:L:66:GLN:NE2	2.04	0.73
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.69	0.73
2:B:807:ARG:H	2:B:1045:SER:HB3	1.53	0.73
2:B:855:PHE:HB3	2:B:970:THR:HG23	1.70	0.73
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.69	0.73
2:B:1033:LYS:O	2:B:1037:LEU:HD12	1.88	0.73
1:A:122:MET:HE2	1:A:122:MET:HA	1.71	0.73
1:A:914:GLU:HG3	1:A:979:SER:O	1.89	0.73
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.71	0.73
7:G:111:THR:HB	7:G:114:LEU:HD23	1.71	0.73
7:G:165:GLU:O	7:G:168:LEU:HD12	1.88	0.73
13:R:1:A:H62	14:T:27:DA:N6	1.85	0.73
1:A:341:MET:HE3	1:A:1401:SER:HB3	1.71	0.73
1:A:1008:GLN:O	1:A:1011:GLN:N	2.20	0.73
2:B:352:ALA:O	2:B:356:LEU:HD12	1.89	0.73
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.71	0.73
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.03	0.72
1:A:1438:THR:CG2	6:F:92:ARG:HB2	2.19	0.72
7:G:13:LEU:CD1	7:G:26:LEU:CD2	2.67	0.72
1:A:149:GLU:OE1	1:A:152:VAL:CG2	2.37	0.72
1:A:208:LEU:HD12	1:A:209:ASN:N	2.04	0.72
1:A:455:MET:HE1	2:B:1134:GLU:HB3	1.71	0.72
1:A:601:LYS:HB2	1:A:603:ASN:CG	2.14	0.72
2:B:367:LEU:N	2:B:367:LEU:HD23	2.03	0.72
5:E:22:MET:HE2	5:E:187:TYR:CD2	2.23	0.72
6:F:109:VAL:HG22	6:F:123:LYS:HE3	1.71	0.72
8:H:13:SER:HB3	8:H:27:GLU:O	1.90	0.72
9:I:8:ARG:HG2	9:I:34:TYR:HE2	1.53	0.72
1:A:1404:GLU:HB3	1:A:1407:GLU:OE2	1.88	0.72
3:C:37:MET:HE1	3:C:232:VAL:HG11	1.69	0.72
1:A:1324:PRO:HB3	5:E:142:VAL:HG21	1.71	0.72
1:A:1450:LEU:HD11	7:G:19:GLY:HA2	1.70	0.72
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.72	0.72
3:C:265:MET:HE1	11:K:21:ILE:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:MET:O	7:G:14:HIS:HE1	1.72	0.72
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.70	0.72
8:H:135:LEU:CD1	8:H:137:GLN:HG2	2.19	0.72
1:A:88:LYS:HD3	1:A:205:GLU:CD	2.14	0.72
1:A:469:ARG:NH2	2:B:991:GLY:O	2.22	0.72
1:A:559:VAL:O	1:A:561:PRO:HD3	1.89	0.72
1:A:1344:GLY:O	1:A:1347:ALA:N	2.22	0.72
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.24	0.72
2:B:978:ASP:OD1	2:B:1099:VAL:HG12	1.89	0.72
2:B:1031:LEU:HD21	2:B:1042:GLY:HA3	1.71	0.72
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.71	0.72
1:A:496:GLU:OE2	7:G:64:THR:HA	1.90	0.72
1:A:579:SER:HB3	1:A:611:GLN:HA	1.70	0.72
2:B:680:THR:HB	2:B:683:SER:HB2	1.70	0.72
1:A:404:TYR:HA	1:A:415:LEU:HD12	1.71	0.72
1:A:806:ARG:HG2	2:B:728:ARG:HA	1.72	0.72
1:A:816:HIS:ND1	2:B:764:SER:HB3	2.04	0.72
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.23	0.72
5:E:175:LEU:HD23	5:E:213:ILE:HB	1.70	0.72
7:G:99:PHE:CD2	7:G:115:MET:HE2	2.25	0.72
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.54	0.72
1:A:346:ASP:HB3	1:A:347:PHE:CD1	2.25	0.72
1:A:596:THR:HG22	1:A:597:LEU:N	2.05	0.72
1:A:1263:ILE:HG23	1:A:1267:MET:HG3	1.72	0.72
2:B:603:LEU:HD23	2:B:609:ILE:HG13	1.70	0.72
2:B:900:ALA:O	2:B:903:VAL:HG23	1.89	0.72
3:C:44:LEU:HD12	3:C:160:LYS:O	1.89	0.72
1:A:728:LYS:HA	1:A:731:ARG:HG2	1.72	0.72
1:A:808:LEU:HD12	1:A:808:LEU:N	2.05	0.72
1:A:911:SER:C	1:A:912:LEU:HD23	2.13	0.72
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.72	0.72
2:B:283:VAL:HG21	2:B:321:GLY:HA3	1.70	0.72
2:B:956:THR:HG22	2:B:961:LEU:C	2.15	0.72
3:C:44:LEU:HD11	3:C:159:ALA:O	1.90	0.72
1:A:870:GLU:OE1	5:E:202:SER:HB2	1.90	0.72
1:A:1363:VAL:HG12	1:A:1364:ASN:H	1.54	0.72
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.20	0.72
2:B:875:GLU:CG	2:B:876:LYS:N	2.53	0.71
4:D:6:SER:OG	4:D:7:THR:N	2.21	0.71
1:A:436:ILE:HG13	1:A:436:ILE:O	1.89	0.71
1:A:441:PRO:HG2	1:A:498:ARG:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:LEU:HD23	4:D:50:LEU:N	2.05	0.71
10:J:16:ASP:CG	10:J:17:LYS:HG3	2.15	0.71
1:A:592:ASP:H	1:A:595:THR:HG21	1.55	0.71
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.72	0.71
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.73	0.71
5:E:12:LEU:O	5:E:12:LEU:HD23	1.90	0.71
1:A:96:ILE:HG13	1:A:97:ALA:H	1.55	0.71
1:A:298:PHE:O	1:A:302:THR:HG22	1.91	0.71
1:A:308:ILE:HG22	1:A:309:ALA:H	1.56	0.71
2:B:707:PRO:HD3	2:B:741:CYS:SG	2.31	0.71
2:B:800:GLN:NE2	10:J:52:THR:OG1	2.23	0.71
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.25	0.71
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.72	0.71
8:H:12:VAL:HG21	8:H:50:ALA:O	1.90	0.71
1:A:592:ASP:O	1:A:595:THR:HG23	1.89	0.71
2:B:44:VAL:HG23	2:B:48:LEU:HD13	1.72	0.71
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.73	0.71
5:E:195:VAL:HG12	5:E:196:VAL:H	1.55	0.71
6:F:72:LYS:HG3	6:F:72:LYS:O	1.89	0.71
1:A:44:THR:HB	1:A:46:THR:OG1	1.91	0.71
1:A:1299:VAL:HG22	1:A:1300:LYS:H	1.54	0.71
1:A:998:LEU:HD13	1:A:1001:ARG:HG3	1.73	0.71
2:B:331:LEU:HB2	2:B:352:ALA:HB3	1.72	0.71
2:B:512:ARG:NH2	2:B:532:ALA:HA	2.05	0.71
7:G:139:ILE:HG12	7:G:140:LYS:HG2	1.72	0.71
1:A:1018:PHE:O	1:A:1021:LEU:N	2.23	0.71
2:B:957:ASN:OD1	2:B:958:GLN:HG3	1.91	0.71
7:G:165:GLU:OE1	7:G:165:GLU:HA	1.91	0.71
2:B:995:ARG:HH12	11:K:9:LEU:CD1	2.03	0.71
7:G:80:LYS:HD3	7:G:82:PHE:CZ	2.26	0.71
10:J:1:MET:O	10:J:2:ILE:HG22	1.91	0.71
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.21	0.70
1:A:598:LEU:HG	1:A:598:LEU:O	1.89	0.70
1:A:1407:GLU:HA	1:A:1410:PHE:HB2	1.70	0.70
2:B:527:THR:OG1	2:B:528:PRO:HD2	1.91	0.70
3:C:11:ARG:HB3	3:C:19:ASP:HB3	1.73	0.70
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.72	0.70
5:E:192:ARG:HA	5:E:214:CYS:O	1.91	0.70
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.72	0.70
1:A:244:PRO:N	1:A:245:PRO:HD2	2.06	0.70
1:A:404:TYR:HA	1:A:415:LEU:CD1	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:HB2	1:A:603:ASN:OD1	1.91	0.70
5:E:4:GLU:HA	5:E:6:GLU:OE1	1.91	0.70
1:A:451:HIS:CE1	1:A:453:MET:HB2	2.26	0.70
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.71	0.70
2:B:1100:ASP:OD1	11:K:1:MET:CB	2.38	0.70
5:E:117:THR:HB	5:E:118:PRO:HD2	1.72	0.70
8:H:97:MET:SD	8:H:142:LEU:HD23	2.30	0.70
1:A:547:LEU:HB3	11:K:58:PHE:CE2	2.26	0.70
7:G:13:LEU:HD11	7:G:26:LEU:HD23	1.73	0.70
7:G:85:GLU:HG3	7:G:85:GLU:O	1.90	0.70
1:A:845:LEU:HD13	1:A:1068:ALA:HB3	1.73	0.70
1:A:1263:ILE:CG2	1:A:1267:MET:HG3	2.22	0.70
3:C:193:TYR:HB3	3:C:197:SER:HA	1.73	0.70
1:A:843:LYS:HE2	1:A:1401:SER:HB2	1.74	0.70
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.73	0.70
4:D:141:LEU:HD13	7:G:46:LEU:O	1.90	0.70
4:D:188:ALA:HA	4:D:191:ALA:HB3	1.72	0.70
1:A:335:ARG:NH2	2:B:1115:THR:CG2	2.55	0.70
1:A:383:TYR:HB3	6:F:115:THR:HA	1.72	0.70
3:C:61:GLU:HA	3:C:64:ALA:CB	2.22	0.70
4:D:176:GLU:O	4:D:180:LEU:HB2	1.92	0.70
1:A:489:LEU:HD23	1:A:490:HIS:O	1.91	0.70
1:A:1057:VAL:HG22	1:A:1058:VAL:O	1.92	0.70
2:B:361:LEU:N	2:B:362:PRO:HD3	2.06	0.70
2:B:846:ILE:C	2:B:846:ILE:HD12	2.17	0.70
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.21	0.70
1:A:453:MET:O	1:A:456:MET:CE	2.40	0.70
1:A:716:ASP:O	1:A:720:ARG:HG2	1.91	0.70
2:B:425:THR:O	2:B:428:ILE:HG13	1.90	0.70
2:B:581:PHE:O	2:B:626:ILE:N	2.21	0.70
5:E:149:LEU:HD12	5:E:149:LEU:O	1.91	0.70
1:A:568:PRO:HG3	8:H:95:TYR:HA	1.74	0.70
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.57	0.70
5:E:65:THR:O	5:E:69:ILE:HG12	1.91	0.70
5:E:136:ASN:O	5:E:140:LEU:HG	1.92	0.70
10:J:36:LEU:HD21	10:J:50:ILE:HG21	1.72	0.70
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.24	0.69
1:A:504:LEU:HD21	6:F:88:TYR:CD1	2.27	0.69
1:A:867:ILE:HG22	1:A:872:GLY:N	2.07	0.69
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.73	0.69
5:E:12:LEU:CD1	5:E:55:ARG:HE	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:PRO:HG2	2:B:705:MET:HE2	1.75	0.69
1:A:942:PHE:CD1	1:A:942:PHE:O	2.46	0.69
1:A:1081:LEU:HD23	1:A:1081:LEU:O	1.92	0.69
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.56	0.69
1:A:1434:ALA:O	1:A:1436:ILE:N	2.25	0.69
2:B:372:SER:OG	2:B:567:GLU:HG3	1.90	0.69
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.26	0.69
2:B:963:PHE:HE2	2:B:965:LYS:CE	2.03	0.69
2:B:999:MET:HG2	2:B:1000:PRO:HD2	1.73	0.69
5:E:26:ARG:O	5:E:75:MET:HE1	1.92	0.69
5:E:178:ILE:O	5:E:214:CYS:HA	1.92	0.69
11:K:112:GLN:HA	11:K:112:GLN:OE1	1.92	0.69
1:A:83:HIS:CA	1:A:241:VAL:HG23	2.23	0.69
1:A:483:ASP:CB	2:B:988:GLY:HA2	2.22	0.69
1:A:833:GLU:HB3	1:A:834:PRO:HD3	1.72	0.69
2:B:590:HIS:NE2	2:B:592:ASN:O	2.21	0.69
2:B:664:THR:HG23	2:B:665:GLU:H	1.58	0.69
3:C:86:CYS:SG	3:C:87:PHE:N	2.62	0.69
2:B:766:ARG:CZ	2:B:1020:ARG:HG2	2.21	0.69
2:B:841:MET:CE	2:B:990:ILE:HD11	2.21	0.69
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.75	0.69
7:G:160:ILE:N	7:G:160:ILE:HD12	2.06	0.69
1:A:335:ARG:HH21	2:B:1115:THR:CG2	2.05	0.69
1:A:500:GLU:O	1:A:504:LEU:HB2	1.93	0.69
1:A:982:THR:HB	1:A:985:ASP:H	1.58	0.69
2:B:1189:ILE:HG13	2:B:1190:ASP:H	1.56	0.69
5:E:169:ARG:C	5:E:170:LEU:HD23	2.18	0.69
8:H:12:VAL:HG21	8:H:50:ALA:C	2.17	0.69
1:A:542:GLU:HG2	1:A:543:LEU:H	1.57	0.69
1:A:1146:VAL:HG13	1:A:1201:ALA:CB	2.21	0.69
2:B:411:PRO:O	2:B:414:ALA:HB3	1.93	0.69
2:B:581:PHE:HB2	2:B:625:LYS:HA	1.75	0.69
2:B:827:ILE:HD12	2:B:1012:ILE:HD12	1.75	0.69
18:E:301:GOL:H32	6:F:80:ALA:HB3	1.74	0.69
9:I:22:ASN:ND2	9:I:24:ARG:HD2	2.08	0.69
2:B:805:THR:HG21	2:B:1041:GLU:HG2	1.74	0.69
3:C:8:VAL:HG13	3:C:22:LEU:HD23	1.74	0.69
1:A:569:LYS:CB	8:H:46:LEU:HD22	2.22	0.69
1:A:703:THR:O	1:A:705:LYS:HD2	1.92	0.69
1:A:1043:ASP:HA	1:A:1046:LEU:HB2	1.73	0.69
1:A:1402:PHE:CE1	1:A:1403:GLU:CG	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:O	2:B:365:THR:HB	1.90	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.69
4:D:48:ILE:HG21	7:G:4:ILE:HD12	1.75	0.69
6:F:109:VAL:CG2	6:F:123:LYS:HE3	2.23	0.69
1:A:359:LEU:HD22	1:A:363:GLN:HG3	1.75	0.69
1:A:1146:VAL:HG13	1:A:1201:ALA:HB3	1.75	0.69
1:A:1263:ILE:O	1:A:1263:ILE:CG2	2.41	0.69
2:B:409:ALA:O	2:B:413:LEU:HD12	1.93	0.69
2:B:613:VAL:HG12	2:B:628:THR:HA	1.75	0.69
1:A:814:PHE:O	1:A:817:ALA:HB3	1.93	0.69
2:B:525:ALA:HB1	2:B:768:THR:OG1	1.92	0.69
8:H:93:TYR:CD1	8:H:143:LEU:HD22	2.27	0.69
9:I:85:PHE:O	9:I:86:PHE:HB3	1.93	0.69
1:A:18:GLN:HE21	1:A:19:PHE:N	1.91	0.68
1:A:569:LYS:HB2	8:H:46:LEU:HD22	1.74	0.68
1:A:737:LEU:N	1:A:737:LEU:HD23	2.08	0.68
2:B:610:ASN:O	2:B:613:VAL:HG22	1.93	0.68
1:A:808:LEU:H	1:A:808:LEU:CD1	2.06	0.68
2:B:1198:TYR:O	2:B:1201:LYS:HB3	1.94	0.68
3:C:51:VAL:HG22	3:C:155:LEU:HB3	1.73	0.68
3:C:100:THR:HG23	3:C:156:THR:HG22	1.74	0.68
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.75	0.68
1:A:446:ARG:HD3	1:A:448:PRO:HD2	1.74	0.68
1:A:1381:LEU:H	1:A:1381:LEU:HD12	1.58	0.68
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.27	0.68
8:H:58:THR:HB	8:H:143:LEU:HD13	1.74	0.68
1:A:483:ASP:OD1	1:A:483:ASP:C	2.35	0.68
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.75	0.68
1:A:491:VAL:HG13	1:A:491:VAL:O	1.92	0.68
2:B:824:ILE:HD11	10:J:44:TYR:HE2	1.57	0.68
6:F:147:SER:HB3	6:F:150:GLU:HG2	1.76	0.68
8:H:97:MET:HG3	8:H:118:PHE:HE2	1.58	0.68
1:A:693:VAL:O	1:A:693:VAL:HG22	1.91	0.68
1:A:784:LEU:O	1:A:786:HIS:N	2.26	0.68
2:B:657:HIS:HA	2:B:660:LYS:HB2	1.74	0.68
3:C:169:LYS:HZ2	12:L:69:ALA:HB3	1.59	0.68
1:A:35:ILE:HG13	1:A:241:VAL:HG11	1.76	0.68
1:A:151:ASP:HA	1:A:163:SER:HA	1.74	0.68
1:A:211:PHE:HA	1:A:214:ILE:HG12	1.74	0.68
1:A:996:ASN:O	1:A:998:LEU:N	2.25	0.68
2:B:307:ASP:O	2:B:311:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:ASP:HB3	2:B:358:LYS:HE3	1.75	0.68
13:R:9:G:H1	14:T:20:DC:N4	1.92	0.68
2:B:216:GLU:HA	2:B:406:LEU:HA	1.76	0.68
3:C:22:LEU:HB3	3:C:25:VAL:HG21	1.74	0.68
3:C:166:GLU:OE1	12:L:70:ARG:NH2	2.27	0.68
1:A:243:PRO:C	1:A:245:PRO:HD2	2.19	0.68
1:A:960:ILE:CG1	1:A:1021:LEU:HD21	2.23	0.68
1:A:1035:TYR:HB3	1:A:1037:LEU:CD1	2.24	0.68
2:B:492:LEU:O	2:B:495:LEU:N	2.26	0.68
2:B:702:LEU:CD2	2:B:737:THR:HG23	2.24	0.68
3:C:44:LEU:HD12	3:C:160:LYS:C	2.18	0.68
3:C:186:LEU:HD23	3:C:223:ALA:HB1	1.75	0.68
3:C:235:VAL:HB	10:J:13:VAL:HG13	1.76	0.68
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.76	0.68
1:A:134:ARG:HD2	1:A:221:SER:O	1.94	0.68
1:A:341:MET:HE3	1:A:1401:SER:CB	2.23	0.68
8:H:101:ALA:HB1	8:H:104:PHE:CZ	2.29	0.68
1:A:377:PRO:HD2	1:A:493:GLN:HG3	1.75	0.67
2:B:36:ALA:O	2:B:39:ARG:HG2	1.92	0.67
2:B:53:GLN:HE22	2:B:58:THR:HG23	1.60	0.67
1:A:448:PRO:HA	14:T:19:DC:O2	1.94	0.67
1:A:618:GLU:OE2	1:A:620:LYS:HE3	1.94	0.67
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.67
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.24	0.67
5:E:170:LEU:HD23	5:E:170:LEU:N	2.10	0.67
9:I:6:PHE:HB3	9:I:12:ASN:O	1.94	0.67
2:B:604:ARG:HG3	2:B:605:ARG:N	2.07	0.67
2:B:658:ILE:HG22	2:B:659:ALA:N	2.09	0.67
2:B:685:LEU:HD12	2:B:686:ASN:N	2.09	0.67
3:C:39:ALA:CB	3:C:164:ALA:HB3	2.23	0.67
4:D:7:THR:HG21	4:D:32:GLU:OE2	1.94	0.67
2:B:416:LEU:O	2:B:420:LEU:HB2	1.94	0.67
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.75	0.67
4:D:66:ARG:HG3	7:G:51:TYR:CD2	2.29	0.67
1:A:1121:GLU:O	1:A:1125:ALA:HB2	1.94	0.67
1:A:1444:MET:HA	7:G:59:GLY:O	1.94	0.67
3:C:33:LEU:O	3:C:37:MET:HG3	1.95	0.67
1:A:19:PHE:HZ	1:A:1397:LEU:HD21	1.60	0.67
1:A:440:ASP:H	1:A:460:VAL:HG23	1.59	0.67
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.58	0.67
2:B:875:GLU:HG3	2:B:876:LYS:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:VAL:O	4:D:164:ILE:HG12	1.94	0.67
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.77	0.67
1:A:946:VAL:HG13	5:E:201:LYS:HD2	1.77	0.67
1:A:1120:LEU:HD11	1:A:1304:TRP:HB2	1.76	0.67
1:A:1267:MET:HA	1:A:1271:ILE:HG13	1.77	0.67
1:A:1418:LEU:HD13	1:A:1419:ASP:N	2.10	0.67
2:B:373:ARG:HB3	2:B:566:LEU:HD11	1.75	0.67
12:L:48:CYS:SG	12:L:51:CYS:N	2.68	0.67
1:A:151:ASP:OD2	1:A:163:SER:N	2.28	0.67
1:A:881:GLN:HA	1:A:961:ARG:NH2	2.09	0.67
1:A:1118:VAL:HG12	1:A:1306:LEU:O	1.95	0.67
1:A:1141:THR:HG23	1:A:1205:LYS:CD	2.24	0.67
2:B:354:ASP:O	2:B:358:LYS:HG3	1.95	0.67
2:B:595:ARG:O	2:B:599:THR:HG23	1.95	0.67
5:E:113:GLN:HA	5:E:137:GLU:HG2	1.76	0.67
6:F:152:ILE:HG22	6:F:153:VAL:N	2.09	0.67
1:A:249:SER:C	1:A:250:ILE:HD12	2.20	0.67
1:A:341:MET:HE1	1:A:1429:ILE:HD11	1.77	0.67
1:A:783:THR:O	1:A:784:LEU:HD23	1.94	0.67
10:J:55:ASP:OD1	10:J:57:ILE:HG22	1.95	0.67
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.27	0.67
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.29	0.67
2:B:171:PRO:HB3	2:B:205:ILE:HD11	1.76	0.67
11:K:82:ASP:OD1	11:K:83:PRO:HD2	1.94	0.67
1:A:962:ARG:HA	1:A:965:GLN:OE1	1.95	0.66
2:B:956:THR:HA	2:B:961:LEU:O	1.95	0.66
4:D:40:HIS:NE2	7:G:73:LYS:HB3	2.10	0.66
2:B:1173:ALA:O	2:B:1175:LEU:N	2.28	0.66
8:H:10:PHE:O	8:H:55:LEU:N	2.28	0.66
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.76	0.66
1:A:504:LEU:HD21	6:F:88:TYR:CE1	2.31	0.66
1:A:739:ASP:CG	8:H:19:ARG:HD3	2.21	0.66
1:A:1363:VAL:HG12	1:A:1364:ASN:N	2.10	0.66
2:B:788:ARG:NH2	2:B:790:ASP:OD2	2.28	0.66
3:C:21:ILE:HD12	3:C:21:ILE:O	1.95	0.66
4:D:130:LEU:HD13	4:D:142:LYS:HA	1.78	0.66
9:I:19:ASP:CB	9:I:24:ARG:HG2	2.24	0.66
1:A:1195:LEU:HD11	1:A:1238:ILE:HD13	1.76	0.66
2:B:841:MET:CE	2:B:990:ILE:CD1	2.73	0.66
5:E:15:ALA:O	5:E:19:VAL:HG23	1.95	0.66
6:F:79:ARG:HD2	6:F:146:TRP:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:O	10:J:60:PHE:HB2	1.94	0.66
1:A:40:THR:HG21	1:A:259:GLU:HG3	1.75	0.66
1:A:83:HIS:HA	1:A:241:VAL:HG23	1.77	0.66
1:A:1238:ILE:N	1:A:1238:ILE:HD12	2.09	0.66
2:B:115:GLN:OE1	2:B:194:GLU:HG2	1.94	0.66
2:B:639:ILE:HD13	2:B:688:GLY:O	1.94	0.66
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.30	0.66
2:B:912:ILE:HB	2:B:939:THR:OG1	1.96	0.66
9:I:86:PHE:C	9:I:99:LEU:HD12	2.21	0.66
1:A:62:ASP:OD1	1:A:65:LEU:HB2	1.94	0.66
1:A:219:PHE:HA	1:A:222:LEU:HB3	1.77	0.66
1:A:714:PHE:CG	9:I:97:MET:HE1	2.30	0.66
2:B:38:PHE:O	2:B:42:GLY:N	2.28	0.66
2:B:222:ILE:HG22	2:B:223:VAL:H	1.59	0.66
2:B:798:TYR:CE2	10:J:4:PRO:HB3	2.31	0.66
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.78	0.66
11:K:47:ARG:HA	11:K:50:LEU:HD12	1.78	0.66
12:L:61:THR:OG1	12:L:63:ARG:HD3	1.95	0.66
1:A:463:ILE:HD12	1:A:469:ARG:HD3	1.78	0.66
1:A:575:LYS:HB3	1:A:612:ILE:HG21	1.76	0.66
4:D:35:LEU:HD11	4:D:46:GLU:HG2	1.76	0.66
9:I:10:CYS:SG	9:I:31:THR:CG2	2.84	0.66
1:A:56:PRO:O	1:A:57:ARG:HG3	1.95	0.66
1:A:1011:GLN:HE22	1:A:1015:VAL:CG1	2.09	0.66
2:B:850:LEU:HD12	2:B:851:PHE:N	2.10	0.66
2:B:941:LEU:HG	2:B:942:ARG:H	1.61	0.66
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.77	0.66
3:C:253:LYS:O	3:C:256:ALA:HB3	1.96	0.66
1:A:476:SER:O	1:A:479:ASN:N	2.26	0.66
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.58	0.66
2:B:784:ASN:ND2	2:B:788:ARG:HG3	2.10	0.66
3:C:10:ILE:HD13	11:K:108:GLU:O	1.95	0.66
4:D:55:ALA:O	4:D:57:LEU:N	2.29	0.66
6:F:116:ASP:O	6:F:120:ILE:HG13	1.95	0.66
1:A:474:VAL:O	1:A:478:TYR:HD2	1.79	0.66
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.31	0.66
1:A:1195:LEU:HD12	1:A:1195:LEU:O	1.95	0.66
3:C:37:MET:HE1	3:C:232:VAL:CG1	2.26	0.66
3:C:50:GLU:HB2	12:L:64:LEU:HD23	1.78	0.66
8:H:58:THR:HG22	8:H:59:ILE:H	1.61	0.66
1:A:447:GLN:O	1:A:448:PRO:C	2.38	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LYS:HE3	1:A:721:PHE:CE1	2.31	0.65
1:A:1436:ILE:O	1:A:1439:GLY:N	2.28	0.65
2:B:37:PHE:HE2	2:B:542:MET:HA	1.60	0.65
2:B:222:ILE:HG22	2:B:223:VAL:N	2.10	0.65
2:B:541:LEU:HD12	2:B:747:MET:CE	2.26	0.65
2:B:654:ARG:O	2:B:657:HIS:N	2.29	0.65
2:B:859:TYR:HB2	2:B:966:VAL:HG22	1.78	0.65
2:B:1204:PHE:CE2	2:B:1216:LEU:HD11	2.31	0.65
6:F:127:GLU:O	6:F:129:LYS:HG2	1.96	0.65
12:L:48:CYS:O	12:L:51:CYS:N	2.29	0.65
1:A:174:ILE:HG12	1:A:202:LEU:HD11	1.77	0.65
2:B:1160:VAL:HG11	2:B:1169:MET:HB3	1.76	0.65
8:H:135:LEU:HD11	8:H:137:GLN:HE21	1.60	0.65
10:J:1:MET:SD	10:J:60:PHE:HE2	2.19	0.65
10:J:57:ILE:HG12	10:J:61:LEU:HD21	1.78	0.65
1:A:910:PRO:HB3	1:A:916:GLY:HA3	1.78	0.65
2:B:459:TYR:CE1	2:B:463:THR:HG21	2.31	0.65
3:C:48:SER:HB3	12:L:66:GLN:CD	2.21	0.65
4:D:68:ARG:O	4:D:72:ARG:HG3	1.97	0.65
4:D:198:LEU:N	4:D:198:LEU:HD23	2.12	0.65
1:A:282:ASN:HD22	1:A:283:GLY:H	1.42	0.65
1:A:869:GLY:C	1:A:871:ASP:H	2.04	0.65
1:A:889:SER:OG	1:A:891:ALA:HB3	1.97	0.65
1:A:910:PRO:C	1:A:912:LEU:H	2.05	0.65
2:B:222:ILE:CG2	2:B:223:VAL:H	2.09	0.65
2:B:657:HIS:HA	2:B:660:LYS:CB	2.27	0.65
4:D:138:ASN:OD1	4:D:141:LEU:HB3	1.97	0.65
1:A:596:THR:HG22	1:A:598:LEU:H	1.61	0.65
1:A:715:GLU:OE1	1:A:774:ARG:HD3	1.96	0.65
1:A:784:LEU:C	1:A:786:HIS:H	2.05	0.65
2:B:31:TRP:NE1	2:B:807:ARG:HG3	2.12	0.65
2:B:170:LEU:HD23	2:B:172:ILE:CD1	2.27	0.65
2:B:199:MET:HE2	2:B:492:LEU:HD21	1.79	0.65
2:B:228:LYS:CG	2:B:229:ALA:H	2.10	0.65
2:B:759:PRO:HB3	2:B:767:ASN:ND2	2.12	0.65
2:B:1204:PHE:O	2:B:1208:MET:HG3	1.96	0.65
1:A:73:GLY:O	1:A:75:ASN:N	2.30	0.65
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.77	0.65
1:A:531:ILE:CD1	1:A:617:VAL:HG11	2.27	0.65
1:A:640:GLN:CD	1:A:640:GLN:H	1.99	0.65
2:B:899:ILE:HD12	2:B:949:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1188:LYS:C	2:B:1191:ILE:HD11	2.21	0.65
5:E:163:GLU:HA	5:E:163:GLU:OE1	1.97	0.65
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.62	0.65
1:A:449:SER:O	2:B:1133:MET:CG	2.45	0.65
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.27	0.65
1:A:946:VAL:HG22	5:E:201:LYS:HB2	1.79	0.65
1:A:1361:SER:O	1:A:1362:TYR:HB3	1.97	0.65
2:B:225:VAL:HA	2:B:237:VAL:O	1.96	0.65
3:C:57:VAL:HG11	10:J:60:PHE:CG	2.32	0.65
11:K:21:ILE:HD12	11:K:21:ILE:O	1.96	0.65
11:K:73:LEU:HD12	11:K:74:ARG:N	2.11	0.65
2:B:225:VAL:HG12	2:B:238:ALA:HA	1.77	0.65
2:B:806:THR:HG22	2:B:1044:ALA:C	2.22	0.65
4:D:56:ARG:H	4:D:148:LEU:HD13	1.62	0.65
5:E:198:ILE:H	5:E:198:ILE:HD12	1.62	0.65
1:A:648:ASN:O	1:A:652:VAL:HG12	1.97	0.65
1:A:678:GLU:HA	1:A:681:GLU:OE1	1.97	0.65
1:A:775:ILE:HG12	1:A:797:LYS:HA	1.79	0.65
1:A:809:THR:HB	1:A:810:PRO:HD2	1.79	0.65
1:A:896:ARG:O	1:A:1029:ARG:HD2	1.97	0.65
1:A:1037:LEU:HD23	1:A:1042:PHE:HB2	1.79	0.65
2:B:546:SER:HB3	2:B:631:GLY:H	1.62	0.65
2:B:903:VAL:HG12	2:B:905:VAL:HG22	1.78	0.65
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.27	0.65
3:C:80:LEU:HD11	3:C:95:CYS:C	2.21	0.65
1:A:899:VAL:HG22	1:A:1029:ARG:NE	2.10	0.65
4:D:202:ILE:HD13	4:D:207:LEU:HD13	1.79	0.65
1:A:660:ASN:OD1	2:B:1082:MET:HB2	1.97	0.64
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.79	0.64
2:B:546:SER:HB3	2:B:632:ARG:H	1.62	0.64
2:B:941:LEU:HG	2:B:942:ARG:N	2.10	0.64
2:B:947:GLY:C	2:B:948:ILE:HD12	2.21	0.64
2:B:1152:MET:O	2:B:1157:ALA:HB2	1.97	0.64
3:C:80:LEU:HD12	3:C:94:LYS:O	1.98	0.64
4:D:56:ARG:HH22	4:D:155:ARG:HD3	1.61	0.64
12:L:31:CYS:SG	12:L:32:ALA:N	2.65	0.64
1:A:457:ALA:HB2	1:A:501:LEU:HD22	1.78	0.64
1:A:640:GLN:OE1	1:A:640:GLN:N	2.22	0.64
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.79	0.64
2:B:357:GLN:CD	2:B:368:GLU:HG3	2.22	0.64
3:C:59:ALA:O	3:C:63:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:GLU:HG2	3:C:180:TYR:N	2.12	0.64
1:A:93:VAL:HG21	1:A:305:ASP:HB3	1.79	0.64
1:A:148:CYS:O	1:A:149:GLU:HG2	1.96	0.64
1:A:566:ILE:O	8:H:96:VAL:HB	1.96	0.64
1:A:1081:LEU:O	1:A:1081:LEU:CD2	2.46	0.64
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	1.98	0.64
2:B:228:LYS:HG3	2:B:229:ALA:N	2.12	0.64
2:B:515:HIS:ND1	2:B:517:THR:OG1	2.28	0.64
2:B:796:LEU:HD23	2:B:798:TYR:H	1.62	0.64
3:C:93:ASP:O	3:C:127:ARG:NH2	2.31	0.64
4:D:207:LEU:HG	4:D:211:LEU:HD23	1.80	0.64
11:K:51:LEU:HD12	11:K:59:ALA:HB3	1.79	0.64
14:T:22:DT:H2'	14:T:23:DC:O4'	1.96	0.64
1:A:404:TYR:N	1:A:415:LEU:HD13	2.12	0.64
1:A:1170:ILE:O	1:A:1170:ILE:HD12	1.98	0.64
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	1.98	0.64
2:B:195:CYS:HB3	2:B:198:ASP:HB2	1.80	0.64
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.80	0.64
2:B:432:MET:HB2	2:B:433:GLN:OE1	1.97	0.64
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.80	0.64
1:A:830:LYS:HE2	1:A:1094:VAL:HG23	1.78	0.64
1:A:960:ILE:HG13	1:A:1021:LEU:CD2	2.27	0.64
1:A:1153:TYR:HB2	1:A:1192:LEU:HB3	1.79	0.64
1:A:1343:ALA:CB	5:E:149:LEU:HD12	2.27	0.64
2:B:639:ILE:HD11	2:B:689:LEU:HA	1.79	0.64
2:B:770:GLN:CD	2:B:983:ARG:HA	2.23	0.64
1:A:340:LEU:C	1:A:342:GLY:H	2.05	0.64
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.98	0.64
2:B:377:PHE:O	2:B:380:TYR:N	2.31	0.64
5:E:185:ALA:O	5:E:189:GLY:N	2.31	0.64
1:A:404:TYR:C	1:A:415:LEU:HD11	2.23	0.64
1:A:1398:MET:CE	1:A:1423:GLY:HA3	2.28	0.64
2:B:301:ILE:HD12	2:B:301:ILE:N	2.13	0.64
2:B:1166:CYS:SG	2:B:1168:LEU:HD11	2.37	0.64
3:C:242:GLN:HA	3:C:245:VAL:HG12	1.78	0.64
7:G:44:TYR:HB3	7:G:46:LEU:HG	1.80	0.64
9:I:103:CYS:SG	9:I:107:SER:N	2.71	0.64
1:A:260:ASP:O	1:A:263:THR:N	2.29	0.64
1:A:534:LEU:HA	1:A:539:THR:HG21	1.80	0.64
1:A:83:HIS:N	1:A:241:VAL:HG23	2.12	0.64
1:A:95:PHE:CD2	1:A:234:MET:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:HA	1:A:302:THR:HG22	1.80	0.64
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.33	0.64
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.78	0.64
1:A:1011:GLN:HE22	1:A:1015:VAL:HG11	1.62	0.64
1:A:1399:ARG:O	1:A:1401:SER:N	2.31	0.64
1:A:1420:ASP:OD1	2:B:1222:ARG:HD3	1.98	0.64
2:B:53:GLN:HG3	2:B:547:VAL:CG1	2.27	0.64
2:B:256:VAL:HG22	2:B:271:ALA:HB2	1.80	0.64
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.22	0.64
3:C:37:MET:CE	3:C:232:VAL:HG11	2.27	0.64
1:A:42:ASP:OD1	1:A:42:ASP:N	2.31	0.63
2:B:1189:ILE:HG13	2:B:1190:ASP:N	2.14	0.63
4:D:37:GLN:HE21	4:D:47:LEU:HD12	1.63	0.63
1:A:116:ASP:OD2	1:A:164:ARG:HD2	1.97	0.63
1:A:878:ILE:HD12	1:A:1366:ARG:HH22	1.63	0.63
2:B:407:ASP:HB3	2:B:411:PRO:HB2	1.80	0.63
2:B:1112:GLN:HG3	2:B:1113:VAL:N	2.09	0.63
3:C:73:GLN:HB3	3:C:131:HIS:H	1.63	0.63
4:D:37:GLN:NE2	4:D:47:LEU:HD12	2.13	0.63
1:A:671:ALA:HB1	1:A:736:ASN:HD22	1.62	0.63
1:A:902:LEU:O	1:A:903:ASN:HB2	1.99	0.63
1:A:1078:GLN:CG	1:A:1078:GLN:O	2.46	0.63
1:A:1336:MET:HG3	1:A:1381:LEU:CD1	2.27	0.63
2:B:48:LEU:HD12	2:B:173:MET:HE1	1.80	0.63
2:B:373:ARG:HA	2:B:566:LEU:HD11	1.81	0.63
3:C:48:SER:HB3	12:L:66:GLN:HE22	1.61	0.63
4:D:37:GLN:HE22	7:G:5:LYS:HD3	1.63	0.63
4:D:129:LEU:O	4:D:133:THR:N	2.31	0.63
9:I:7:CYS:SG	9:I:9:ASP:N	2.66	0.63
1:A:56:PRO:O	1:A:57:ARG:CB	2.47	0.63
1:A:384:ASN:O	1:A:387:ARG:N	2.22	0.63
1:A:446:ARG:NH1	1:A:480:ALA:HA	2.13	0.63
1:A:1265:ASN:O	1:A:1268:LEU:N	2.32	0.63
2:B:206:ASN:OD1	2:B:458:LYS:HE2	1.99	0.63
2:B:874:PHE:HB3	2:B:897:GLY:HA3	1.80	0.63
3:C:68:GLY:O	3:C:169:LYS:HB2	1.97	0.63
4:D:48:ILE:HD12	4:D:48:ILE:N	2.12	0.63
1:A:525:GLN:HA	2:B:1015:HIS:CD2	2.34	0.63
2:B:365:THR:OG1	2:B:367:LEU:HG	1.98	0.63
7:G:106:MET:HE3	7:G:108:VAL:HG23	1.78	0.63
11:K:40:HIS:HE1	11:K:63:VAL:HG21	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:32:ALA:CB	12:L:55:ILE:HG21	2.29	0.63
12:L:48:CYS:SG	15:L:101:ZN:ZN	1.79	0.63
1:A:282:ASN:ND2	1:A:283:GLY:H	1.95	0.63
1:A:948:VAL:O	1:A:950:GLY:N	2.32	0.63
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.28	0.63
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.80	0.63
2:B:1060:ARG:HH21	3:C:202:PRO:HB3	1.63	0.63
3:C:238:ILE:HD11	3:C:246:ARG:NH2	2.14	0.63
7:G:116:PRO:HG3	7:G:164:LYS:HA	1.79	0.63
9:I:73:ARG:O	9:I:81:ARG:HA	1.97	0.63
1:A:374:LEU:O	1:A:436:ILE:HG23	1.98	0.63
1:A:1027:ALA:HB3	1:A:1030:ARG:HB2	1.78	0.63
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.34	0.63
2:B:102:VAL:HB	2:B:112:LEU:HD22	1.81	0.63
2:B:512:ARG:HH21	2:B:532:ALA:HA	1.63	0.63
2:B:1110:PRO:O	2:B:1111:MET:HE2	1.97	0.63
3:C:147:LEU:HD23	3:C:151:GLN:HB3	1.81	0.63
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.34	0.63
1:A:375:THR:OG1	1:A:433:GLU:HB3	1.98	0.63
2:B:50:SER:OG	2:B:410:GLY:N	2.30	0.63
2:B:865:LYS:HG2	2:B:866:TYR:N	2.13	0.63
10:J:1:MET:SD	10:J:60:PHE:CE2	2.92	0.63
1:A:557:ASP:CG	1:A:559:VAL:HG22	2.24	0.63
1:A:973:ILE:HD12	1:A:973:ILE:O	1.98	0.63
1:A:1011:GLN:O	1:A:1015:VAL:HG22	1.98	0.63
1:A:1089:VAL:HG23	1:A:1090:ALA:H	1.63	0.63
1:A:476:SER:HB2	1:A:477:PRO:CD	2.29	0.62
2:B:217:ARG:NH1	2:B:405:ARG:CB	2.61	0.62
2:B:397:ASP:HB3	2:B:400:HIS:HB2	1.80	0.62
2:B:830:TYR:CE1	2:B:1000:PRO:HD3	2.33	0.62
3:C:68:GLY:HA3	12:L:69:ALA:HB1	1.81	0.62
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.24	0.62
9:I:10:CYS:SG	9:I:31:THR:HG21	2.38	0.62
9:I:58:VAL:HG22	9:I:58:VAL:O	1.96	0.62
1:A:452:LYS:HG3	2:B:1140:ALA:HB1	1.80	0.62
1:A:1442:ASP:CG	7:G:60:ARG:HH21	2.07	0.62
2:B:1082:MET:HE1	19:H:203:HOH:O	1.99	0.62
2:B:1106:ARG:HG3	2:B:1106:ARG:HH11	1.63	0.62
3:C:12:GLU:H	3:C:19:ASP:HB3	1.64	0.62
1:A:99:ILE:HG23	1:A:211:PHE:HE2	1.65	0.62
1:A:391:LEU:O	1:A:394:ASN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CZ	1:A:1366:ARG:HD2	2.34	0.62
2:B:832:GLY:O	2:B:835:GLN:HG3	2.00	0.62
7:G:81:PRO:HG3	7:G:106:MET:SD	2.39	0.62
12:L:48:CYS:SG	12:L:51:CYS:CA	2.88	0.62
1:A:567:LYS:C	1:A:569:LYS:N	2.57	0.62
2:B:1030:LEU:HD21	2:B:1056:SER:OG	1.99	0.62
5:E:55:ARG:HD3	5:E:113:GLN:OE1	1.99	0.62
11:K:73:LEU:HD12	11:K:74:ARG:H	1.64	0.62
12:L:46:VAL:C	12:L:47:ARG:CG	2.72	0.62
1:A:752:LYS:HD2	2:B:1019:SER:HB2	1.81	0.62
1:A:868:TYR:CE2	1:A:1366:ARG:HD2	2.34	0.62
1:A:1363:VAL:CG1	1:A:1364:ASN:H	2.11	0.62
3:C:57:VAL:HG11	10:J:60:PHE:CD2	2.35	0.62
3:C:259:LEU:HD22	3:C:259:LEU:H	1.65	0.62
4:D:190:GLU:HB2	7:G:167:TYR:CD1	2.35	0.62
1:A:19:PHE:CZ	1:A:1397:LEU:HD21	2.33	0.62
3:C:58:LEU:HB3	3:C:62:PHE:CD1	2.34	0.62
5:E:22:MET:SD	5:E:26:ARG:NH2	2.72	0.62
8:H:139:ASN:O	8:H:140:ALA:HB2	1.98	0.62
10:J:9:SER:OG	10:J:45:CYS:HB2	2.00	0.62
1:A:491:VAL:O	1:A:491:VAL:CG1	2.48	0.62
1:A:530:GLY:HA2	1:A:533:LYS:HG3	1.80	0.62
1:A:569:LYS:HG2	8:H:46:LEU:HD21	1.80	0.62
1:A:671:ALA:O	1:A:673:GLY:N	2.32	0.62
1:A:833:GLU:O	1:A:837:ILE:HG12	2.00	0.62
1:A:880:LYS:HA	1:A:954:TRP:O	1.99	0.62
1:A:998:LEU:O	1:A:1053:PHE:HE1	1.83	0.62
1:A:1398:MET:HE1	1:A:1423:GLY:CA	2.29	0.62
2:B:360:PHE:CE2	2:B:361:LEU:HD12	2.35	0.62
2:B:837:ASP:OD1	2:B:1016:ALA:CB	2.45	0.62
1:A:308:ILE:HG22	1:A:309:ALA:N	2.14	0.62
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.82	0.62
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.35	0.62
2:B:619:ILE:H	2:B:619:ILE:HD12	1.64	0.62
2:B:995:ARG:HD3	11:K:6:ARG:HH22	1.64	0.62
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.82	0.62
10:J:6:ARG:HA	10:J:14:VAL:H	1.65	0.62
12:L:60:ARG:HG3	12:L:61:THR:O	1.99	0.62
1:A:875:ALA:HA	1:A:1366:ARG:NH2	2.14	0.62
2:B:864:LYS:H	2:B:872:GLU:CD	2.08	0.62
11:K:19:LEU:HD12	11:K:19:LEU:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:HB2	2:B:988:GLY:N	2.14	0.62
1:A:970:THR:HG22	1:A:971:PHE:CD1	2.34	0.62
2:B:304:ASP:O	2:B:306:ASN:N	2.28	0.62
2:B:522:VAL:HG12	2:B:523:CYS:N	2.14	0.62
11:K:10:PHE:CD1	11:K:11:LEU:N	2.68	0.62
1:A:361:LEU:HD21	1:A:511:ILE:HD11	1.80	0.61
1:A:1116:LEU:CD1	1:A:1311:VAL:HA	2.30	0.61
1:A:1148:ILE:CG2	1:A:1196:GLU:HG2	2.30	0.61
1:A:1313:LEU:HD22	1:A:1338:VAL:HG11	1.81	0.61
3:C:99:LEU:HD23	3:C:120:ILE:HA	1.82	0.61
12:L:65:VAL:HG23	12:L:67:PHE:CZ	2.35	0.61
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.81	0.61
1:A:867:ILE:CG2	1:A:872:GLY:N	2.64	0.61
1:A:1011:GLN:NE2	1:A:1015:VAL:HG11	2.15	0.61
1:A:1384:VAL:C	1:A:1385:THR:CG2	2.73	0.61
2:B:217:ARG:N	2:B:405:ARG:O	2.33	0.61
7:G:13:LEU:CD1	7:G:26:LEU:HD21	2.26	0.61
1:A:1215:ARG:O	1:A:1219:THR:HG23	2.00	0.61
2:B:1006:ILE:HG13	10:J:43:ARG:HD2	1.83	0.61
3:C:70:ILE:HG23	3:C:71:PRO:HD2	1.82	0.61
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.34	0.61
5:E:171:LYS:HD3	5:E:173:SER:HB3	1.80	0.61
5:E:196:VAL:HG13	5:E:198:ILE:CD1	2.30	0.61
1:A:208:LEU:HD12	1:A:208:LEU:C	2.26	0.61
1:A:466:SER:HB2	2:B:1099:VAL:HG22	1.82	0.61
1:A:739:ASP:OD1	8:H:19:ARG:HD3	2.00	0.61
1:A:1284:MET:HB3	1:A:1306:LEU:HD23	1.80	0.61
2:B:424:LEU:O	2:B:428:ILE:HG23	2.00	0.61
2:B:680:THR:HB	2:B:683:SER:CB	2.30	0.61
7:G:18:PHE:CD1	7:G:22:MET:HE2	2.35	0.61
1:A:525:GLN:NE2	2:B:836:GLU:OE2	2.34	0.61
1:A:1376:THR:O	1:A:1378:GLN:N	2.33	0.61
2:B:29:ASP:CG	2:B:658:ILE:HG12	2.25	0.61
4:D:118:THR:O	4:D:121:LYS:HB3	2.00	0.61
8:H:16:ASP:C	8:H:16:ASP:OD1	2.44	0.61
1:A:49:LYS:HE2	1:A:61:ILE:HG22	1.82	0.61
1:A:251:SER:HB2	1:A:257:ARG:HH11	1.66	0.61
1:A:711:ARG:HH11	9:I:97:MET:HG2	1.65	0.61
1:A:1399:ARG:C	1:A:1401:SER:H	2.07	0.61
2:B:291:ILE:HG21	2:B:300:HIS:CD2	2.35	0.61
2:B:1007:VAL:HG12	2:B:1008:PRO:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:HH12	2:B:1110:PRO:HD2	1.66	0.61
8:H:125:LEU:C	8:H:125:LEU:HD12	2.25	0.61
10:J:36:LEU:HD21	10:J:50:ILE:CG2	2.30	0.61
11:K:108:GLU:OE1	11:K:111:LEU:HD12	2.01	0.61
12:L:32:ALA:HB2	12:L:55:ILE:HD13	1.82	0.61
1:A:102:VAL:HG23	1:A:211:PHE:CZ	2.36	0.61
1:A:864:ILE:O	1:A:865:GLN:HG3	1.99	0.61
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.64	0.61
3:C:134:ILE:HG13	3:C:134:ILE:O	1.99	0.61
1:A:601:LYS:HB3	1:A:603:ASN:HD21	1.65	0.61
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.80	0.61
1:A:1444:MET:HE1	6:F:135:ARG:NH1	2.16	0.61
2:B:226:PHE:HE1	2:B:396:ASP:HB2	1.64	0.61
2:B:635:ARG:HH21	2:B:637:LEU:CD1	2.13	0.61
2:B:1036:ALA:HB1	10:J:44:TYR:HB2	1.82	0.61
2:B:1166:CYS:HB2	2:B:1168:LEU:HD11	1.82	0.61
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.81	0.61
4:D:54:GLU:O	4:D:58:VAL:HG12	2.00	0.61
4:D:168:LYS:HE3	4:D:177:VAL:HG11	1.83	0.61
7:G:96:GLN:HG3	7:G:121:PHE:CZ	2.36	0.61
10:J:37:SER:OG	10:J:47:ARG:NH2	2.23	0.61
1:A:139:TRP:O	1:A:142:CYS:N	2.34	0.61
1:A:455:MET:HE1	2:B:1134:GLU:HG2	1.83	0.61
1:A:989:GLY:O	1:A:992:ASP:N	2.33	0.61
1:A:998:LEU:O	1:A:999:VAL:HG23	2.01	0.61
2:B:120:ARG:NH2	2:B:956:THR:O	2.30	0.61
2:B:217:ARG:O	2:B:405:ARG:N	2.34	0.61
2:B:803:LEU:HG	10:J:52:THR:HG21	1.82	0.61
3:C:88:CYS:O	3:C:89:GLU:C	2.43	0.61
4:D:56:ARG:N	4:D:59:ILE:CD1	2.64	0.61
4:D:69:ALA:O	4:D:72:ARG:HB2	2.01	0.61
5:E:127:ILE:HG22	5:E:127:ILE:O	2.01	0.61
7:G:91:VAL:HG22	7:G:101:VAL:HG12	1.83	0.61
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.36	0.61
9:I:111:THR:HG21	9:I:118:ARG:HG2	1.82	0.61
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.01	0.61
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.00	0.61
1:A:687:LYS:O	1:A:691:LEU:N	2.33	0.61
1:A:987:VAL:CG1	1:A:1028:THR:OG1	2.49	0.61
2:B:226:PHE:CE1	2:B:396:ASP:HB2	2.36	0.61
1:A:545:GLN:HE21	1:A:549:MET:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG2	5:E:212:ARG:HE	1.66	0.60
2:B:248:SER:OG	2:B:249:ARG:N	2.34	0.60
2:B:446:LEU:O	2:B:447:ALA:HB3	2.00	0.60
3:C:48:SER:HB3	12:L:66:GLN:OE1	2.01	0.60
7:G:1:MET:HB2	7:G:3:PHE:HE1	1.66	0.60
7:G:119:LEU:HD13	7:G:131:GLN:O	2.02	0.60
9:I:92:ARG:HB3	9:I:95:THR:HG23	1.83	0.60
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.35	0.60
12:L:48:CYS:SG	12:L:48:CYS:O	2.59	0.60
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.82	0.60
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.65	0.60
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.83	0.60
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.60
1:A:349:ALA:HB3	1:A:489:LEU:HB3	1.83	0.60
1:A:542:GLU:HG2	1:A:543:LEU:N	2.16	0.60
1:A:738:LYS:HD2	1:A:740:LEU:HB2	1.84	0.60
1:A:867:ILE:HG22	1:A:872:GLY:H	1.64	0.60
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.00	0.60
2:B:396:ASP:HB3	2:B:403:LYS:HZ3	1.65	0.60
5:E:55:ARG:CZ	5:E:113:GLN:NE2	2.63	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.37	0.60
1:A:96:ILE:HG13	1:A:97:ALA:N	2.16	0.60
1:A:568:PRO:HD3	8:H:96:VAL:HG23	1.84	0.60
2:B:170:LEU:HD23	2:B:172:ILE:HD13	1.84	0.60
8:H:15:VAL:HA	8:H:26:ILE:HD12	1.83	0.60
12:L:61:THR:C	12:L:63:ARG:H	2.09	0.60
1:A:1128:GLN:HG3	1:A:1304:TRP:CZ2	2.36	0.60
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.83	0.60
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.32	0.60
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.14	0.60
2:B:1058:LEU:H	2:B:1058:LEU:HD12	1.66	0.60
7:G:127:PRO:HG2	7:G:139:ILE:HG21	1.82	0.60
1:A:451:HIS:CD2	1:A:454:SER:HB2	2.36	0.60
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.83	0.60
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.84	0.60
2:B:431:TYR:CZ	2:B:447:ALA:HB3	2.35	0.60
2:B:651:LEU:O	2:B:651:LEU:HG	2.01	0.60
8:H:113:ALA:HA	8:H:125:LEU:O	2.01	0.60
1:A:419:LYS:HG3	1:A:420:ARG:N	2.16	0.60
1:A:820:GLY:O	1:A:824:LEU:N	2.34	0.60
1:A:1139:GLU:O	1:A:1139:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.83	0.60
2:B:405:ARG:NH1	2:B:629:ASP:OD2	2.35	0.60
2:B:1006:ILE:HD11	10:J:43:ARG:HG2	1.84	0.60
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.37	0.60
1:A:1138:ILE:O	1:A:1140:HIS:N	2.35	0.60
2:B:108:VAL:HG23	2:B:109:THR:H	1.67	0.60
2:B:832:GLY:C	2:B:835:GLN:HG3	2.27	0.60
5:E:29:PHE:O	5:E:30:ILE:HD13	2.02	0.60
7:G:99:PHE:O	7:G:99:PHE:CD1	2.54	0.60
8:H:7:ASP:C	8:H:7:ASP:OD1	2.45	0.60
1:A:272:ALA:HB2	1:A:299:HIS:HD2	1.67	0.60
1:A:830:LYS:HE2	1:A:1094:VAL:CG2	2.32	0.60
2:B:331:LEU:HB2	2:B:352:ALA:CB	2.31	0.60
2:B:582:VAL:HA	2:B:626:ILE:O	2.02	0.60
2:B:878:GLN:C	2:B:885:MET:HE1	2.26	0.60
11:K:63:VAL:O	11:K:65:HIS:N	2.34	0.60
12:L:40:LEU:HD21	12:L:44:ASP:HB3	1.82	0.60
1:A:453:MET:O	1:A:456:MET:HE2	1.99	0.60
1:A:928:LEU:HD13	1:A:988:LEU:HD11	1.82	0.60
1:A:1339:LEU:HD13	5:E:147:HIS:HD2	1.66	0.60
1:A:1386:ARG:HB3	1:A:1403:GLU:HB2	1.83	0.60
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.32	0.60
2:B:498:THR:O	2:B:498:THR:OG1	2.19	0.60
2:B:498:THR:HG23	2:B:537:LYS:O	2.01	0.60
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.84	0.60
1:A:741:ASN:O	1:A:745:GLN:HG3	2.02	0.59
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.42	0.59
2:B:431:TYR:OH	2:B:447:ALA:HB3	2.01	0.59
2:B:541:LEU:HD12	2:B:747:MET:HE3	1.83	0.59
2:B:706:GLN:HB3	2:B:709:ASP:HB2	1.84	0.59
2:B:798:TYR:CD2	10:J:4:PRO:HB3	2.36	0.59
2:B:1046:PRO:C	2:B:1048:THR:HG23	2.27	0.59
10:J:43:ARG:HB3	10:J:45:CYS:SG	2.41	0.59
2:B:773:MET:HE1	2:B:987:LYS:HE2	1.82	0.59
5:E:3:GLN:HG3	5:E:5:ASN:H	1.68	0.59
7:G:163:ILE:O	7:G:163:ILE:HG22	2.01	0.59
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.75	0.59
1:A:216:VAL:HA	1:A:219:PHE:CE1	2.37	0.59
1:A:353:ILE:CG2	1:A:487:MET:HB2	2.32	0.59
1:A:446:ARG:NH2	1:A:485:ASP:OD2	2.31	0.59
1:A:569:LYS:HD3	3:C:221:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:OE1	1:A:774:ARG:CD	2.51	0.59
1:A:1402:PHE:CD1	1:A:1403:GLU:CG	2.86	0.59
3:C:73:GLN:HE21	3:C:75:MET:H	1.50	0.59
1:A:507:VAL:N	1:A:508:PRO:CD	2.65	0.59
1:A:830:LYS:HB2	1:A:830:LYS:HZ2	1.67	0.59
2:B:953:LEU:CD2	2:B:955:THR:HG22	2.33	0.59
1:A:843:LYS:HE2	1:A:1401:SER:CB	2.31	0.59
1:A:1384:VAL:O	1:A:1385:THR:HG22	2.01	0.59
2:B:222:ILE:O	2:B:240:ILE:HD12	2.02	0.59
5:E:86:PRO:HB3	5:E:114:ASN:HB2	1.83	0.59
5:E:153:HIS:HB3	5:E:196:VAL:CG2	2.33	0.59
8:H:25:ARG:HG3	8:H:26:ILE:N	2.16	0.59
8:H:145:ARG:O	8:H:146:ARG:HB2	2.03	0.59
1:A:501:LEU:HD23	1:A:505:CYS:HB2	1.84	0.59
1:A:789:LYS:HG2	1:A:790:ASP:H	1.66	0.59
1:A:1261:LYS:NZ	2:B:265:SER:OG	2.36	0.59
2:B:173:MET:HG3	2:B:176:SER:HB3	1.83	0.59
2:B:805:THR:CG2	2:B:1041:GLU:HG2	2.31	0.59
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.17	0.59
3:C:176:ILE:HG12	3:C:232:VAL:HG13	1.84	0.59
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.85	0.59
5:E:80:VAL:HG23	5:E:109:ILE:O	2.03	0.59
7:G:96:GLN:CG	7:G:121:PHE:CZ	2.85	0.59
1:A:423:ASP:OD1	1:A:424:ILE:N	2.35	0.59
1:A:1004:ASN:HB3	5:E:167:ARG:CZ	2.33	0.59
1:A:1332:PHE:HD1	1:A:1381:LEU:HD21	1.67	0.59
2:B:549:THR:HG22	2:B:550:ASP:N	2.18	0.59
2:B:735:ALA:O	2:B:737:THR:HG22	2.03	0.59
2:B:841:MET:HE3	2:B:990:ILE:CD1	2.33	0.59
2:B:846:ILE:HA	2:B:850:LEU:HB3	1.84	0.59
2:B:1013:ASN:HD22	2:B:1014:PRO:HD2	1.68	0.59
8:H:43:ASN:OD1	8:H:44:VAL:N	2.35	0.59
12:L:55:ILE:HG23	12:L:56:LEU:N	2.17	0.59
1:A:525:GLN:CG	2:B:836:GLU:OE2	2.49	0.59
1:A:827:THR:HG21	1:A:1084:PHE:HB3	1.84	0.59
2:B:780:VAL:CG2	2:B:799:PRO:HG2	2.33	0.59
2:B:813:LYS:HA	2:B:816:GLU:OE1	2.03	0.59
2:B:859:TYR:O	2:B:965:LYS:HA	2.02	0.59
3:C:248:ILE:HG12	11:K:101:LEU:HD23	1.85	0.59
4:D:8:PHE:CD2	4:D:38:ILE:HB	2.37	0.59
4:D:40:HIS:CE1	7:G:73:LYS:HE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:HB3	1:A:133:LYS:HE2	1.85	0.59
1:A:350:ARG:HD2	2:B:1128:LEU:HD11	1.84	0.59
1:A:693:VAL:HG22	1:A:714:PHE:CE1	2.37	0.59
1:A:1011:GLN:NE2	1:A:1015:VAL:CG1	2.66	0.59
2:B:843:GLN:N	2:B:994:TYR:O	2.34	0.59
2:B:1010:LEU:HD23	2:B:1011:ILE:N	2.18	0.59
3:C:142:VAL:HG23	10:J:16:ASP:N	2.17	0.59
4:D:8:PHE:CD2	4:D:38:ILE:HD12	2.37	0.59
8:H:56:THR:HG22	8:H:57:VAL:N	2.13	0.59
1:A:453:MET:O	1:A:456:MET:HE3	2.03	0.59
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.68	0.59
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.32	0.59
1:A:1402:PHE:HD1	1:A:1403:GLU:H	1.49	0.59
1:A:1424:VAL:HG13	1:A:1425:SER:N	2.18	0.59
2:B:1168:LEU:HD12	2:B:1168:LEU:O	2.03	0.59
5:E:12:LEU:HD11	5:E:55:ARG:HE	1.66	0.59
1:A:114:LEU:HD21	1:A:171:GLN:HG3	1.84	0.58
1:A:171:GLN:C	1:A:185:TRP:HE1	2.11	0.58
1:A:455:MET:CE	2:B:1130:PHE:HE1	2.15	0.58
1:A:499:ALA:HA	1:A:502:SER:OG	2.03	0.58
1:A:669:THR:O	1:A:805:LEU:HD12	2.03	0.58
1:A:843:LYS:CE	1:A:1401:SER:HB2	2.32	0.58
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.84	0.58
2:B:520:GLY:H	2:B:748:ILE:HG22	1.68	0.58
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.33	0.58
7:G:51:TYR:C	7:G:51:TYR:HD1	2.11	0.58
8:H:135:LEU:HD12	8:H:137:GLN:HG2	1.84	0.58
9:I:35:VAL:CG1	9:I:36:GLU:N	2.66	0.58
1:A:419:LYS:HG3	1:A:420:ARG:H	1.67	0.58
1:A:1118:VAL:CG1	1:A:1306:LEU:HB2	2.33	0.58
1:A:1143:LEU:HD11	1:A:1147:THR:CG2	2.34	0.58
2:B:1175:LEU:HD12	2:B:1176:ASN:N	2.18	0.58
9:I:17:ARG:HH22	9:I:20:LYS:HE3	1.68	0.58
1:A:350:ARG:HD2	2:B:1128:LEU:CD1	2.33	0.58
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.38	0.58
1:A:890:ASP:HB2	1:A:1296:GLY:HA3	1.85	0.58
1:A:999:VAL:HG12	1:A:1000:LEU:N	2.18	0.58
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.18	0.58
1:A:1043:ASP:N	1:A:1043:ASP:OD1	2.35	0.58
2:B:128:LEU:HB2	2:B:168:GLY:H	1.69	0.58
2:B:217:ARG:NH1	2:B:405:ARG:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:O	2:B:654:ARG:HG3	2.04	0.58
2:B:865:LYS:HG2	2:B:866:TYR:H	1.68	0.58
2:B:1106:ARG:HH21	2:B:1111:MET:HE2	1.68	0.58
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.30	0.58
1:A:18:GLN:NE2	1:A:18:GLN:HA	2.19	0.58
1:A:456:MET:CE	1:A:477:PRO:HB2	2.33	0.58
1:A:1037:LEU:HD23	1:A:1042:PHE:CA	2.33	0.58
2:B:552:MET:O	2:B:555:ILE:HG13	2.03	0.58
2:B:578:THR:HG22	2:B:622:LYS:HB3	1.85	0.58
2:B:832:GLY:CA	2:B:835:GLN:HG3	2.33	0.58
4:D:67:ARG:HG2	4:D:67:ARG:NH1	2.11	0.58
5:E:4:GLU:HA	5:E:6:GLU:CD	2.28	0.58
7:G:23:LYS:CG	7:G:56:ILE:HD13	2.33	0.58
8:H:43:ASN:OD1	8:H:45:GLU:N	2.35	0.58
1:A:122:MET:O	1:A:126:LEU:HB2	2.03	0.58
1:A:278:THR:O	1:A:279:LEU:C	2.46	0.58
1:A:450:LEU:CD1	1:A:1074:GLU:HG2	2.34	0.58
1:A:523:ILE:N	1:A:523:ILE:HD12	2.18	0.58
1:A:524:VAL:HG13	1:A:525:GLN:N	2.18	0.58
1:A:714:PHE:O	1:A:718:VAL:HG23	2.02	0.58
1:A:780:VAL:CG2	1:A:789:LYS:HE2	2.34	0.58
1:A:1438:THR:HG22	6:F:92:ARG:HB2	1.85	0.58
2:B:266:ALA:O	2:B:268:THR:HG22	2.03	0.58
2:B:284:ILE:CD1	2:B:333:PHE:HD2	2.16	0.58
2:B:533:CYS:O	2:B:535:LEU:N	2.36	0.58
5:E:93:MET:O	5:E:97:VAL:HG12	2.03	0.58
6:F:83:PRO:HA	6:F:146:TRP:CZ3	2.39	0.58
9:I:92:ARG:HG3	9:I:94:ASP:OD1	2.03	0.58
1:A:415:LEU:HD12	1:A:415:LEU:N	2.17	0.58
1:A:595:THR:HG22	1:A:603:ASN:CB	2.30	0.58
1:A:821:ARG:O	1:A:825:ILE:N	2.36	0.58
1:A:823:GLY:O	1:A:827:THR:HG23	2.03	0.58
1:A:1339:LEU:CD1	5:E:147:HIS:CD2	2.86	0.58
1:A:1364:ASN:O	1:A:1365:TYR:C	2.47	0.58
2:B:350:GLN:O	2:B:352:ALA:N	2.36	0.58
2:B:1060:ARG:HD3	2:B:1060:ARG:C	2.29	0.58
3:C:183:TRP:O	3:C:185:LYS:N	2.37	0.58
4:D:5:THR:HG23	7:G:42:PHE:CE2	2.38	0.58
6:F:114:GLU:O	6:F:120:ILE:HD11	2.04	0.58
7:G:34:VAL:HG11	7:G:74:TYR:CE2	2.39	0.58
7:G:51:TYR:C	7:G:51:TYR:CD1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:HD3	11:K:61:TYR:CD1	2.37	0.58
1:A:463:ILE:CD1	1:A:469:ARG:HD3	2.33	0.58
1:A:596:THR:CG2	1:A:597:LEU:N	2.66	0.58
2:B:308:TRP:CZ2	9:I:52:ILE:HD11	2.39	0.58
5:E:112:TYR:CD2	5:E:116:ILE:HD12	2.38	0.58
5:E:153:HIS:HB3	5:E:196:VAL:HG21	1.86	0.58
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.86	0.58
1:A:122:MET:HE2	1:A:122:MET:CA	2.34	0.58
1:A:886:ILE:HG23	1:A:887:GLY:H	1.68	0.58
2:B:221:ASN:N	2:B:241:ARG:O	2.33	0.58
2:B:632:ARG:CZ	2:B:632:ARG:HB2	2.34	0.58
2:B:973:ILE:HG22	2:B:974:PRO:CD	2.34	0.58
3:C:56:THR:HA	3:C:151:GLN:CD	2.28	0.58
6:F:143:PHE:O	6:F:143:PHE:HD1	1.87	0.58
7:G:96:GLN:HG2	7:G:121:PHE:CE2	2.38	0.58
7:G:106:MET:HE3	7:G:108:VAL:CG2	2.33	0.58
9:I:76:PRO:HD2	9:I:108:HIS:CE1	2.39	0.58
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.86	0.58
2:B:766:ARG:NH1	2:B:1020:ARG:HG2	2.19	0.58
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.86	0.58
3:C:68:GLY:CA	12:L:69:ALA:HB1	2.34	0.58
4:D:167:LEU:O	4:D:170:THR:HG23	2.03	0.58
7:G:102:GLN:NE2	7:G:107:LYS:HG2	2.18	0.58
1:A:276:LEU:HD22	1:A:293:GLU:HA	1.86	0.58
1:A:393:ARG:HB3	1:A:393:ARG:NH1	2.18	0.58
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.38	0.58
1:A:649:ILE:O	1:A:653:VAL:HG23	2.04	0.58
1:A:1427:ASN:O	1:A:1428:VAL:C	2.47	0.58
2:B:97:VAL:HA	2:B:127:GLY:O	2.03	0.58
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.34	0.58
2:B:757:PRO:HA	2:B:1044:ALA:HB1	1.85	0.58
3:C:238:ILE:HG13	3:C:239:PRO:HD2	1.85	0.58
1:A:10:PRO:HD2	2:B:1191:ILE:O	2.04	0.57
1:A:76:GLU:HB2	2:B:1159:ARG:HH22	1.68	0.57
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.85	0.57
2:B:34:ILE:HD13	2:B:747:MET:SD	2.44	0.57
2:B:50:SER:HG	2:B:410:GLY:H	1.52	0.57
2:B:242:SER:OG	2:B:362:PRO:HD2	2.04	0.57
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.85	0.57
2:B:639:ILE:CD1	2:B:688:GLY:O	2.52	0.57
2:B:780:VAL:HG21	10:J:56:LEU:HD13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:O	3:C:144:ILE:HD12	2.04	0.57
4:D:202:ILE:O	4:D:202:ILE:HG23	2.04	0.57
6:F:127:GLU:HB2	6:F:129:LYS:HG3	1.86	0.57
7:G:119:LEU:HD12	7:G:130:TYR:HB3	1.86	0.57
1:A:377:PRO:CD	1:A:493:GLN:HG3	2.34	0.57
1:A:997:LEU:HD22	1:A:1053:PHE:CG	2.39	0.57
1:A:1384:VAL:C	1:A:1385:THR:HG23	2.29	0.57
2:B:53:GLN:NE2	2:B:58:THR:HG23	2.20	0.57
2:B:872:GLU:O	2:B:873:THR:HB	2.03	0.57
2:B:1212:ILE:HG13	2:B:1212:ILE:O	2.04	0.57
7:G:13:LEU:HD11	7:G:26:LEU:CD2	2.34	0.57
12:L:32:ALA:HB2	12:L:55:ILE:HG21	1.85	0.57
1:A:412:ARG:O	1:A:413:ILE:HD13	2.04	0.57
1:A:455:MET:HE1	2:B:1134:GLU:CB	2.34	0.57
1:A:1091:SER:HA	1:A:1095:THR:OG1	2.04	0.57
2:B:180:TYR:O	2:B:183:GLU:HB3	2.04	0.57
2:B:1101:ASP:O	2:B:1122:ARG:CZ	2.52	0.57
5:E:192:ARG:HB3	5:E:215:MET:O	2.04	0.57
1:A:250:ILE:HD12	1:A:250:ILE:N	2.18	0.57
2:B:217:ARG:NH1	2:B:405:ARG:HB3	2.19	0.57
2:B:405:ARG:CZ	2:B:632:ARG:HG3	2.33	0.57
2:B:1020:ARG:NH1	17:B:2501:ATP:O3G	2.37	0.57
6:F:103:MET:HB3	7:G:14:HIS:CE1	2.39	0.57
9:I:85:PHE:CB	9:I:99:LEU:HD21	2.32	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.68	0.57
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.20	0.57
1:A:1342:GLU:HG3	5:E:198:ILE:HG12	1.86	0.57
2:B:190:TYR:O	2:B:193:LYS:N	2.37	0.57
2:B:203:PHE:N	2:B:203:PHE:CD1	2.73	0.57
2:B:287:ARG:O	2:B:327:ARG:HG3	2.04	0.57
2:B:701:ILE:HD12	2:B:703:ILE:HD11	1.87	0.57
2:B:1106:ARG:CZ	2:B:1126:GLY:HA2	2.35	0.57
2:B:1179:GLN:HG3	2:B:1188:LYS:NZ	2.18	0.57
3:C:5:GLY:O	3:C:7:GLN:HG3	2.03	0.57
4:D:192:LYS:NZ	4:D:199:ASN:O	2.29	0.57
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.86	0.57
6:F:105:ALA:HA	7:G:16:SER:HA	1.86	0.57
7:G:27:LYS:O	7:G:31:LEU:HG	2.05	0.57
1:A:450:LEU:C	1:A:450:LEU:HD12	2.30	0.57
1:A:946:VAL:HG13	5:E:201:LYS:CD	2.34	0.57
2:B:812:LEU:O	2:B:813:LYS:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HD12	2:B:851:PHE:H	1.69	0.57
2:B:1194:ILE:HD12	2:B:1196:ILE:HG21	1.85	0.57
3:C:169:LYS:C	3:C:171:GLY:H	2.12	0.57
5:E:117:THR:CB	5:E:118:PRO:HD2	2.34	0.57
1:A:41:MET:HG3	1:A:41:MET:O	2.04	0.57
1:A:331:GLY:O	1:A:332:LYS:HB2	2.04	0.57
1:A:590:ARG:NH1	1:A:621:THR:HG23	2.19	0.57
2:B:802:PRO:HG3	2:B:814:PHE:HE2	1.69	0.57
5:E:179:GLN:O	5:E:182:ASP:HB2	2.05	0.57
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.85	0.57
1:A:899:VAL:O	1:A:929:LEU:HD12	2.05	0.57
1:A:907:THR:HG22	1:A:908:LEU:N	2.18	0.57
1:A:1279:ILE:HG22	1:A:1279:ILE:O	2.03	0.57
2:B:247:GLY:C	2:B:418:LYS:NZ	2.63	0.57
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.87	0.57
11:K:85:ASP:O	11:K:88:LYS:HB3	2.05	0.57
1:A:567:LYS:O	1:A:569:LYS:N	2.38	0.57
1:A:693:VAL:O	1:A:693:VAL:CG2	2.52	0.57
1:A:741:ASN:OD1	1:A:742:ASN:N	2.38	0.57
1:A:789:LYS:HG2	1:A:790:ASP:N	2.20	0.57
1:A:1400:CYS:SG	1:A:1409:LEU:HD11	2.45	0.57
1:A:1427:ASN:O	1:A:1430:LEU:N	2.37	0.57
2:B:20:ASP:OD1	2:B:20:ASP:N	2.36	0.57
2:B:34:ILE:O	2:B:37:PHE:N	2.37	0.57
2:B:875:GLU:CG	2:B:876:LYS:H	2.17	0.57
3:C:39:ALA:HB1	3:C:164:ALA:HB3	1.86	0.57
3:C:73:GLN:N	3:C:131:HIS:O	2.35	0.57
4:D:48:ILE:HG21	7:G:4:ILE:CG1	2.34	0.57
7:G:112:LYS:C	7:G:112:LYS:HD3	2.29	0.57
10:J:37:SER:HG	10:J:47:ARG:HH21	1.49	0.57
10:J:53:HIS:CD2	10:J:54:VAL:N	2.73	0.57
1:A:139:TRP:O	1:A:140:THR:C	2.47	0.57
1:A:354:SER:HB2	1:A:469:ARG:NH1	2.19	0.57
1:A:455:MET:CE	2:B:1134:GLU:HG2	2.35	0.57
1:A:586:ILE:HD12	1:A:633:VAL:HG12	1.87	0.57
1:A:690:VAL:O	1:A:690:VAL:HG12	2.05	0.57
1:A:1148:ILE:HG22	1:A:1196:GLU:HG2	1.87	0.57
1:A:1195:LEU:HD23	1:A:1267:MET:HE1	1.86	0.57
3:C:164:ALA:HA	3:C:167:HIS:O	2.04	0.57
4:D:52:LEU:HD22	4:D:148:LEU:HD23	1.87	0.57
4:D:55:ALA:O	4:D:58:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:66:PRO:O	9:I:67:THR:C	2.45	0.57
13:R:1:A:H62	14:T:27:DA:H62	1.50	0.57
1:A:44:THR:HG22	1:A:44:THR:O	2.05	0.56
1:A:82:GLY:C	1:A:241:VAL:HG23	2.30	0.56
1:A:286:HIS:O	1:A:290:GLU:HG3	2.05	0.56
1:A:424:ILE:O	1:A:424:ILE:HG23	2.04	0.56
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.39	0.56
1:A:607:ILE:HG13	1:A:607:ILE:O	2.03	0.56
1:A:1141:THR:HG23	1:A:1205:LYS:HZ2	1.70	0.56
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.87	0.56
1:A:1371:LEU:O	1:A:1374:VAL:HB	2.05	0.56
1:A:1447:GLU:HA	1:A:1450:LEU:HB3	1.87	0.56
2:B:222:ILE:CG2	2:B:223:VAL:N	2.68	0.56
2:B:525:ALA:O	2:B:768:THR:HG23	2.05	0.56
2:B:616:ILE:HD12	2:B:697:GLU:HA	1.87	0.56
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.87	0.56
8:H:93:TYR:H	8:H:93:TYR:HD1	1.53	0.56
1:A:40:THR:CG2	1:A:259:GLU:HG3	2.35	0.56
1:A:1141:THR:HG23	1:A:1205:LYS:HD2	1.86	0.56
2:B:313:MET:C	2:B:315:LYS:H	2.13	0.56
3:C:52:GLU:O	3:C:53:THR:HG23	2.06	0.56
4:D:134:THR:HG23	4:D:134:THR:O	2.05	0.56
13:R:10:G:O6	14:T:19:DC:N4	2.38	0.56
1:A:103:CYS:O	1:A:108:MET:HE1	2.04	0.56
1:A:362:ASP:OD1	1:A:362:ASP:N	2.24	0.56
1:A:910:PRO:C	1:A:912:LEU:N	2.64	0.56
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.06	0.56
2:B:529:GLU:OE1	2:B:769:TYR:CE1	2.58	0.56
2:B:642:ASP:OD1	2:B:642:ASP:N	2.37	0.56
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.56
3:C:99:LEU:HD21	3:C:120:ILE:HG12	1.86	0.56
3:C:107:SER:HB3	3:C:111:THR:HB	1.86	0.56
3:C:166:GLU:O	11:K:6:ARG:HD3	2.04	0.56
4:D:59:ILE:HD12	4:D:59:ILE:N	2.19	0.56
8:H:40:LEU:HD13	8:H:123:MET:SD	2.46	0.56
9:I:14:LEU:HD22	9:I:29:CYS:HB2	1.87	0.56
10:J:13:VAL:HG23	10:J:13:VAL:O	2.05	0.56
10:J:51:LEU:HD23	10:J:51:LEU:O	2.05	0.56
1:A:225:ASN:OD1	1:A:228:PHE:N	2.35	0.56
1:A:512:VAL:HA	1:A:519:PRO:HA	1.85	0.56
1:A:537:ARG:HG3	8:H:20:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:GLN:O	1:A:1011:GLN:HB3	2.06	0.56
1:A:1259:MET:O	1:A:1262:LYS:HB2	2.05	0.56
1:A:1402:PHE:CD1	1:A:1403:GLU:N	2.67	0.56
2:B:840:ILE:HG12	2:B:1011:ILE:HB	1.87	0.56
11:K:40:HIS:CE1	11:K:63:VAL:HG21	2.39	0.56
13:R:1:A:N6	14:T:27:DA:H62	2.04	0.56
1:A:23:SER:O	1:A:27:VAL:HG23	2.06	0.56
1:A:452:LYS:HG3	2:B:1140:ALA:CB	2.36	0.56
1:A:456:MET:HE1	1:A:477:PRO:HB2	1.88	0.56
1:A:775:ILE:CG1	1:A:797:LYS:HA	2.35	0.56
1:A:839:ARG:HH22	1:A:1402:PHE:HA	1.70	0.56
1:A:846:GLU:O	1:A:848:ILE:N	2.38	0.56
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.88	0.56
1:A:1195:LEU:CD1	1:A:1238:ILE:HD13	2.36	0.56
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.56
1:A:1345:ARG:NH1	1:A:1373:ASP:OD2	2.39	0.56
2:B:299:GLU:OE1	2:B:570:VAL:CG1	2.53	0.56
2:B:363:HIS:O	2:B:585:VAL:HG22	2.06	0.56
2:B:1189:ILE:CG1	2:B:1190:ASP:N	2.69	0.56
4:D:5:THR:HG23	7:G:42:PHE:HE2	1.70	0.56
1:A:642:CYS:O	1:A:645:LEU:HB3	2.06	0.56
1:A:783:THR:HG21	1:A:796:SER:OG	2.05	0.56
1:A:914:GLU:O	1:A:916:GLY:N	2.39	0.56
2:B:123:THR:HG22	2:B:205:ILE:HG23	1.88	0.56
2:B:283:VAL:HG23	2:B:284:ILE:N	2.20	0.56
2:B:752:ALA:O	2:B:754:SER:N	2.38	0.56
2:B:824:ILE:O	2:B:1009:ASP:HB2	2.04	0.56
3:C:138:GLU:OE1	3:C:140:ASN:ND2	2.38	0.56
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.45	0.56
5:E:63:ASN:CB	5:E:64:PRO:CD	2.83	0.56
7:G:106:MET:HG3	7:G:157:ILE:O	2.05	0.56
1:A:987:VAL:HG13	1:A:1028:THR:OG1	2.05	0.56
1:A:1042:PHE:CE2	1:A:1046:LEU:HD13	2.40	0.56
1:A:1302:PRO:O	1:A:1303:GLU:HB3	2.05	0.56
1:A:1330:ASN:O	1:A:1332:PHE:N	2.38	0.56
2:B:1027:ILE:CD1	2:B:1052:VAL:HG22	2.36	0.56
2:B:1125:ASP:O	2:B:1125:ASP:CG	2.48	0.56
5:E:39:LEU:HA	5:E:42:PHE:HB3	1.86	0.56
7:G:3:PHE:HB2	7:G:78:VAL:CG2	2.36	0.56
13:R:9:G:H1	14:T:20:DC:H42	1.54	0.56
1:A:618:GLU:OE2	1:A:620:LYS:CE	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.06	0.56
1:A:1053:PHE:O	1:A:1056:SER:N	2.38	0.56
2:B:385:LEU:HD23	2:B:385:LEU:C	2.31	0.56
2:B:1055:ILE:O	2:B:1058:LEU:HD12	2.05	0.56
8:H:63:LEU:C	8:H:63:LEU:HD12	2.30	0.56
1:A:262:LEU:HD21	1:A:325:ILE:HG12	1.88	0.56
1:A:314:ALA:O	1:A:322:VAL:HG12	2.05	0.56
1:A:507:VAL:N	1:A:508:PRO:HD3	2.20	0.56
1:A:845:LEU:CD2	1:A:848:ILE:HD12	2.35	0.56
1:A:1132:LYS:HG3	1:A:1284:MET:HE1	1.88	0.56
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.87	0.56
2:B:792:MET:O	2:B:793:ALA:HB2	2.05	0.56
4:D:119:ARG:HG3	4:D:121:LYS:H	1.70	0.56
5:E:75:MET:O	5:E:75:MET:HG2	2.05	0.56
9:I:83:ASN:CB	9:I:103:CYS:HA	2.36	0.56
1:A:29:ALA:C	1:A:31:SER:H	2.13	0.56
1:A:181:LEU:O	1:A:202:LEU:N	2.37	0.56
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.39	0.56
1:A:998:LEU:HD13	1:A:1001:ARG:CG	2.35	0.56
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.88	0.56
2:B:43:LEU:O	2:B:496:ARG:NH1	2.39	0.56
2:B:302:CYS:SG	2:B:310:MET:CE	2.94	0.56
2:B:766:ARG:HG2	2:B:1022:THR:CG2	2.36	0.56
2:B:950:ASP:OD1	2:B:969:ARG:HD3	2.06	0.56
2:B:1027:ILE:HD13	2:B:1052:VAL:HG22	1.88	0.56
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.36	0.56
3:C:99:LEU:CD2	3:C:120:ILE:HG12	2.36	0.56
3:C:124:LEU:HD11	3:C:127:ARG:O	2.06	0.56
4:D:29:LEU:HD23	4:D:33:PHE:HB3	1.87	0.56
5:E:94:LYS:HA	5:E:97:VAL:HG12	1.87	0.56
6:F:79:ARG:HD2	6:F:146:TRP:CZ2	2.40	0.56
8:H:56:THR:OG1	8:H:146:ARG:NH2	2.39	0.56
8:H:143:LEU:O	8:H:144:ILE:HD13	2.06	0.56
10:J:45:CYS:O	10:J:48:ARG:NE	2.35	0.56
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.46	0.55
1:A:80:HIS:O	1:A:243:PRO:HB3	2.05	0.55
1:A:896:ARG:NH1	1:A:1034:GLU:OE2	2.40	0.55
2:B:520:GLY:HA2	2:B:748:ILE:HG22	1.88	0.55
2:B:843:GLN:HB2	2:B:993:THR:HB	1.88	0.55
2:B:1106:ARG:HD2	2:B:1126:GLY:O	2.05	0.55
2:B:1176:ASN:O	2:B:1177:HIS:ND1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PHE:HD2	4:D:38:ILE:CD1	2.19	0.55
7:G:135:ASP:O	7:G:136:VAL:HG23	2.06	0.55
8:H:93:TYR:CD1	8:H:93:TYR:N	2.74	0.55
10:J:6:ARG:HA	10:J:14:VAL:N	2.21	0.55
1:A:131:SER:OG	1:A:132:LYS:N	2.39	0.55
1:A:1332:PHE:CD1	1:A:1381:LEU:HD21	2.41	0.55
1:A:1336:MET:SD	1:A:1336:MET:C	2.89	0.55
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.87	0.55
1:A:1402:PHE:CE1	1:A:1403:GLU:HG2	2.40	0.55
2:B:247:GLY:CA	2:B:418:LYS:HZ2	2.14	0.55
2:B:1046:PRO:O	2:B:1048:THR:HG23	2.06	0.55
6:F:152:ILE:CG2	6:F:153:VAL:N	2.69	0.55
7:G:47:CYS:HB3	7:G:77:VAL:HG12	1.88	0.55
10:J:5:VAL:O	10:J:6:ARG:HG2	2.06	0.55
12:L:46:VAL:C	12:L:47:ARG:HG2	2.32	0.55
1:A:49:LYS:HE2	1:A:61:ILE:CG2	2.36	0.55
1:A:610:GLY:C	1:A:611:GLN:HG2	2.32	0.55
2:B:552:MET:HA	2:B:555:ILE:CG1	2.37	0.55
8:H:8:ASP:OD1	8:H:30:SER:OG	2.22	0.55
11:K:57:LEU:HD13	11:K:76:GLN:HE21	1.71	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.54	0.55
1:A:107:CYS:HA	1:A:171:GLN:OE1	2.06	0.55
1:A:199:LEU:HD23	1:A:199:LEU:O	2.06	0.55
1:A:330:LYS:HG2	1:A:331:GLY:N	2.20	0.55
1:A:747:VAL:HG13	1:A:753:GLY:O	2.07	0.55
1:A:756:ILE:HG21	1:A:1086:PHE:HE2	1.70	0.55
2:B:211:VAL:HG12	2:B:212:LEU:H	1.72	0.55
3:C:14:SER:HA	11:K:114:LEU:HD12	1.88	0.55
3:C:49:VAL:N	12:L:66:GLN:OE1	2.39	0.55
7:G:44:TYR:HE2	7:G:106:MET:HB2	1.72	0.55
9:I:19:ASP:HB2	9:I:24:ARG:HG3	1.86	0.55
1:A:341:MET:HE2	1:A:1429:ILE:HD11	1.87	0.55
1:A:617:VAL:HG13	1:A:622:VAL:HB	1.89	0.55
1:A:692:ASP:C	1:A:694:THR:H	2.15	0.55
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.06	0.55
1:A:1339:LEU:CD1	5:E:147:HIS:HD2	2.19	0.55
2:B:97:VAL:CG2	2:B:128:LEU:HD23	2.37	0.55
2:B:283:VAL:HG21	2:B:321:GLY:CA	2.36	0.55
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.42	0.55
3:C:178:PHE:HD1	3:C:179:GLU:N	2.04	0.55
6:F:152:ILE:O	6:F:153:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.87	0.55
7:G:120:THR:O	7:G:120:THR:HG23	2.07	0.55
8:H:9:ILE:HG13	8:H:56:THR:HA	1.87	0.55
1:A:98:LYS:HA	1:A:101:LYS:HB2	1.87	0.55
1:A:265:LYS:O	1:A:269:ILE:HG13	2.07	0.55
1:A:340:LEU:C	1:A:342:GLY:N	2.61	0.55
1:A:899:VAL:HG11	1:A:908:LEU:CG	2.37	0.55
1:A:1037:LEU:HD23	1:A:1042:PHE:CB	2.35	0.55
2:B:217:ARG:CZ	2:B:405:ARG:HB2	2.37	0.55
2:B:272:THR:C	2:B:273:LEU:HD22	2.32	0.55
2:B:1072:MET:HG3	2:B:1085:ILE:HD12	1.89	0.55
5:E:150:VAL:HG13	5:E:150:VAL:O	2.07	0.55
5:E:178:ILE:HG22	5:E:213:ILE:O	2.06	0.55
1:A:147:VAL:HA	1:A:170:THR:HA	1.88	0.55
1:A:447:GLN:HG2	14:T:20:DC:H1'	1.88	0.55
1:A:1097:GLY:H	1:A:1099:PRO:HD2	1.71	0.55
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.36	0.55
2:B:590:HIS:CG	2:B:591:ARG:N	2.75	0.55
2:B:995:ARG:HH12	11:K:9:LEU:HD11	1.72	0.55
3:C:179:GLU:HG2	3:C:180:TYR:H	1.72	0.55
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.88	0.55
5:E:119:SER:HA	5:E:122:LYS:HE3	1.87	0.55
6:F:133:VAL:HG21	7:G:58:ARG:NH1	2.22	0.55
9:I:34:TYR:CD1	9:I:35:VAL:N	2.75	0.55
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.89	0.55
1:A:44:THR:C	1:A:46:THR:H	2.14	0.55
1:A:139:TRP:O	1:A:141:LEU:N	2.39	0.55
1:A:564:ALA:O	1:A:565:ILE:HD13	2.06	0.55
1:A:642:CYS:O	1:A:645:LEU:N	2.40	0.55
1:A:666:ILE:C	1:A:666:ILE:CD1	2.75	0.55
1:A:845:LEU:HD23	1:A:848:ILE:HD12	1.89	0.55
2:B:210:LYS:HG3	2:B:482:VAL:HG12	1.89	0.55
2:B:617:ARG:HB2	2:B:624:LEU:HD13	1.88	0.55
2:B:1037:LEU:HD22	2:B:1062:HIS:HB3	1.89	0.55
4:D:155:ARG:H	4:D:219:THR:HG21	1.72	0.55
9:I:65:ASP:CG	9:I:67:THR:HG1	2.14	0.55
1:A:172:PRO:HG2	1:A:174:ILE:HG13	1.89	0.55
1:A:690:VAL:HG21	1:A:718:VAL:HG13	1.87	0.55
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.88	0.55
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.06	0.55
1:A:1344:GLY:O	1:A:1345:ARG:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ILE:HA	2:B:740:HIS:O	2.05	0.55
8:H:135:LEU:HD11	8:H:137:GLN:HG2	1.88	0.55
1:A:108:MET:HA	1:A:210:ILE:HG21	1.89	0.55
1:A:118:HIS:O	1:A:119:ASN:HB2	2.06	0.55
1:A:344:ARG:NH1	14:T:21:DC:OP1	2.40	0.55
1:A:379:VAL:HG12	1:A:380:VAL:H	1.72	0.55
1:A:380:VAL:HG12	1:A:428:TYR:HD1	1.71	0.55
2:B:53:GLN:HE22	2:B:58:THR:CG2	2.20	0.55
2:B:510:LYS:N	2:B:513:GLN:OE1	2.40	0.55
2:B:522:VAL:CG1	2:B:523:CYS:N	2.70	0.55
2:B:1142:GLY:O	2:B:1144:ALA:N	2.40	0.55
8:H:16:ASP:OD1	8:H:17:PRO:N	2.40	0.55
8:H:96:VAL:HG12	8:H:97:MET:H	1.72	0.55
9:I:6:PHE:HA	9:I:14:LEU:HG	1.88	0.55
1:A:1267:MET:HA	1:A:1271:ILE:CG1	2.36	0.54
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.88	0.54
1:A:1445:ILE:HD11	7:G:70:PHE:CE1	2.42	0.54
2:B:203:PHE:CD2	2:B:461:LEU:HD11	2.42	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.07	0.54
2:B:1103:ILE:HG13	2:B:1104:HIS:H	1.72	0.54
4:D:202:ILE:HD13	4:D:207:LEU:CD1	2.38	0.54
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.42	0.54
5:E:96:PHE:CD1	5:E:96:PHE:C	2.86	0.54
9:I:75:CYS:O	9:I:79:HIS:ND1	2.40	0.54
11:K:12:LEU:HD21	11:K:18:LYS:CG	2.37	0.54
1:A:105:CYS:SG	1:A:139:TRP:HA	2.48	0.54
1:A:122:MET:HG3	1:A:126:LEU:HD13	1.88	0.54
1:A:219:PHE:H	1:A:219:PHE:HD1	1.51	0.54
1:A:359:LEU:CD2	1:A:363:GLN:HG3	2.38	0.54
1:A:909:ASP:C	1:A:909:ASP:OD1	2.50	0.54
1:A:1447:GLU:OE1	7:G:23:LYS:HD2	2.06	0.54
2:B:378:LEU:O	2:B:382:ILE:HG13	2.08	0.54
2:B:745:PRO:O	2:B:748:ILE:HG12	2.06	0.54
3:C:82:TYR:O	3:C:83:SER:C	2.50	0.54
3:C:153:LEU:CD1	3:C:155:LEU:HD23	2.38	0.54
5:E:200:ARG:HG3	5:E:201:LYS:O	2.07	0.54
9:I:26:LEU:HD23	9:I:26:LEU:H	1.73	0.54
11:K:55:LYS:HB3	11:K:78:THR:OG1	2.07	0.54
11:K:57:LEU:HD13	11:K:76:GLN:NE2	2.23	0.54
1:A:392:VAL:O	1:A:394:ASN:N	2.40	0.54
1:A:863:VAL:HG12	1:A:865:GLN:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:HD23	1:A:952:ALA:O	2.08	0.54
1:A:1080:THR:HG23	1:A:1080:THR:O	2.05	0.54
1:A:1116:LEU:HD21	1:A:1313:LEU:HB2	1.88	0.54
1:A:1120:LEU:HB2	1:A:1125:ALA:HB1	1.88	0.54
2:B:197:PHE:CD2	2:B:817:LEU:HD11	2.42	0.54
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.25	0.54
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.06	0.54
2:B:753:ALA:C	2:B:755:ILE:H	2.16	0.54
3:C:9:LYS:HA	11:K:108:GLU:HG3	1.89	0.54
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.54
7:G:1:MET:CG	7:G:2:PHE:H	2.13	0.54
12:L:28:LYS:HE2	12:L:41:SER:HA	1.88	0.54
1:A:83:HIS:N	1:A:241:VAL:CG2	2.70	0.54
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.89	0.54
1:A:1152:ILE:HD12	9:I:44:TYR:HB3	1.88	0.54
2:B:179:CYS:SG	2:B:181:LEU:N	2.79	0.54
2:B:254:LEU:HD11	2:B:360:PHE:CE1	2.41	0.54
2:B:492:LEU:HA	2:B:495:LEU:HD12	1.89	0.54
2:B:789:MET:HB2	2:B:967:ARG:HD3	1.89	0.54
5:E:6:GLU:HA	5:E:9:ILE:HB	1.90	0.54
6:F:97:ARG:HG3	6:F:101:ILE:HD12	1.89	0.54
12:L:32:ALA:O	12:L:34:CYS:N	2.40	0.54
1:A:450:LEU:HD22	1:A:1074:GLU:HA	1.89	0.54
1:A:827:THR:O	1:A:831:THR:HB	2.07	0.54
1:A:1138:ILE:C	1:A:1140:HIS:H	2.15	0.54
1:A:1143:LEU:CD1	1:A:1147:THR:CG2	2.85	0.54
1:A:1194:ARG:O	1:A:1194:ARG:HG2	2.06	0.54
2:B:368:GLU:O	2:B:370:PHE:N	2.40	0.54
2:B:976:ILE:HD11	2:B:993:THR:N	2.21	0.54
2:B:1202:LEU:O	2:B:1203:LEU:C	2.50	0.54
3:C:162:GLY:O	3:C:170:TRP:HB3	2.07	0.54
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.43	0.54
3:C:189:THR:HG23	3:C:189:THR:O	2.07	0.54
4:D:5:THR:O	7:G:42:PHE:CE2	2.61	0.54
4:D:138:ASN:OD1	4:D:141:LEU:CB	2.55	0.54
7:G:157:ILE:O	7:G:157:ILE:HG23	2.07	0.54
8:H:18:GLY:C	8:H:20:TYR:H	2.16	0.54
9:I:75:CYS:SG	9:I:108:HIS:HE1	2.31	0.54
1:A:167:CYS:SG	1:A:168:GLY:N	2.79	0.54
1:A:924:LYS:O	1:A:927:VAL:CG1	2.55	0.54
1:A:1378:GLN:HG3	1:A:1378:GLN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:VAL:HG23	1:A:1436:ILE:HD11	1.89	0.54
2:B:213:ILE:HD12	2:B:499:ASN:HB2	1.89	0.54
2:B:247:GLY:CA	2:B:418:LYS:HZ1	2.21	0.54
2:B:247:GLY:C	2:B:418:LYS:HZ1	2.14	0.54
2:B:453:ILE:HD12	2:B:453:ILE:H	1.72	0.54
4:D:211:LEU:O	4:D:215:SER:OG	2.26	0.54
9:I:7:CYS:SG	9:I:8:ARG:N	2.79	0.54
1:A:174:ILE:HA	1:A:182:VAL:O	2.08	0.54
1:A:226:GLU:CG	1:A:226:GLU:O	2.56	0.54
1:A:889:SER:OG	1:A:891:ALA:CB	2.55	0.54
1:A:1339:LEU:CD2	5:E:147:HIS:CD2	2.91	0.54
2:B:1209:ALA:C	2:B:1211:ASN:H	2.16	0.54
6:F:109:VAL:CG1	6:F:123:LYS:HD3	2.37	0.54
9:I:6:PHE:HD1	9:I:13:MET:HA	1.71	0.54
11:K:18:LYS:NZ	11:K:36:GLU:O	2.40	0.54
1:A:56:PRO:O	1:A:57:ARG:HB2	2.07	0.54
1:A:415:LEU:O	1:A:417:TYR:N	2.40	0.54
1:A:446:ARG:CD	1:A:448:PRO:HD2	2.37	0.54
1:A:455:MET:HE1	2:B:1134:GLU:CG	2.38	0.54
2:B:37:PHE:CD2	2:B:542:MET:HG2	2.42	0.54
7:G:40:GLY:O	7:G:80:LYS:NZ	2.40	0.54
7:G:80:LYS:CD	7:G:82:PHE:CE1	2.90	0.54
1:A:88:LYS:O	1:A:90:VAL:HG13	2.08	0.54
1:A:121:LEU:HB3	1:A:141:LEU:CD1	2.38	0.54
1:A:629:LEU:HD12	1:A:629:LEU:O	2.08	0.54
1:A:775:ILE:HG13	1:A:797:LYS:HG2	1.90	0.54
1:A:825:ILE:HD13	2:B:512:ARG:HB2	1.90	0.54
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.88	0.54
1:A:1363:VAL:CG1	1:A:1364:ASN:N	2.71	0.54
2:B:420:LEU:C	2:B:422:LYS:N	2.65	0.54
2:B:533:CYS:C	2:B:535:LEU:H	2.16	0.54
4:D:119:ARG:HG3	4:D:121:LYS:N	2.23	0.54
5:E:171:LYS:HE2	5:E:172:GLU:HB2	1.89	0.54
8:H:18:GLY:O	8:H:20:TYR:HD1	1.91	0.54
9:I:19:ASP:CB	9:I:24:ARG:CG	2.86	0.54
11:K:31:VAL:O	11:K:74:ARG:HA	2.08	0.54
2:B:285:ILE:O	2:B:289:LEU:HG	2.08	0.54
2:B:655:LYS:HA	2:B:658:ILE:HB	1.90	0.54
4:D:63:LEU:HD22	4:D:133:THR:OG1	2.07	0.54
11:K:114:LEU:HD13	11:K:115:ALA:N	2.22	0.54
1:A:354:SER:O	1:A:469:ARG:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:THR:CG2	1:A:1205:LYS:CD	2.86	0.53
1:A:1146:VAL:HG22	1:A:1201:ALA:HB1	1.90	0.53
1:A:1161:THR:O	1:A:1162:VAL:C	2.50	0.53
1:A:1398:MET:HE3	1:A:1423:GLY:HA3	1.91	0.53
2:B:128:LEU:CB	2:B:167:ILE:HB	2.39	0.53
2:B:211:VAL:HG12	2:B:212:LEU:N	2.23	0.53
2:B:684:LEU:C	2:B:690:VAL:HG22	2.32	0.53
2:B:769:TYR:O	2:B:770:GLN:C	2.50	0.53
2:B:874:PHE:CE1	2:B:914:LYS:HB2	2.43	0.53
2:B:1134:GLU:O	2:B:1135:ARG:C	2.51	0.53
3:C:21:ILE:HD12	3:C:21:ILE:C	2.33	0.53
4:D:8:PHE:CE1	7:G:6:ASP:O	2.61	0.53
7:G:16:SER:O	7:G:17:PHE:CD1	2.61	0.53
12:L:29:TYR:O	12:L:38:LEU:HB3	2.07	0.53
1:A:49:LYS:CE	1:A:61:ILE:HG22	2.38	0.53
1:A:83:HIS:HA	1:A:239:LEU:O	2.07	0.53
1:A:519:PRO:HG3	1:A:631:HIS:HB2	1.91	0.53
1:A:525:GLN:HB3	2:B:1015:HIS:CD2	2.43	0.53
1:A:670:ILE:HG22	1:A:805:LEU:HD11	1.90	0.53
1:A:825:ILE:HG23	1:A:829:VAL:HG21	1.89	0.53
1:A:948:VAL:C	1:A:950:GLY:H	2.17	0.53
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.74	0.53
2:B:23:ALA:O	2:B:654:ARG:HB3	2.08	0.53
2:B:332:ASP:OD1	2:B:332:ASP:O	2.25	0.53
2:B:890:TYR:O	2:B:892:LYS:N	2.41	0.53
2:B:944:THR:OG1	2:B:945:GLU:HG3	2.08	0.53
2:B:1127:GLY:C	2:B:1128:LEU:HD23	2.33	0.53
7:G:154:VAL:HG13	7:G:155:SER:N	2.23	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HG	2.42	0.53
1:A:92:HIS:HB2	1:A:236:LEU:CD1	2.37	0.53
1:A:670:ILE:HG13	1:A:670:ILE:O	2.09	0.53
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.09	0.53
1:A:834:PRO:HA	1:A:837:ILE:HG12	1.90	0.53
1:A:858:ASN:OD1	1:A:860:LEU:N	2.40	0.53
2:B:859:TYR:HB2	2:B:966:VAL:CG2	2.38	0.53
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.90	0.53
4:D:179:GLN:HB3	4:D:195:ILE:HD11	1.91	0.53
10:J:46:CYS:O	10:J:49:MET:HB2	2.08	0.53
1:A:337:ARG:HD2	1:A:839:ARG:NH1	2.23	0.53
1:A:344:ARG:O	2:B:1155:SER:HB3	2.07	0.53
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:C	1:A:404:TYR:CD1	2.86	0.53
1:A:504:LEU:CD2	6:F:88:TYR:HE1	2.21	0.53
1:A:523:ILE:N	1:A:523:ILE:CD1	2.71	0.53
1:A:843:LYS:HD2	2:B:1135:ARG:HH22	1.73	0.53
1:A:1107:VAL:HG12	1:A:1108:ALA:N	2.24	0.53
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.90	0.53
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.39	0.53
9:I:65:ASP:O	9:I:66:PRO:C	2.52	0.53
11:K:44:ASN:HA	11:K:61:TYR:CE1	2.43	0.53
1:A:5:GLN:CD	2:B:1175:LEU:HD11	2.34	0.53
1:A:106:VAL:HG22	1:A:107:CYS:N	2.23	0.53
1:A:231:PRO:O	1:A:233:TRP:N	2.42	0.53
1:A:504:LEU:CD2	6:F:88:TYR:CE1	2.91	0.53
1:A:528:LEU:O	1:A:531:ILE:HG22	2.09	0.53
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.73	0.53
2:B:132:VAL:HG11	2:B:165:VAL:HG11	1.91	0.53
2:B:604:ARG:O	2:B:607:GLY:N	2.42	0.53
2:B:635:ARG:NH2	2:B:742:GLU:OE1	2.40	0.53
2:B:875:GLU:HG2	2:B:876:LYS:N	2.24	0.53
2:B:890:TYR:O	2:B:893:LEU:HG	2.09	0.53
4:D:48:ILE:HG21	7:G:4:ILE:CD1	2.38	0.53
4:D:57:LEU:C	4:D:57:LEU:HD23	2.33	0.53
4:D:138:ASN:OD1	4:D:138:ASN:O	2.26	0.53
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.89	0.53
12:L:53:HIS:O	12:L:55:ILE:N	2.41	0.53
1:A:149:GLU:HB2	1:A:164:ARG:NE	2.23	0.53
1:A:1239:ARG:NH1	1:A:1239:ARG:HG2	2.23	0.53
2:B:855:PHE:HB3	2:B:970:THR:CG2	2.37	0.53
4:D:194:LEU:HD22	7:G:86:VAL:HG21	1.90	0.53
5:E:177:ARG:HG2	5:E:213:ILE:HG22	1.90	0.53
1:A:19:PHE:HE1	2:B:1214:PRO:HB3	1.74	0.53
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.73	0.53
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.39	0.53
1:A:681:GLU:O	1:A:685:GLU:N	2.36	0.53
1:A:837:ILE:O	1:A:841:LEU:HG	2.08	0.53
1:A:837:ILE:HD11	1:A:1102:LYS:HD2	1.90	0.53
1:A:878:ILE:CD1	1:A:1366:ARG:HH22	2.21	0.53
1:A:1055:ARG:HE	6:F:154:ASP:CG	2.16	0.53
1:A:1128:GLN:HG3	1:A:1304:TRP:CE2	2.44	0.53
2:B:354:ASP:HB3	2:B:358:LYS:CE	2.37	0.53
2:B:431:TYR:CE1	2:B:447:ALA:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:759:PRO:CB	2:B:767:ASN:HD21	2.21	0.53
3:C:249:ASP:O	3:C:253:LYS:HG2	2.09	0.53
4:D:52:LEU:O	4:D:148:LEU:HD22	2.08	0.53
9:I:83:ASN:HB2	9:I:103:CYS:HA	1.91	0.53
10:J:60:PHE:O	10:J:63:TYR:HD1	1.91	0.53
1:A:46:THR:HG22	1:A:48:ALA:H	1.73	0.53
1:A:344:ARG:NH2	2:B:1120:GLU:HG3	2.23	0.53
1:A:858:ASN:OD1	1:A:858:ASN:C	2.48	0.53
1:A:1065:GLY:C	1:A:1067:LEU:H	2.16	0.53
1:A:1105:LEU:CD2	1:A:1384:VAL:HG21	2.36	0.53
2:B:165:VAL:HG21	2:B:446:LEU:HD12	1.90	0.53
2:B:487:THR:HG22	2:B:488:TYR:N	2.23	0.53
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.23	0.53
2:B:1058:LEU:O	2:B:1061:GLU:HG2	2.08	0.53
3:C:183:TRP:CD1	3:C:183:TRP:H	2.24	0.53
6:F:90:ARG:O	6:F:93:ILE:N	2.42	0.53
9:I:84:VAL:HG22	9:I:85:PHE:H	1.74	0.53
11:K:103:THR:O	11:K:107:THR:HG23	2.08	0.53
1:A:43:GLU:HB3	1:A:50:ILE:HD13	1.91	0.53
1:A:526:ASP:HB2	2:B:835:GLN:HE22	1.74	0.53
1:A:642:CYS:O	1:A:643:ALA:C	2.52	0.53
1:A:862:ASN:CG	5:E:174:GLN:HA	2.33	0.53
1:A:1450:LEU:HD11	7:G:19:GLY:CA	2.38	0.53
2:B:349:ILE:HG22	2:B:349:ILE:O	2.09	0.53
2:B:872:GLU:OE1	2:B:914:LYS:HD2	2.09	0.53
5:E:196:VAL:HG13	5:E:198:ILE:HD12	1.90	0.53
8:H:125:LEU:HD11	8:H:130:ARG:NH1	2.24	0.53
9:I:14:LEU:HD22	9:I:28:GLU:O	2.08	0.53
14:T:25:DC:H2"	14:T:26:DG:H8	1.73	0.53
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.90	0.53
1:A:453:MET:N	1:A:453:MET:SD	2.82	0.53
1:A:534:LEU:O	1:A:539:THR:HG21	2.08	0.53
1:A:671:ALA:C	1:A:673:GLY:H	2.16	0.53
1:A:715:GLU:CD	1:A:774:ARG:HH11	2.15	0.53
1:A:853:ASP:O	1:A:854:ASN:HB2	2.07	0.53
1:A:1013:ASP:OD1	5:E:207:ARG:HD2	2.09	0.53
1:A:1405:THR:O	1:A:1409:LEU:HD12	2.09	0.53
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.56	0.53
2:B:27:ALA:O	2:B:29:ASP:N	2.42	0.53
2:B:53:GLN:HG3	2:B:547:VAL:HG11	1.90	0.53
2:B:465:ASN:HA	2:B:477:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:HIS:CG	2:B:591:ARG:H	2.27	0.53
6:F:143:PHE:O	6:F:143:PHE:CD1	2.62	0.53
7:G:22:MET:HG2	7:G:26:LEU:CD1	2.39	0.53
11:K:55:LYS:HB3	11:K:78:THR:CG2	2.39	0.53
1:A:299:HIS:HA	1:A:302:THR:CG2	2.39	0.52
1:A:722:LEU:O	1:A:725:ALA:HB3	2.09	0.52
1:A:896:ARG:HD2	1:A:897:TYR:CE2	2.44	0.52
1:A:1014:ALA:HA	5:E:205:SER:OG	2.08	0.52
2:B:459:TYR:CZ	2:B:463:THR:HG21	2.44	0.52
2:B:510:LYS:HB2	2:B:511:PRO:HD2	1.91	0.52
2:B:770:GLN:HG2	2:B:983:ARG:O	2.09	0.52
2:B:780:VAL:HG23	2:B:799:PRO:HG2	1.90	0.52
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.42	0.52
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.91	0.52
2:B:1175:LEU:O	2:B:1177:HIS:N	2.42	0.52
3:C:255:VAL:O	3:C:258:ILE:HB	2.08	0.52
7:G:103:VAL:O	7:G:103:VAL:HG12	2.08	0.52
1:A:531:ILE:HD11	1:A:617:VAL:HG11	1.91	0.52
1:A:691:LEU:O	1:A:694:THR:HB	2.09	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD12	1.91	0.52
1:A:1055:ARG:HH21	6:F:154:ASP:CG	2.14	0.52
2:B:205:ILE:O	2:B:206:ASN:C	2.52	0.52
2:B:360:PHE:H	2:B:362:PRO:HG3	1.75	0.52
2:B:996:ARG:CB	2:B:996:ARG:HH11	2.21	0.52
2:B:1167:GLY:H	2:B:1215:ARG:HG2	1.73	0.52
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.90	0.52
7:G:13:LEU:HB3	7:G:17:PHE:HD2	1.72	0.52
8:H:106:GLU:O	8:H:107:VAL:HG13	2.09	0.52
9:I:14:LEU:CD2	9:I:29:CYS:HB2	2.39	0.52
9:I:26:LEU:HD23	9:I:26:LEU:N	2.24	0.52
11:K:50:LEU:CD1	11:K:75:ILE:HD11	2.39	0.52
1:A:338:GLY:O	2:B:1129:ARG:NH1	2.39	0.52
1:A:404:TYR:C	1:A:415:LEU:CD1	2.82	0.52
1:A:432:VAL:HG22	1:A:432:VAL:O	2.09	0.52
1:A:448:PRO:HG3	17:B:2501:ATP:O2'	2.09	0.52
1:A:1100:ARG:HH22	1:A:1111:MET:HE2	1.75	0.52
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.92	0.52
1:A:1352:VAL:HG12	1:A:1368:MET:HE2	1.90	0.52
2:B:817:LEU:O	2:B:818:PRO:O	2.27	0.52
2:B:1209:ALA:C	2:B:1211:ASN:N	2.68	0.52
3:C:135:GLN:NE2	3:C:235:VAL:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:LYS:HA	5:E:97:VAL:CG1	2.38	0.52
6:F:109:VAL:HG21	6:F:123:LYS:HG2	1.90	0.52
11:K:64:GLU:O	11:K:65:HIS:HB2	2.10	0.52
1:A:525:GLN:HA	2:B:1015:HIS:HD2	1.74	0.52
1:A:605:MET:HE2	1:A:621:THR:HG21	1.91	0.52
1:A:1055:ARG:NE	6:F:154:ASP:OD2	2.38	0.52
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.35	0.52
2:B:459:TYR:CE2	2:B:470:LYS:HD3	2.44	0.52
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.24	0.52
2:B:890:TYR:HD1	2:B:890:TYR:H	1.56	0.52
2:B:1033:LYS:HD2	2:B:1087:PHE:O	2.10	0.52
3:C:5:GLY:O	3:C:7:GLN:N	2.42	0.52
3:C:38:ILE:HG22	3:C:39:ALA:N	2.24	0.52
3:C:48:SER:O	3:C:49:VAL:CG2	2.57	0.52
5:E:90:VAL:HG23	5:E:123:LEU:HD22	1.92	0.52
8:H:6:PHE:O	8:H:58:THR:HG23	2.09	0.52
1:A:388:LEU:HD22	1:A:432:VAL:HG11	1.92	0.52
1:A:590:ARG:NH1	1:A:621:THR:CG2	2.73	0.52
1:A:671:ALA:HB1	1:A:736:ASN:ND2	2.25	0.52
1:A:869:GLY:HA2	1:A:1366:ARG:HG2	1.92	0.52
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.45	0.52
1:A:1443:VAL:HG12	6:F:134:ILE:HD13	1.91	0.52
2:B:419:THR:O	2:B:422:LYS:HB3	2.10	0.52
2:B:460:ALA:C	2:B:462:ALA:N	2.67	0.52
2:B:515:HIS:CE1	2:B:517:THR:HG1	2.23	0.52
2:B:590:HIS:HE2	2:B:592:ASN:C	2.15	0.52
2:B:653:VAL:HG23	2:B:657:HIS:HB2	1.92	0.52
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.45	0.52
3:C:52:GLU:C	3:C:53:THR:HG23	2.34	0.52
5:E:55:ARG:HA	5:E:58:MET:HE3	1.91	0.52
5:E:175:LEU:HD12	5:E:176:PRO:HD2	1.91	0.52
8:H:93:TYR:CD2	8:H:143:LEU:HB3	2.45	0.52
11:K:43:GLY:O	11:K:45:LEU:N	2.42	0.52
12:L:52:GLY:C	12:L:53:HIS:ND1	2.68	0.52
1:A:134:ARG:O	1:A:138:ILE:HG13	2.10	0.52
1:A:306:ASN:HB2	1:A:324:SER:HB2	1.90	0.52
1:A:318:SER:HG	1:A:321:PRO:N	2.08	0.52
1:A:601:LYS:CB	1:A:603:ASN:ND2	2.64	0.52
1:A:899:VAL:CG1	1:A:908:LEU:HG	2.40	0.52
2:B:45:SER:O	2:B:47:GLN:N	2.42	0.52
2:B:603:LEU:HG	2:B:608:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:ASN:O	2:B:795:ILE:HD13	2.09	0.52
2:B:1106:ARG:NH1	2:B:1106:ARG:HG3	2.25	0.52
3:C:52:GLU:O	3:C:53:THR:CG2	2.58	0.52
8:H:55:LEU:HD13	8:H:146:ARG:O	2.10	0.52
8:H:77:ARG:NH1	8:H:78:SER:H	2.08	0.52
1:A:368:LYS:O	1:A:371:ALA:N	2.42	0.52
1:A:377:PRO:HG2	1:A:493:GLN:CG	2.40	0.52
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.44	0.52
4:D:24:ALA:H	4:D:28:GLN:HB3	1.75	0.52
4:D:51:ASN:HB2	4:D:181:GLY:O	2.09	0.52
8:H:135:LEU:HD11	8:H:137:GLN:NE2	2.24	0.52
1:A:32:VAL:HG23	1:A:33:ALA:N	2.21	0.52
1:A:57:ARG:HB3	1:A:69:THR:OG1	2.10	0.52
1:A:67:CYS:HB3	1:A:70:CYS:O	2.09	0.52
1:A:75:ASN:O	1:A:76:GLU:HB3	2.09	0.52
1:A:899:VAL:CG2	1:A:1029:ARG:HB2	2.40	0.52
1:A:982:THR:O	1:A:985:ASP:HB2	2.10	0.52
1:A:1074:GLU:O	1:A:1075:PRO:C	2.53	0.52
2:B:313:MET:O	2:B:316:PRO:HD2	2.10	0.52
2:B:401:PHE:CD2	2:B:521:LEU:HD12	2.45	0.52
2:B:525:ALA:O	2:B:768:THR:HA	2.10	0.52
2:B:659:ALA:O	2:B:661:LEU:N	2.41	0.52
6:F:127:GLU:HB3	6:F:129:LYS:NZ	2.25	0.52
10:J:6:ARG:HB2	10:J:12:LYS:C	2.34	0.52
1:A:385:ILE:HD12	1:A:428:TYR:CE1	2.45	0.52
1:A:391:LEU:O	1:A:392:VAL:C	2.50	0.52
3:C:36:VAL:HG12	3:C:40:GLU:OE1	2.10	0.52
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.09	0.52
5:E:213:ILE:HG12	5:E:214:CYS:H	1.74	0.52
7:G:44:TYR:CZ	7:G:105:PRO:HB2	2.45	0.52
9:I:75:CYS:SG	9:I:108:HIS:CE1	3.03	0.52
1:A:103:CYS:HB3	1:A:108:MET:HE1	1.92	0.52
1:A:336:ILE:HG21	1:A:1400:CYS:O	2.10	0.52
1:A:378:GLU:O	1:A:431:LYS:HA	2.10	0.52
1:A:457:ALA:HB3	1:A:505:CYS:O	2.09	0.52
1:A:577:ILE:O	1:A:580:VAL:HG23	2.09	0.52
1:A:1242:VAL:HG22	1:A:1260:LEU:HD13	1.91	0.52
1:A:1384:VAL:O	1:A:1385:THR:CG2	2.58	0.52
2:B:116:GLU:O	2:B:120:ARG:HB2	2.09	0.52
2:B:390:LEU:O	2:B:391:ASP:C	2.53	0.52
2:B:855:PHE:CD2	2:B:972:LYS:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:HD11	3:C:95:CYS:HA	1.92	0.52
5:E:151:PRO:HB2	5:E:198:ILE:HG23	1.92	0.52
5:E:187:TYR:CD1	5:E:187:TYR:O	2.63	0.52
1:A:870:GLU:OE1	5:E:202:SER:CB	2.56	0.51
1:A:916:GLY:O	1:A:919:ILE:HG22	2.10	0.51
1:A:1065:GLY:C	1:A:1067:LEU:N	2.68	0.51
2:B:132:VAL:CG1	2:B:165:VAL:HG11	2.39	0.51
3:C:57:VAL:HG21	10:J:60:PHE:HB3	1.92	0.51
4:D:125:SER:O	4:D:128:VAL:CG1	2.58	0.51
6:F:86:THR:HG23	6:F:89:GLU:CD	2.35	0.51
11:K:80:GLY:O	11:K:81:TYR:C	2.53	0.51
1:A:481:ASP:OD1	1:A:481:ASP:N	2.43	0.51
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.10	0.51
1:A:1078:GLN:O	1:A:1078:GLN:HG3	2.11	0.51
1:A:1317:MET:HB3	5:E:142:VAL:HG11	1.92	0.51
1:A:1341:ILE:O	1:A:1344:GLY:N	2.42	0.51
2:B:40:GLU:OE1	2:B:681:TRP:HB3	2.09	0.51
2:B:293:PRO:HB2	2:B:296:GLU:HB2	1.92	0.51
2:B:588:GLY:C	2:B:589:VAL:CG2	2.83	0.51
2:B:601:ARG:O	2:B:605:ARG:HG3	2.10	0.51
2:B:619:ILE:HD13	9:I:65:ASP:OD2	2.09	0.51
2:B:757:PRO:O	2:B:1024:ALA:HB1	2.10	0.51
2:B:972:LYS:C	2:B:973:ILE:HG13	2.33	0.51
12:L:32:ALA:CB	12:L:55:ILE:HD13	2.40	0.51
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.45	0.51
2:B:29:ASP:OD1	2:B:658:ILE:HG12	2.10	0.51
2:B:243:ALA:HB2	2:B:250:PHE:O	2.10	0.51
2:B:274:PRO:O	2:B:275:TYR:HB2	2.11	0.51
2:B:770:GLN:HG2	2:B:983:ARG:C	2.35	0.51
2:B:899:ILE:CD1	2:B:949:VAL:HG21	2.39	0.51
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.25	0.51
3:C:222:LYS:HG2	3:C:222:LYS:O	2.10	0.51
5:E:88:VAL:HG13	5:E:92:THR:OG1	2.10	0.51
6:F:104:ASN:O	7:G:16:SER:HB3	2.11	0.51
9:I:111:THR:HG21	9:I:118:ARG:H	1.74	0.51
1:A:58:LEU:HD22	1:A:80:HIS:O	2.10	0.51
1:A:89:PRO:O	1:A:204:THR:HG21	2.10	0.51
1:A:132:LYS:O	1:A:135:PHE:HB3	2.11	0.51
1:A:297:GLN:O	1:A:297:GLN:HG2	2.09	0.51
1:A:741:ASN:OD1	1:A:743:VAL:N	2.44	0.51
1:A:1004:ASN:OD1	1:A:1007:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.45	0.51
2:B:357:GLN:NE2	2:B:368:GLU:HG3	2.25	0.51
2:B:1152:MET:HE3	2:B:1157:ALA:HA	1.91	0.51
5:E:66:GLU:HA	5:E:69:ILE:HD11	1.92	0.51
10:J:6:ARG:HB3	10:J:13:VAL:HA	1.92	0.51
1:A:447:GLN:CG	14:T:20:DC:H1'	2.40	0.51
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.91	0.51
1:A:683:ILE:HD12	1:A:801:GLU:OE2	2.11	0.51
1:A:807:GLY:O	2:B:728:ARG:HD2	2.10	0.51
1:A:904:THR:HG23	1:A:905:ASP:OD1	2.10	0.51
1:A:1103:GLU:O	1:A:1104:ILE:C	2.54	0.51
1:A:1116:LEU:HD12	1:A:1310:GLY:O	2.10	0.51
2:B:266:ALA:O	2:B:268:THR:N	2.38	0.51
2:B:296:GLU:O	2:B:299:GLU:HG2	2.10	0.51
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.92	0.51
2:B:952:VAL:CG1	2:B:966:VAL:HG12	2.40	0.51
3:C:142:VAL:O	3:C:142:VAL:CG1	2.57	0.51
5:E:109:ILE:O	5:E:109:ILE:HG13	2.09	0.51
8:H:135:LEU:HD11	8:H:137:GLN:CG	2.40	0.51
9:I:6:PHE:HB3	9:I:12:ASN:C	2.36	0.51
1:A:542:GLU:CG	1:A:543:LEU:H	2.23	0.51
1:A:678:GLU:OE2	1:A:732:LEU:HD23	2.11	0.51
1:A:1195:LEU:HD12	1:A:1195:LEU:C	2.35	0.51
1:A:1313:LEU:O	1:A:1314:SER:C	2.53	0.51
2:B:242:SER:OG	2:B:362:PRO:CD	2.58	0.51
2:B:496:ARG:CD	2:B:751:VAL:CG2	2.84	0.51
2:B:520:GLY:N	2:B:748:ILE:HG22	2.26	0.51
2:B:550:ASP:CG	2:B:551:PRO:HD2	2.36	0.51
2:B:635:ARG:NH2	2:B:637:LEU:HD13	2.22	0.51
2:B:636:PRO:O	2:B:743:ILE:HD11	2.11	0.51
2:B:702:LEU:HD23	2:B:737:THR:HG23	1.91	0.51
3:C:142:VAL:O	3:C:142:VAL:HG13	2.09	0.51
3:C:259:LEU:O	3:C:262:LEU:HB3	2.10	0.51
5:E:18:THR:HA	5:E:21:GLU:HB2	1.93	0.51
7:G:86:VAL:HA	7:G:146:LYS:HA	1.92	0.51
10:J:46:CYS:O	10:J:49:MET:N	2.42	0.51
10:J:61:LEU:C	10:J:63:TYR:H	2.19	0.51
11:K:29:ASN:O	11:K:76:GLN:HB2	2.11	0.51
1:A:15:LYS:CD	2:B:1218:THR:O	2.59	0.51
1:A:35:ILE:HB	1:A:83:HIS:O	2.11	0.51
1:A:239:LEU:HG	1:A:240:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HG2	2:B:1129:ARG:HA	1.92	0.51
1:A:470:LEU:HD12	1:A:470:LEU:O	2.10	0.51
1:A:635:ARG:NH1	1:A:876:ALA:O	2.44	0.51
1:A:779:PHE:CZ	1:A:785:PRO:CD	2.93	0.51
2:B:702:LEU:HD22	2:B:737:THR:HG23	1.91	0.51
2:B:785:TYR:HE1	10:J:60:PHE:CZ	2.28	0.51
5:E:55:ARG:NE	5:E:113:GLN:OE1	2.43	0.51
7:G:27:LYS:HD2	7:G:51:TYR:HE1	1.76	0.51
7:G:80:LYS:CE	7:G:82:PHE:HE1	2.24	0.51
1:A:408:ASP:N	1:A:408:ASP:OD1	2.36	0.51
1:A:492:PRO:CG	1:A:498:ARG:HG2	2.41	0.51
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.46	0.51
1:A:1325:THR:O	5:E:148:GLU:HG3	2.11	0.51
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.93	0.51
2:B:789:MET:CB	2:B:967:ARG:HD3	2.41	0.51
2:B:862:GLN:OE1	2:B:963:PHE:HE1	1.93	0.51
2:B:1051:THR:OG1	2:B:1054:GLY:N	2.43	0.51
2:B:1166:CYS:CB	2:B:1168:LEU:HD11	2.41	0.51
3:C:8:VAL:CG1	3:C:22:LEU:HD23	2.39	0.51
6:F:127:GLU:HB3	6:F:129:LYS:HZ3	1.75	0.51
7:G:1:MET:HE3	7:G:80:LYS:H	1.76	0.51
8:H:139:ASN:O	8:H:140:ALA:CB	2.59	0.51
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.92	0.51
1:A:375:THR:O	1:A:376:TYR:HB2	2.11	0.51
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.93	0.51
1:A:504:LEU:HD21	6:F:88:TYR:HD1	1.75	0.51
1:A:598:LEU:HD12	8:H:122:LEU:HB3	1.93	0.51
1:A:789:LYS:HE3	9:I:67:THR:CB	2.34	0.51
1:A:825:ILE:O	1:A:829:VAL:HB	2.11	0.51
1:A:1018:PHE:CE2	1:A:1053:PHE:HD2	2.29	0.51
1:A:1037:LEU:HD23	1:A:1042:PHE:HA	1.91	0.51
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.93	0.51
2:B:756:ILE:HB	2:B:759:PRO:HG3	1.93	0.51
2:B:1108:ARG:CZ	2:B:1108:ARG:HB2	2.41	0.51
6:F:125:LEU:HA	6:F:130:ILE:CD1	2.40	0.51
11:K:100:ALA:O	11:K:104:ASN:CG	2.54	0.51
12:L:61:THR:OG1	12:L:63:ARG:HB2	2.11	0.51
1:A:363:GLN:HA	1:A:459:ARG:O	2.11	0.51
1:A:568:PRO:O	1:A:569:LYS:HB2	2.11	0.51
1:A:807:GLY:HA2	2:B:760:ASP:O	2.10	0.51
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:O	2:B:59:LEU:N	2.44	0.51
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.93	0.51
2:B:118:ARG:HE	2:B:204:ILE:CD1	2.23	0.51
2:B:757:PRO:CB	2:B:1028:GLU:HG3	2.41	0.51
2:B:769:TYR:C	2:B:771:SER:N	2.68	0.51
4:D:183:LEU:HD23	4:D:194:LEU:HD13	1.92	0.51
5:E:196:VAL:CG1	5:E:198:ILE:HD11	2.41	0.51
7:G:9:LEU:CD2	7:G:11:ILE:HD11	2.41	0.51
12:L:61:THR:C	12:L:63:ARG:N	2.67	0.51
1:A:144:THR:O	1:A:146:MET:HG2	2.10	0.50
1:A:391:LEU:HG	1:A:400:PRO:O	2.10	0.50
1:A:569:LYS:CB	8:H:46:LEU:CD2	2.88	0.50
1:A:657:LEU:O	1:A:661:GLY:N	2.35	0.50
1:A:693:VAL:HG22	1:A:714:PHE:CD1	2.46	0.50
1:A:1141:THR:HG23	1:A:1205:LYS:NZ	2.26	0.50
1:A:1398:MET:CE	1:A:1423:GLY:CA	2.88	0.50
2:B:51:PHE:O	2:B:54:PHE:HB3	2.10	0.50
2:B:210:LYS:NZ	2:B:462:ALA:HA	2.26	0.50
2:B:733:HIS:O	2:B:734:HIS:HB2	2.11	0.50
2:B:953:LEU:HD21	2:B:955:THR:CG2	2.41	0.50
4:D:157:GLN:O	4:D:160:VAL:HG22	2.11	0.50
8:H:23:VAL:HG12	8:H:24:CYS:N	2.27	0.50
8:H:114:VAL:O	8:H:124:ARG:HA	2.11	0.50
10:J:2:ILE:HG13	10:J:3:VAL:N	2.26	0.50
1:A:397:ASN:OD1	1:A:397:ASN:N	2.43	0.50
1:A:439:ASN:HA	1:A:459:ARG:HB3	1.93	0.50
1:A:663:SER:O	1:A:664:THR:HB	2.10	0.50
1:A:847:ASP:OD2	1:A:859:SER:HB2	2.11	0.50
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.11	0.50
1:A:1427:ASN:O	1:A:1431:GLY:N	2.42	0.50
2:B:25:ILE:HG22	2:B:651:LEU:HD12	1.93	0.50
2:B:272:THR:OG1	2:B:279:ASP:OD2	2.29	0.50
7:G:47:CYS:HB3	7:G:77:VAL:CG1	2.41	0.50
8:H:12:VAL:HG21	8:H:50:ALA:CA	2.42	0.50
8:H:130:ARG:N	8:H:130:ARG:HD2	2.26	0.50
9:I:19:ASP:HB2	9:I:24:ARG:CG	2.41	0.50
9:I:42:LEU:C	9:I:42:LEU:HD23	2.35	0.50
9:I:65:ASP:OD1	9:I:67:THR:HG23	2.11	0.50
1:A:324:SER:O	1:A:325:ILE:C	2.54	0.50
1:A:575:LYS:O	1:A:579:SER:OG	2.29	0.50
1:A:1386:ARG:O	1:A:1390:ASN:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:LEU:N	1:A:1397:LEU:HD23	2.26	0.50
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.45	0.50
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.36	0.50
3:C:29:MET:HE2	11:K:98:LEU:HD21	1.92	0.50
4:D:59:ILE:HG22	4:D:63:LEU:HD12	1.93	0.50
4:D:188:ALA:O	4:D:191:ALA:N	2.44	0.50
5:E:145:THR:HG21	5:E:187:TYR:CE1	2.46	0.50
5:E:169:ARG:HD2	18:E:301:GOL:O2	2.11	0.50
5:E:185:ALA:HA	5:E:190:LEU:CD1	2.41	0.50
6:F:81:THR:OG1	6:F:136:ARG:NH1	2.44	0.50
1:A:5:GLN:NE2	2:B:1175:LEU:CD1	2.74	0.50
1:A:490:HIS:CG	2:B:1150:ARG:HH12	2.29	0.50
1:A:1099:PRO:HA	1:A:1102:LYS:HB2	1.93	0.50
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	1.93	0.50
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.45	0.50
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.25	0.50
2:B:37:PHE:CE2	2:B:542:MET:HG2	2.46	0.50
2:B:170:LEU:HD12	2:B:457:LEU:HD13	1.93	0.50
2:B:700:SER:C	2:B:701:ILE:HG23	2.37	0.50
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.93	0.50
4:D:138:ASN:CG	4:D:141:LEU:HB3	2.35	0.50
6:F:125:LEU:CA	6:F:130:ILE:HD11	2.40	0.50
8:H:43:ASN:OD1	8:H:43:ASN:C	2.54	0.50
11:K:12:LEU:H	11:K:12:LEU:HD12	1.75	0.50
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.50
1:A:821:ARG:O	1:A:824:LEU:N	2.43	0.50
1:A:899:VAL:HG11	1:A:908:LEU:HG	1.94	0.50
1:A:1116:LEU:HD11	1:A:1311:VAL:HA	1.93	0.50
1:A:1267:MET:O	1:A:1271:ILE:HB	2.11	0.50
2:B:27:ALA:O	2:B:30:SER:N	2.36	0.50
2:B:759:PRO:CB	2:B:767:ASN:ND2	2.73	0.50
2:B:980:PHE:HE1	2:B:1094:ARG:HG3	1.76	0.50
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.12	0.50
5:E:204:THR:OG1	5:E:205:SER:N	2.33	0.50
8:H:96:VAL:HG12	8:H:97:MET:N	2.27	0.50
11:K:12:LEU:HD21	11:K:18:LYS:HG3	1.93	0.50
1:A:22:PHE:CD2	2:B:1213:THR:HG22	2.47	0.50
1:A:46:THR:C	1:A:48:ALA:H	2.19	0.50
1:A:92:HIS:HB2	1:A:236:LEU:HD13	1.93	0.50
1:A:119:ASN:H	1:A:123:ARG:HH11	1.59	0.50
1:A:351:THR:CG2	1:A:468:PHE:H	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:O	1:A:374:LEU:HB2	2.11	0.50
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.92	0.50
1:A:677:ARG:O	1:A:680:THR:OG1	2.29	0.50
1:A:1422:ARG:NH2	2:B:1223:ASP:O	2.42	0.50
2:B:214:ALA:HB1	2:B:406:LEU:HD13	1.93	0.50
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.52	0.50
2:B:885:MET:HA	2:B:936:ASP:HB2	1.94	0.50
6:F:101:ILE:HG22	6:F:117:PRO:HB3	1.93	0.50
1:A:106:VAL:HG23	1:A:112:LYS:O	2.12	0.50
1:A:483:ASP:HB2	2:B:988:GLY:HA2	1.93	0.50
1:A:508:PRO:O	1:A:511:ILE:HG12	2.12	0.50
1:A:592:ASP:H	1:A:595:THR:CG2	2.22	0.50
1:A:857:ARG:HD3	1:A:861:GLY:O	2.12	0.50
1:A:923:LEU:HD23	1:A:923:LEU:H	1.77	0.50
2:B:419:THR:O	2:B:422:LYS:CB	2.60	0.50
2:B:464:GLY:HA2	2:B:480:SER:H	1.77	0.50
2:B:639:ILE:CD1	2:B:689:LEU:HA	2.40	0.50
2:B:860:MET:HG3	2:B:965:LYS:NZ	2.26	0.50
4:D:146:GLN:O	4:D:149:THR:OG1	2.27	0.50
7:G:154:VAL:HG13	7:G:155:SER:H	1.77	0.50
8:H:143:LEU:C	8:H:144:ILE:HG12	2.37	0.50
11:K:56:VAL:HA	11:K:77:THR:HA	1.93	0.50
1:A:313:GLN:O	1:A:314:ALA:C	2.55	0.50
1:A:344:ARG:HH12	14:T:21:DC:P	2.34	0.50
1:A:510:GLN:OE1	2:B:1141:HIS:CE1	2.65	0.50
1:A:598:LEU:CD1	8:H:122:LEU:HB3	2.42	0.50
1:A:926:GLN:HG3	1:A:926:GLN:O	2.12	0.50
2:B:97:VAL:HG22	2:B:127:GLY:O	2.11	0.50
2:B:132:VAL:HG12	2:B:165:VAL:CG1	2.41	0.50
2:B:530:GLY:C	2:B:532:ALA:H	2.20	0.50
2:B:963:PHE:CE2	2:B:965:LYS:CE	2.87	0.50
3:C:61:GLU:HA	3:C:64:ALA:HB2	1.91	0.50
3:C:135:GLN:OE1	10:J:13:VAL:HG21	2.12	0.50
3:C:235:VAL:HB	10:J:13:VAL:CG1	2.41	0.50
4:D:211:LEU:CD1	4:D:214:LEU:HD22	2.42	0.50
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.77	0.50
8:H:93:TYR:HB3	8:H:144:ILE:O	2.11	0.50
9:I:75:CYS:H	9:I:79:HIS:HA	1.76	0.50
1:A:343:LYS:HE3	2:B:1151:LEU:HA	1.93	0.50
1:A:563:PRO:HD2	8:H:79:TRP:CD1	2.46	0.50
1:A:679:ILE:HG22	1:A:679:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:HD11	1:A:815:PHE:CZ	2.47	0.50
1:A:868:TYR:CD1	1:A:1064:VAL:HG21	2.47	0.50
1:A:1343:ALA:HA	5:E:149:LEU:O	2.12	0.50
2:B:433:GLN:OE1	2:B:433:GLN:N	2.45	0.50
2:B:620:ARG:NH2	9:I:89:GLN:OE1	2.44	0.50
2:B:801:LYS:O	10:J:52:THR:HB	2.11	0.50
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.70	0.50
3:C:111:THR:HG22	3:C:147:LEU:O	2.12	0.50
6:F:93:ILE:O	6:F:94:LEU:C	2.54	0.50
8:H:56:THR:CG2	8:H:57:VAL:H	2.19	0.50
8:H:97:MET:HE2	8:H:118:PHE:CD2	2.47	0.50
9:I:12:ASN:ND2	9:I:31:THR:OG1	2.44	0.50
10:J:53:HIS:HD2	10:J:54:VAL:N	2.10	0.50
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.42	0.49
1:A:347:PHE:HB3	1:A:491:VAL:HG12	1.94	0.49
1:A:756:ILE:HG21	1:A:1086:PHE:CE2	2.47	0.49
1:A:1018:PHE:CE2	1:A:1053:PHE:CD2	3.00	0.49
1:A:1116:LEU:HD12	1:A:1311:VAL:HA	1.93	0.49
1:A:1436:ILE:O	1:A:1438:THR:N	2.45	0.49
2:B:128:LEU:HB2	2:B:167:ILE:HB	1.93	0.49
2:B:460:ALA:C	2:B:462:ALA:H	2.19	0.49
2:B:803:LEU:HD12	2:B:822:ASN:HB3	1.94	0.49
2:B:806:THR:HB	2:B:1045:SER:HA	1.94	0.49
2:B:987:LYS:NZ	13:R:10:G:P	2.85	0.49
6:F:72:LYS:O	6:F:72:LYS:CG	2.58	0.49
11:K:40:HIS:HE1	11:K:63:VAL:CG2	2.26	0.49
1:A:135:PHE:CE1	1:A:222:LEU:HD11	2.48	0.49
1:A:432:VAL:O	1:A:434:ARG:N	2.45	0.49
1:A:674:PRO:HA	1:A:677:ARG:HB3	1.94	0.49
1:A:1345:ARG:HH11	1:A:1373:ASP:CG	2.21	0.49
2:B:797:TYR:HB3	2:B:798:TYR:HD1	1.76	0.49
2:B:863:GLU:OE2	2:B:962:LYS:HD2	2.12	0.49
2:B:894:ASP:HB2	2:B:896:ASP:OD1	2.12	0.49
3:C:50:GLU:HA	12:L:65:VAL:O	2.12	0.49
3:C:193:TYR:CD2	3:C:197:SER:N	2.80	0.49
8:H:27:GLU:OE1	8:H:39:THR:CG2	2.60	0.49
12:L:42:ARG:HB2	12:L:43:THR:HG23	1.95	0.49
13:R:1:A:N6	14:T:27:DA:N6	2.56	0.49
1:A:380:VAL:HG12	1:A:428:TYR:CD1	2.47	0.49
1:A:525:GLN:CB	2:B:1015:HIS:HD2	2.24	0.49
1:A:566:ILE:O	1:A:567:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ASP:O	1:A:729:ALA:N	2.41	0.49
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.41	0.49
2:B:44:VAL:HG23	2:B:48:LEU:CD1	2.40	0.49
2:B:305:VAL:HG13	2:B:572:HIS:CE1	2.47	0.49
2:B:309:GLN:O	2:B:312:GLU:HG3	2.12	0.49
2:B:424:LEU:HD13	2:B:424:LEU:C	2.37	0.49
2:B:493:SER:CB	2:B:775:LYS:HE2	2.43	0.49
2:B:523:CYS:SG	2:B:750:GLY:N	2.85	0.49
2:B:805:THR:O	2:B:1044:ALA:N	2.32	0.49
3:C:21:ILE:O	3:C:21:ILE:CD1	2.61	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.94	0.49
7:G:18:PHE:HD1	7:G:22:MET:HE2	1.74	0.49
9:I:89:GLN:O	9:I:89:GLN:HG2	2.11	0.49
10:J:5:VAL:HG12	10:J:6:ARG:HD2	1.93	0.49
13:R:6:G:H1	14:T:23:DC:N4	2.01	0.49
1:A:15:LYS:HD3	2:B:1218:THR:O	2.12	0.49
1:A:184:SER:O	1:A:185:TRP:CG	2.66	0.49
1:A:1313:LEU:C	1:A:1315:GLU:N	2.70	0.49
2:B:48:LEU:O	2:B:51:PHE:N	2.44	0.49
2:B:849:GLY:HA2	2:B:852:ARG:NE	2.28	0.49
2:B:1020:ARG:C	2:B:1021:MET:HG3	2.37	0.49
3:C:3:GLU:HG2	3:C:4:GLU:OE1	2.12	0.49
8:H:130:ARG:NH1	8:H:130:ARG:HG3	2.28	0.49
1:A:44:THR:C	1:A:46:THR:N	2.68	0.49
1:A:106:VAL:HG23	1:A:112:LYS:C	2.38	0.49
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.94	0.49
1:A:816:HIS:CE1	2:B:764:SER:H	2.30	0.49
1:A:846:GLU:OE2	1:A:1425:SER:OG	2.29	0.49
1:A:1153:TYR:CD2	1:A:1192:LEU:HD23	2.47	0.49
2:B:209:GLU:CD	2:B:485:ARG:NH1	2.70	0.49
2:B:419:THR:C	2:B:422:LYS:HB2	2.37	0.49
2:B:800:GLN:HA	10:J:52:THR:O	2.13	0.49
2:B:814:PHE:O	2:B:816:GLU:N	2.45	0.49
2:B:816:GLU:C	2:B:817:LEU:HD12	2.38	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.93	0.49
3:C:56:THR:HG21	3:C:145:CYS:SG	2.52	0.49
7:G:1:MET:CE	7:G:80:LYS:N	2.76	0.49
7:G:1:MET:HE1	7:G:80:LYS:N	2.28	0.49
8:H:93:TYR:CD1	8:H:143:LEU:CD2	2.94	0.49
10:J:60:PHE:O	10:J:63:TYR:CD1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:LYS:O	11:K:33:ILE:HA	2.13	0.49
1:A:452:LYS:C	1:A:454:SER:H	2.21	0.49
1:A:500:GLU:HG2	2:B:1143:ALA:HA	1.93	0.49
1:A:1284:MET:HB3	1:A:1306:LEU:CD2	2.43	0.49
1:A:1317:MET:HE3	5:E:142:VAL:CG1	2.43	0.49
1:A:1390:ASN:OD1	1:A:1402:PHE:CB	2.56	0.49
2:B:466:TRP:O	2:B:468:GLU:HG2	2.12	0.49
2:B:520:GLY:O	2:B:521:LEU:HD23	2.13	0.49
2:B:653:VAL:O	2:B:654:ARG:CG	2.60	0.49
2:B:971:THR:HG22	2:B:972:LYS:N	2.28	0.49
3:C:26:ASP:O	3:C:29:MET:HB3	2.13	0.49
4:D:33:PHE:CD1	4:D:33:PHE:N	2.80	0.49
5:E:152:LYS:HA	5:E:152:LYS:HE3	1.95	0.49
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.47	0.49
1:A:337:ARG:HH12	2:B:1132:GLU:HG3	1.77	0.49
1:A:568:PRO:HG3	8:H:96:VAL:H	1.77	0.49
1:A:702:LEU:HD23	1:A:710:LEU:HG	1.95	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:CG2	2.96	0.49
1:A:999:VAL:HG12	1:A:1000:LEU:HD12	1.95	0.49
1:A:1147:THR:HG22	1:A:1195:LEU:HD13	1.95	0.49
1:A:1336:MET:HE1	5:E:179:GLN:NE2	2.28	0.49
2:B:217:ARG:HH12	2:B:405:ARG:HB3	1.78	0.49
2:B:245:GLU:HG3	2:B:245:GLU:O	2.12	0.49
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.28	0.49
2:B:874:PHE:HA	2:B:913:GLY:O	2.11	0.49
1:A:102:VAL:O	1:A:106:VAL:HG12	2.13	0.49
1:A:135:PHE:HD1	1:A:222:LEU:O	1.95	0.49
1:A:184:SER:O	1:A:185:TRP:CD1	2.66	0.49
1:A:244:PRO:N	1:A:245:PRO:CD	2.75	0.49
1:A:531:ILE:HD13	1:A:617:VAL:HG11	1.94	0.49
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.37	0.49
1:A:1329:THR:HG22	1:A:1335:ILE:HD11	1.94	0.49
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.95	0.49
2:B:39:ARG:NH2	2:B:665:GLU:HG3	2.18	0.49
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.77	0.49
2:B:301:ILE:N	2:B:301:ILE:CD1	2.74	0.49
2:B:424:LEU:O	2:B:424:LEU:HD22	2.12	0.49
2:B:428:ILE:C	2:B:428:ILE:HD12	2.37	0.49
2:B:663:ALA:O	2:B:664:THR:C	2.56	0.49
4:D:37:GLN:OE1	7:G:5:LYS:HD2	2.11	0.49
4:D:66:ARG:NH2	7:G:48:VAL:HG12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ILE:HD13	4:D:164:ILE:N	2.28	0.49
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.48	0.49
5:E:113:GLN:CA	5:E:137:GLU:HG2	2.42	0.49
5:E:185:ALA:CB	5:E:190:LEU:HD12	2.43	0.49
7:G:3:PHE:HB2	7:G:78:VAL:HG22	1.94	0.49
7:G:21:ARG:HB3	7:G:24:GLN:HB2	1.94	0.49
7:G:109:PHE:O	7:G:161:GLY:N	2.44	0.49
9:I:19:ASP:HB3	9:I:24:ARG:H	1.77	0.49
1:A:83:HIS:CA	1:A:241:VAL:CG2	2.90	0.49
1:A:583:PRO:O	1:A:585:GLY:N	2.45	0.49
1:A:1265:ASN:O	1:A:1266:THR:C	2.56	0.49
1:A:1424:VAL:HG21	2:B:1139:ILE:CD1	2.42	0.49
2:B:103:ASN:OD1	2:B:109:THR:N	2.45	0.49
2:B:1146:PHE:O	2:B:1146:PHE:CG	2.66	0.49
4:D:28:GLN:C	4:D:29:LEU:HD12	2.38	0.49
5:E:78:LEU:HD23	5:E:78:LEU:C	2.38	0.49
6:F:72:LYS:O	6:F:73:ALA:HB3	2.12	0.49
7:G:59:GLY:CA	7:G:70:PHE:CE1	2.95	0.49
11:K:82:ASP:OD1	11:K:83:PRO:CD	2.60	0.49
12:L:44:ASP:OD1	12:L:44:ASP:O	2.29	0.49
1:A:331:GLY:O	1:A:333:GLU:N	2.46	0.49
1:A:405:VAL:O	1:A:413:ILE:HB	2.13	0.49
1:A:564:ALA:N	1:A:576:GLN:HE22	2.11	0.49
1:A:711:ARG:NH1	9:I:97:MET:HG2	2.28	0.49
1:A:777:PHE:HA	1:A:782:ARG:O	2.13	0.49
1:A:922:ASP:OD1	1:A:924:LYS:HG2	2.13	0.49
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.42	0.49
2:B:128:LEU:HD12	2:B:168:GLY:C	2.38	0.49
2:B:292:ILE:HB	2:B:293:PRO:HD3	1.95	0.49
2:B:401:PHE:HB3	2:B:517:THR:HB	1.95	0.49
2:B:952:VAL:HG13	2:B:966:VAL:HG12	1.94	0.49
2:B:1107:ALA:C	2:B:1108:ARG:O	2.56	0.49
4:D:202:ILE:HG21	4:D:207:LEU:HD13	1.95	0.49
1:A:375:THR:O	1:A:376:TYR:CB	2.61	0.48
1:A:450:LEU:CD1	1:A:450:LEU:C	2.86	0.48
1:A:727:ASP:C	1:A:729:ALA:H	2.21	0.48
1:A:775:ILE:HG21	1:A:815:PHE:CD1	2.48	0.48
1:A:815:PHE:CD1	1:A:818:MET:CE	2.96	0.48
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.48	0.48
2:B:766:ARG:NH1	17:B:2501:ATP:PG	2.86	0.48
2:B:789:MET:HG3	2:B:789:MET:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:MET:HA	11:K:45:LEU:HD22	1.95	0.48
5:E:157:SER:H	5:E:160:GLU:HB2	1.76	0.48
7:G:87:VAL:HG23	7:G:145:VAL:HG22	1.95	0.48
10:J:31:ASP:OD1	10:J:32:GLU:N	2.46	0.48
11:K:65:HIS:ND1	11:K:66:PRO:N	2.61	0.48
1:A:92:HIS:O	1:A:96:ILE:HG23	2.13	0.48
1:A:357:PRO:HB3	1:A:654:ASN:ND2	2.29	0.48
1:A:446:ARG:HG2	1:A:447:GLN:H	1.78	0.48
1:A:729:ALA:HA	1:A:732:LEU:CD1	2.44	0.48
1:A:789:LYS:O	1:A:790:ASP:C	2.55	0.48
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.94	0.48
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.47	0.48
2:B:25:ILE:HG22	2:B:651:LEU:CD1	2.42	0.48
2:B:363:HIS:O	2:B:585:VAL:CG2	2.61	0.48
2:B:484:ASN:OD1	2:B:486:TYR:CD2	2.65	0.48
2:B:620:ARG:O	2:B:621:GLU:OE2	2.30	0.48
2:B:703:ILE:HG23	2:B:741:CYS:HA	1.94	0.48
2:B:789:MET:HE3	2:B:967:ARG:HB2	1.95	0.48
2:B:805:THR:HG21	2:B:1041:GLU:OE2	2.14	0.48
2:B:953:LEU:HD21	2:B:955:THR:HG22	1.94	0.48
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.25	0.48
4:D:73:SER:HB2	7:G:21:ARG:HH22	1.78	0.48
5:E:117:THR:HB	5:E:118:PRO:CD	2.43	0.48
7:G:34:VAL:HG11	7:G:74:TYR:CZ	2.49	0.48
7:G:121:PHE:CZ	7:G:123:ALA:HB2	2.49	0.48
11:K:47:ARG:O	11:K:50:LEU:HB2	2.13	0.48
1:A:219:PHE:HB2	1:A:224:PHE:HB2	1.95	0.48
1:A:351:THR:HG21	1:A:468:PHE:H	1.77	0.48
1:A:466:SER:HB2	2:B:1099:VAL:CG2	2.43	0.48
1:A:835:GLY:HA3	14:T:18:DT:H1'	1.94	0.48
1:A:846:GLU:HG2	1:A:1424:VAL:HG11	1.95	0.48
1:A:962:ARG:O	1:A:965:GLN:OE1	2.31	0.48
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.95	0.48
1:A:1343:ALA:O	5:E:149:LEU:CD1	2.53	0.48
1:A:1398:MET:HE1	1:A:1423:GLY:HA2	1.94	0.48
2:B:100:PRO:HD3	2:B:178:ASN:O	2.14	0.48
2:B:751:VAL:O	2:B:812:LEU:HD21	2.13	0.48
5:E:81:GLU:HB3	5:E:96:PHE:CD2	2.49	0.48
1:A:203:SER:O	1:A:206:GLU:HG2	2.14	0.48
1:A:566:ILE:O	1:A:568:PRO:HD2	2.13	0.48
1:A:1100:ARG:HH22	1:A:1111:MET:CE	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:VAL:O	2:B:256:VAL:HG12	2.14	0.48
2:B:1104:HIS:CD2	2:B:1122:ARG:HA	2.48	0.48
3:C:15:LYS:HD2	11:K:114:LEU:CD1	2.43	0.48
3:C:105:GLY:O	3:C:149:LYS:HA	2.12	0.48
8:H:43:ASN:ND2	8:H:46:LEU:HG	2.28	0.48
8:H:93:TYR:CD2	8:H:143:LEU:CB	2.96	0.48
8:H:125:LEU:HD12	8:H:125:LEU:O	2.14	0.48
8:H:144:ILE:HG22	8:H:145:ARG:N	2.28	0.48
1:A:1385:THR:O	1:A:1387:HIS:N	2.47	0.48
1:A:1389:PHE:CZ	1:A:1402:PHE:HE2	2.30	0.48
1:A:1402:PHE:HD1	1:A:1403:GLU:N	2.08	0.48
2:B:235:SER:OG	2:B:258:LEU:HD23	2.14	0.48
2:B:1204:PHE:CD2	2:B:1216:LEU:HD11	2.48	0.48
3:C:242:GLN:CB	3:C:246:ARG:NH2	2.72	0.48
5:E:31:THR:CG2	5:E:34:GLU:H	2.25	0.48
5:E:113:GLN:HB2	5:E:137:GLU:OE2	2.14	0.48
9:I:111:THR:CG2	9:I:118:ARG:H	2.27	0.48
1:A:236:LEU:HD21	1:A:304:MET:HE1	1.96	0.48
1:A:525:GLN:CA	2:B:1015:HIS:CD2	2.96	0.48
1:A:787:PHE:CD2	1:A:796:SER:HB2	2.48	0.48
2:B:222:ILE:O	2:B:240:ILE:HA	2.14	0.48
2:B:536:VAL:HG23	2:B:536:VAL:O	2.12	0.48
2:B:904:ARG:NH1	12:L:67:PHE:HD1	2.12	0.48
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.13	0.48
3:C:238:ILE:CG1	3:C:246:ARG:HH21	2.27	0.48
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.48	0.48
4:D:153:ARG:O	4:D:154:PHE:CD1	2.66	0.48
7:G:16:SER:O	7:G:17:PHE:HD1	1.96	0.48
9:I:17:ARG:O	9:I:25:LEU:HD12	2.14	0.48
9:I:81:ARG:N	9:I:81:ARG:HD2	2.29	0.48
12:L:55:ILE:CG2	12:L:56:LEU:H	2.23	0.48
1:A:18:GLN:HE21	1:A:18:GLN:C	2.22	0.48
1:A:427:GLN:OE1	1:A:430:TRP:CZ2	2.66	0.48
1:A:618:GLU:O	1:A:622:VAL:HG12	2.13	0.48
1:A:869:GLY:C	1:A:871:ASP:N	2.70	0.48
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.28	0.48
1:A:1441:PHE:CE1	6:F:92:ARG:HD3	2.48	0.48
2:B:527:THR:CG2	2:B:534:GLY:H	2.25	0.48
2:B:600:LEU:O	2:B:603:LEU:N	2.37	0.48
2:B:893:LEU:HA	2:B:898:LEU:O	2.13	0.48
2:B:997:GLU:HB3	3:C:38:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:HD2	2:B:1127:GLY:N	2.29	0.48
3:C:51:VAL:CG1	12:L:60:ARG:NH2	2.76	0.48
3:C:208:GLU:CD	3:C:208:GLU:H	2.22	0.48
4:D:51:ASN:HB2	4:D:182:SER:HG	1.78	0.48
7:G:16:SER:C	7:G:17:PHE:CD1	2.91	0.48
7:G:88:ASP:OD1	7:G:144:ARG:HG3	2.12	0.48
1:A:353:ILE:HG22	1:A:468:PHE:CB	2.43	0.48
1:A:483:ASP:HB2	2:B:988:GLY:CA	2.43	0.48
1:A:510:GLN:OE1	2:B:1141:HIS:HE1	1.96	0.48
1:A:537:ARG:N	1:A:575:LYS:HZ1	2.11	0.48
1:A:638:GLY:O	1:A:639:PRO:C	2.57	0.48
2:B:222:ILE:C	2:B:240:ILE:HD12	2.39	0.48
2:B:299:GLU:OE1	2:B:570:VAL:HG11	2.14	0.48
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.95	0.48
2:B:581:PHE:N	2:B:624:LEU:O	2.47	0.48
2:B:890:TYR:N	2:B:890:TYR:CD1	2.81	0.48
8:H:80:ARG:HG2	8:H:81:PRO:HD2	1.96	0.48
8:H:130:ARG:HG3	8:H:130:ARG:HH11	1.78	0.48
1:A:341:MET:HE3	1:A:1401:SER:OG	2.14	0.48
1:A:787:PHE:CE2	1:A:796:SER:HB2	2.49	0.48
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.95	0.48
1:A:1387:HIS:HA	1:A:1391:ARG:HG3	1.96	0.48
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.78	0.48
2:B:766:ARG:HD3	2:B:1020:ARG:HB3	1.96	0.48
2:B:807:ARG:N	2:B:1045:SER:HB3	2.26	0.48
2:B:947:GLY:CA	2:B:948:ILE:HD12	2.43	0.48
3:C:37:MET:HE1	3:C:232:VAL:HG21	1.96	0.48
4:D:120:GLU:O	4:D:123:LEU:HD23	2.14	0.48
4:D:176:GLU:HG2	4:D:198:LEU:HD21	1.95	0.48
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.44	0.48
5:E:78:LEU:HD23	5:E:78:LEU:O	2.13	0.48
5:E:171:LYS:O	5:E:174:GLN:HG3	2.12	0.48
13:R:8:G:H2'	13:R:9:G:H8	1.77	0.48
1:A:251:SER:HB2	1:A:257:ARG:NH1	2.29	0.48
1:A:878:ILE:HD12	1:A:1366:ARG:NH2	2.27	0.48
1:A:882:SER:HA	1:A:953:ASN:HA	1.96	0.48
1:A:1080:THR:O	1:A:1080:THR:OG1	2.23	0.48
2:B:286:PHE:O	2:B:289:LEU:HB2	2.13	0.48
2:B:976:ILE:HD11	2:B:993:THR:H	1.78	0.48
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.49	0.48
5:E:13:TRP:CZ2	5:E:38:PRO:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:PHE:CE1	8:H:57:VAL:HG11	2.48	0.48
9:I:83:ASN:HA	9:I:104:LEU:H	1.79	0.48
1:A:18:GLN:NE2	1:A:18:GLN:CA	2.77	0.47
1:A:89:PRO:C	1:A:90:VAL:HG13	2.38	0.47
1:A:231:PRO:C	1:A:233:TRP:N	2.72	0.47
1:A:1441:PHE:HE1	6:F:92:ARG:HD3	1.79	0.47
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.54	0.47
2:B:1155:SER:O	2:B:1156:ASP:C	2.57	0.47
3:C:198:ALA:O	3:C:200:GLU:N	2.47	0.47
4:D:61:GLU:HA	4:D:64:VAL:HG12	1.95	0.47
4:D:204:ASP:O	4:D:205:ASP:C	2.57	0.47
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.95	0.47
1:A:305:ASP:OD1	1:A:306:ASN:N	2.47	0.47
1:A:492:PRO:HG2	1:A:498:ARG:HG2	1.95	0.47
1:A:737:LEU:O	1:A:744:LYS:NZ	2.38	0.47
1:A:842:VAL:HG23	1:A:843:LYS:N	2.28	0.47
1:A:1050:GLU:O	1:A:1054:LEU:HD12	2.13	0.47
1:A:1263:ILE:HA	1:A:1266:THR:HB	1.96	0.47
2:B:55:VAL:O	2:B:56:ASP:C	2.56	0.47
2:B:862:GLN:HB3	2:B:963:PHE:CD1	2.48	0.47
2:B:1033:LYS:O	2:B:1037:LEU:CD1	2.61	0.47
4:D:8:PHE:CD1	7:G:6:ASP:O	2.66	0.47
4:D:127:ASP:OD1	4:D:127:ASP:O	2.31	0.47
7:G:3:PHE:CD1	7:G:3:PHE:N	2.80	0.47
8:H:14:GLU:O	8:H:26:ILE:HD12	2.13	0.47
12:L:42:ARG:O	12:L:43:THR:C	2.56	0.47
1:A:231:PRO:C	1:A:233:TRP:H	2.22	0.47
1:A:508:PRO:HA	1:A:511:ILE:HG12	1.97	0.47
1:A:960:ILE:O	1:A:962:ARG:N	2.47	0.47
1:A:1073:GLY:O	1:A:1074:GLU:C	2.57	0.47
1:A:1129:GLU:O	1:A:1132:LYS:HB2	2.14	0.47
2:B:269:ILE:HG22	2:B:282:ILE:CG2	2.44	0.47
2:B:653:VAL:C	2:B:654:ARG:HG3	2.40	0.47
2:B:658:ILE:CG2	2:B:659:ALA:N	2.77	0.47
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.78	0.47
2:B:893:LEU:HD23	2:B:899:ILE:HG23	1.97	0.47
2:B:953:LEU:HD23	2:B:955:THR:HG22	1.95	0.47
2:B:1027:ILE:O	2:B:1028:GLU:C	2.58	0.47
3:C:51:VAL:HG12	12:L:60:ARG:NH2	2.30	0.47
5:E:19:VAL:HG22	5:E:140:LEU:HD13	1.95	0.47
5:E:132:ILE:O	5:E:132:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:LYS:HD2	6:F:79:ARG:HH21	1.75	0.47
6:F:108:PHE:HD1	6:F:124:GLU:OE2	1.96	0.47
7:G:88:ASP:OD1	7:G:144:ARG:CG	2.62	0.47
10:J:59:LYS:O	10:J:63:TYR:CE1	2.67	0.47
12:L:66:GLN:C	12:L:67:PHE:CD1	2.92	0.47
1:A:266:LEU:HD23	1:A:269:ILE:HD12	1.96	0.47
1:A:483:ASP:CA	2:B:988:GLY:HA2	2.44	0.47
1:A:738:LYS:C	1:A:740:LEU:H	2.22	0.47
1:A:924:LYS:O	1:A:927:VAL:HG12	2.14	0.47
1:A:1116:LEU:N	1:A:1308:THR:OG1	2.47	0.47
2:B:215:GLN:NE2	2:B:499:ASN:HB3	2.29	0.47
2:B:588:GLY:C	2:B:589:VAL:HG23	2.39	0.47
2:B:593:PRO:O	2:B:594:ALA:C	2.57	0.47
2:B:912:ILE:HD11	2:B:966:VAL:HG13	1.94	0.47
2:B:995:ARG:NH1	11:K:6:ARG:HH21	2.13	0.47
2:B:1056:SER:HB3	2:B:1066:SER:O	2.14	0.47
3:C:37:MET:HE2	3:C:176:ILE:CD1	2.41	0.47
4:D:61:GLU:HA	4:D:64:VAL:CG1	2.44	0.47
4:D:125:SER:O	4:D:128:VAL:HG12	2.14	0.47
4:D:190:GLU:HB2	7:G:167:TYR:CE1	2.49	0.47
5:E:135:PHE:HB3	5:E:140:LEU:HD21	1.96	0.47
9:I:86:PHE:CD2	9:I:87:GLN:O	2.68	0.47
11:K:114:LEU:HD22	11:K:115:ALA:N	2.30	0.47
12:L:32:ALA:HB3	12:L:55:ILE:HG21	1.96	0.47
1:A:127:ALA:O	1:A:129:LYS:N	2.47	0.47
1:A:680:THR:O	1:A:683:ILE:CG1	2.62	0.47
1:A:1386:ARG:HE	14:T:15:DA:H1'	1.80	0.47
1:A:1389:PHE:O	1:A:1392:SER:HB2	2.14	0.47
1:A:1445:ILE:HD11	7:G:70:PHE:HE1	1.79	0.47
2:B:375:ALA:C	2:B:377:PHE:N	2.72	0.47
2:B:549:THR:HG22	2:B:550:ASP:H	1.80	0.47
2:B:602:THR:HA	2:B:605:ARG:HB2	1.95	0.47
2:B:634:TYR:CE2	2:B:692:TYR:CD2	3.01	0.47
2:B:978:ASP:OD2	2:B:1098:MET:HG3	2.15	0.47
2:B:1045:SER:O	2:B:1048:THR:HG21	2.13	0.47
3:C:10:ILE:HG23	11:K:108:GLU:HB3	1.95	0.47
5:E:26:ARG:O	5:E:26:ARG:HG3	2.14	0.47
7:G:80:LYS:CE	7:G:82:PHE:CE1	2.97	0.47
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.95	0.47
11:K:89:ASN:OD1	11:K:89:ASN:N	2.47	0.47
1:A:219:PHE:CD1	1:A:219:PHE:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ILE:O	1:A:607:ILE:CG1	2.62	0.47
1:A:932:GLU:OE2	1:A:1028:THR:HB	2.15	0.47
1:A:948:VAL:C	1:A:950:GLY:N	2.73	0.47
1:A:1126:ALA:O	1:A:1128:GLN:OE1	2.32	0.47
2:B:268:THR:OG1	2:B:320:ASP:OD2	2.32	0.47
2:B:370:PHE:O	2:B:372:SER:N	2.48	0.47
10:J:6:ARG:HA	10:J:14:VAL:HG12	1.96	0.47
1:A:35:ILE:HD13	1:A:35:ILE:HA	1.76	0.47
1:A:35:ILE:HD13	1:A:52:GLY:O	2.14	0.47
1:A:37:PHE:N	1:A:37:PHE:CD1	2.83	0.47
1:A:99:ILE:HG23	1:A:211:PHE:CE2	2.45	0.47
1:A:135:PHE:O	1:A:138:ILE:N	2.48	0.47
1:A:452:LYS:C	1:A:454:SER:N	2.72	0.47
1:A:733:ALA:O	1:A:735:VAL:N	2.48	0.47
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.26	0.47
1:A:842:VAL:HG12	1:A:1069:ALA:CB	2.44	0.47
1:A:909:ASP:OD1	1:A:911:SER:OG	2.26	0.47
1:A:1118:VAL:HG13	1:A:1306:LEU:HB2	1.95	0.47
1:A:1391:ARG:O	1:A:1392:SER:O	2.32	0.47
2:B:173:MET:HE3	2:B:201:GLY:HA2	1.96	0.47
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.49	0.47
2:B:210:LYS:CG	2:B:482:VAL:HG12	2.44	0.47
2:B:246:LYS:HG3	2:B:246:LYS:O	2.14	0.47
2:B:390:LEU:O	2:B:392:ARG:N	2.48	0.47
2:B:651:LEU:HG	2:B:654:ARG:HE	1.79	0.47
2:B:789:MET:HB3	2:B:967:ARG:HH11	1.79	0.47
2:B:857:ARG:NH2	14:T:24:DT:OP1	2.47	0.47
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.79	0.47
2:B:948:ILE:HD12	2:B:948:ILE:N	2.30	0.47
2:B:976:ILE:HG12	2:B:990:ILE:HG22	1.96	0.47
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.29	0.47
2:B:1181:GLU:HB2	2:B:1188:LYS:HE2	1.96	0.47
3:C:16:ASP:C	3:C:17:ASN:OD1	2.58	0.47
3:C:92:CYS:N	3:C:95:CYS:SG	2.87	0.47
3:C:186:LEU:CD2	3:C:223:ALA:HB1	2.45	0.47
4:D:58:VAL:HG22	4:D:58:VAL:O	2.14	0.47
5:E:16:PHE:CE2	5:E:20:LYS:CE	2.98	0.47
5:E:161:LYS:C	5:E:163:GLU:H	2.22	0.47
6:F:85:MET:HE1	6:F:148:VAL:HG22	1.97	0.47
6:F:86:THR:O	6:F:87:LYS:C	2.58	0.47
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:94:CYS:SG	7:G:130:TYR:CE2	3.08	0.47
7:G:153:GLN:O	7:G:154:VAL:HG12	2.15	0.47
8:H:79:TRP:CH2	8:H:81:PRO:HA	2.50	0.47
9:I:58:VAL:C	9:I:62:ILE:HG21	2.39	0.47
12:L:30:ILE:CG2	12:L:31:CYS:N	2.66	0.47
1:A:142:CYS:C	1:A:144:THR:H	2.22	0.47
1:A:452:LYS:CG	2:B:1140:ALA:HB1	2.43	0.47
1:A:896:ARG:CD	1:A:1030:ARG:HD2	2.39	0.47
1:A:997:LEU:HD23	1:A:997:LEU:HA	1.62	0.47
1:A:1342:GLU:HG2	5:E:212:ARG:NE	2.29	0.47
2:B:60:GLN:O	2:B:62:ILE:N	2.48	0.47
2:B:103:ASN:OD1	2:B:108:VAL:HB	2.15	0.47
2:B:257:LYS:HG3	2:B:259:TYR:HE1	1.80	0.47
2:B:969:ARG:O	2:B:970:THR:HB	2.15	0.47
3:C:61:GLU:O	3:C:64:ALA:HB3	2.14	0.47
3:C:88:CYS:O	3:C:90:ASP:O	2.33	0.47
3:C:193:TYR:CB	3:C:197:SER:HA	2.44	0.47
4:D:5:THR:HG23	4:D:5:THR:O	2.15	0.47
4:D:35:LEU:O	4:D:37:GLN:N	2.47	0.47
4:D:119:ARG:C	4:D:121:LYS:H	2.23	0.47
5:E:184:VAL:HA	5:E:187:TYR:HB3	1.96	0.47
6:F:94:LEU:HD13	6:F:122:MET:HG2	1.96	0.47
8:H:101:ALA:CB	8:H:104:PHE:CZ	2.98	0.47
8:H:130:ARG:HD2	8:H:130:ARG:H	1.80	0.47
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.96	0.47
1:A:285:PRO:O	1:A:286:HIS:C	2.57	0.47
1:A:538:ASP:OD1	8:H:22:LYS:HB2	2.14	0.47
2:B:118:ARG:HE	2:B:204:ILE:HD11	1.80	0.47
2:B:215:GLN:HG3	2:B:476:ARG:HD2	1.95	0.47
2:B:515:HIS:CE1	2:B:517:THR:OG1	2.66	0.47
2:B:554:ILE:HA	2:B:557:PHE:HB2	1.95	0.47
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.97	0.47
2:B:1013:ASN:HD22	2:B:1014:PRO:CD	2.26	0.47
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.15	0.47
2:B:1082:MET:HA	3:C:189:THR:CA	2.28	0.47
2:B:1200:ALA:O	2:B:1201:LYS:C	2.58	0.47
3:C:32:SER:OG	11:K:45:LEU:HD22	2.15	0.47
3:C:132:PRO:O	3:C:133:ILE:C	2.57	0.47
6:F:106:PRO:HD3	7:G:16:SER:HA	1.95	0.47
1:A:18:GLN:N	2:B:1215:ARG:O	2.48	0.47
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HD13	1:A:432:VAL:HG12	1.97	0.47
1:A:512:VAL:O	1:A:512:VAL:HG23	2.15	0.47
1:A:875:ALA:HA	1:A:1366:ARG:HH21	1.78	0.47
1:A:1261:LYS:HA	1:A:1264:GLU:HB2	1.96	0.47
1:A:1385:THR:O	1:A:1388:GLY:N	2.48	0.47
2:B:211:VAL:N	2:B:481:GLN:O	2.41	0.47
2:B:460:ALA:O	2:B:461:LEU:C	2.56	0.47
2:B:579:ARG:HB3	2:B:586:TRP:NE1	2.30	0.47
4:D:7:THR:OG1	4:D:8:PHE:N	2.47	0.47
4:D:136:GLY:C	4:D:138:ASN:H	2.23	0.47
7:G:23:LYS:O	7:G:27:LYS:HG3	2.14	0.47
11:K:50:LEU:HD11	11:K:75:ILE:HD11	1.95	0.47
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.61	0.46
1:A:337:ARG:HH11	1:A:337:ARG:CG	2.26	0.46
1:A:583:PRO:O	1:A:584:ASN:C	2.58	0.46
1:A:770:VAL:O	1:A:772:GLY:N	2.48	0.46
1:A:810:PRO:HG2	2:B:705:MET:CE	2.45	0.46
1:A:980:ASP:H	1:A:981:LEU:HD12	1.79	0.46
1:A:1239:ARG:HG2	1:A:1239:ARG:HH11	1.79	0.46
1:A:1419:ASP:OD1	1:A:1426:GLU:HG2	2.16	0.46
2:B:223:VAL:HA	2:B:239:GLU:O	2.15	0.46
2:B:566:LEU:HD23	2:B:567:GLU:N	2.30	0.46
2:B:910:VAL:HA	2:B:940:PRO:HA	1.97	0.46
2:B:1166:CYS:SG	2:B:1168:LEU:CD1	3.02	0.46
3:C:48:SER:O	3:C:49:VAL:HG23	2.15	0.46
3:C:261:ALA:HA	3:C:264:GLN:HG3	1.97	0.46
4:D:39:ASN:OD1	4:D:41:GLN:N	2.39	0.46
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.97	0.46
5:E:198:ILE:HD13	5:E:212:ARG:HG3	1.96	0.46
1:A:380:VAL:CG1	1:A:428:TYR:HA	2.45	0.46
1:A:568:PRO:O	1:A:569:LYS:CB	2.63	0.46
1:A:837:ILE:HD13	1:A:840:ARG:NH1	2.30	0.46
1:A:1120:LEU:HB2	1:A:1125:ALA:CB	2.46	0.46
1:A:1228:TRP:CD2	1:A:1228:TRP:N	2.80	0.46
1:A:1345:ARG:HA	1:A:1376:THR:HG21	1.97	0.46
2:B:275:TYR:CZ	2:B:359:GLU:OE1	2.68	0.46
2:B:579:ARG:NH2	2:B:621:GLU:O	2.48	0.46
2:B:768:THR:O	2:B:768:THR:HG22	2.15	0.46
3:C:11:ARG:N	3:C:19:ASP:O	2.33	0.46
3:C:88:CYS:O	3:C:90:ASP:N	2.48	0.46
5:E:4:GLU:OE2	5:E:6:GLU:OE2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:GLU:O	5:E:167:ARG:HG2	2.14	0.46
6:F:154:ASP:O	6:F:155:LEU:C	2.58	0.46
12:L:32:ALA:C	12:L:34:CYS:N	2.71	0.46
1:A:346:ASP:CB	1:A:347:PHE:HD1	2.20	0.46
1:A:643:ALA:O	1:A:644:LYS:C	2.58	0.46
1:A:694:THR:HG22	1:A:695:LYS:N	2.30	0.46
1:A:907:THR:CG2	1:A:908:LEU:H	2.23	0.46
1:A:910:PRO:O	1:A:912:LEU:N	2.49	0.46
1:A:971:PHE:CD1	1:A:971:PHE:N	2.84	0.46
2:B:458:LYS:O	2:B:459:TYR:C	2.58	0.46
2:B:753:ALA:C	2:B:755:ILE:N	2.73	0.46
3:C:129:ILE:HG23	3:C:130:GLY:N	2.28	0.46
4:D:181:GLY:C	4:D:182:SER:HG	2.20	0.46
12:L:48:CYS:HB3	12:L:53:HIS:H	1.80	0.46
1:A:637:LYS:O	1:A:641:VAL:CG2	2.63	0.46
1:A:640:GLN:O	1:A:643:ALA:HB3	2.16	0.46
1:A:786:HIS:CD2	2:B:705:MET:SD	3.09	0.46
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.46
1:A:1031:VAL:O	1:A:1035:TYR:HB2	2.16	0.46
1:A:1106:ASN:O	1:A:1107:VAL:HB	2.15	0.46
1:A:1143:LEU:HG	1:A:1147:THR:HG21	1.98	0.46
2:B:235:SER:C	2:B:236:HIS:ND1	2.73	0.46
2:B:254:LEU:HD11	2:B:360:PHE:HE1	1.80	0.46
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.96	0.46
2:B:560:GLU:O	2:B:561:TRP:CD1	2.68	0.46
2:B:664:THR:HG23	2:B:665:GLU:N	2.27	0.46
2:B:827:ILE:HG13	2:B:1012:ILE:HG13	1.98	0.46
2:B:1172:ILE:O	2:B:1172:ILE:HG13	2.15	0.46
2:B:1199:ALA:O	2:B:1200:ALA:C	2.58	0.46
8:H:55:LEU:N	8:H:55:LEU:HD23	2.31	0.46
8:H:97:MET:CG	8:H:118:PHE:CE2	2.97	0.46
1:A:18:GLN:HG2	1:A:228:PHE:CE2	2.50	0.46
1:A:415:LEU:O	1:A:416:ARG:C	2.57	0.46
1:A:456:MET:HE1	1:A:477:PRO:CB	2.46	0.46
1:A:517:ASN:O	1:A:517:ASN:ND2	2.48	0.46
1:A:569:LYS:HG2	8:H:46:LEU:CD2	2.45	0.46
1:A:1138:ILE:HG22	1:A:1276:VAL:HG23	1.97	0.46
1:A:1152:ILE:HB	9:I:44:TYR:HB3	1.97	0.46
2:B:293:PRO:HD2	2:B:296:GLU:HG2	1.98	0.46
2:B:784:ASN:HB3	10:J:63:TYR:HE2	1.81	0.46
2:B:1202:LEU:O	2:B:1204:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:THR:O	3:C:254:LYS:HG2	2.15	0.46
5:E:117:THR:CB	5:E:118:PRO:CD	2.93	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.15	0.46
11:K:112:GLN:OE1	11:K:112:GLN:CA	2.63	0.46
1:A:249:SER:CA	1:A:250:ILE:HD12	2.46	0.46
1:A:391:LEU:O	1:A:394:ASN:HB2	2.16	0.46
1:A:555:ASP:OD2	1:A:644:LYS:HG2	2.15	0.46
1:A:607:ILE:HG22	1:A:612:ILE:HA	1.98	0.46
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.98	0.46
1:A:1053:PHE:O	1:A:1055:ARG:N	2.49	0.46
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.15	0.46
2:B:31:TRP:HA	2:B:31:TRP:HE3	1.79	0.46
2:B:269:ILE:HG22	2:B:282:ILE:HG21	1.97	0.46
2:B:520:GLY:CA	2:B:748:ILE:HG22	2.46	0.46
2:B:805:THR:O	2:B:805:THR:HG23	2.16	0.46
2:B:977:GLY:O	2:B:1099:VAL:HB	2.16	0.46
3:C:241:ASP:O	3:C:245:VAL:HG12	2.16	0.46
4:D:138:ASN:OD1	4:D:138:ASN:C	2.58	0.46
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.50	0.46
10:J:6:ARG:CA	10:J:14:VAL:HG12	2.46	0.46
1:A:335:ARG:O	1:A:340:LEU:HB2	2.16	0.46
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.51	0.46
1:A:869:GLY:O	5:E:204:THR:OG1	2.26	0.46
1:A:921:GLY:O	1:A:922:ASP:C	2.58	0.46
1:A:1051:ALA:O	1:A:1054:LEU:N	2.49	0.46
1:A:1135:ARG:NH1	1:A:1139:GLU:OE2	2.49	0.46
1:A:1282:VAL:HG12	1:A:1283:VAL:N	2.31	0.46
1:A:1385:THR:O	1:A:1386:ARG:C	2.59	0.46
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.64	0.46
2:B:551:PRO:O	2:B:554:ILE:HG12	2.16	0.46
2:B:864:LYS:O	2:B:865:LYS:O	2.33	0.46
2:B:1004:GLU:HB2	2:B:1006:ILE:CD1	2.46	0.46
3:C:142:VAL:HG23	10:J:15:GLY:C	2.41	0.46
4:D:40:HIS:NE2	7:G:73:LYS:CB	2.78	0.46
5:E:3:GLN:O	5:E:6:GLU:OE2	2.34	0.46
5:E:113:GLN:HB2	5:E:137:GLU:CD	2.41	0.46
6:F:104:ASN:O	7:G:16:SER:CB	2.63	0.46
8:H:12:VAL:CG2	8:H:50:ALA:O	2.58	0.46
10:J:2:ILE:O	10:J:53:HIS:CE1	2.68	0.46
11:K:53:ASP:OD1	11:K:81:TYR:OH	2.30	0.46
1:A:249:SER:HB3	1:A:259:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:O	1:A:351:THR:HB	2.16	0.46
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.98	0.46
1:A:646:PHE:O	1:A:650:GLN:HG3	2.16	0.46
1:A:816:HIS:CE1	2:B:764:SER:HB3	2.51	0.46
1:A:1056:SER:O	1:A:1057:VAL:C	2.58	0.46
1:A:1111:MET:SD	1:A:1331:SER:HA	2.55	0.46
2:B:34:ILE:HG12	2:B:542:MET:CE	2.46	0.46
2:B:129:PHE:CE1	2:B:166:PHE:CD1	3.04	0.46
2:B:228:LYS:CG	2:B:229:ALA:N	2.75	0.46
2:B:275:TYR:CE1	2:B:359:GLU:OE1	2.69	0.46
2:B:941:LEU:CG	2:B:942:ARG:N	2.79	0.46
3:C:38:ILE:HG22	3:C:39:ALA:HB2	1.98	0.46
3:C:61:GLU:CA	3:C:64:ALA:HB3	2.45	0.46
5:E:3:GLN:O	5:E:6:GLU:OE1	2.34	0.46
1:A:226:GLU:O	1:A:226:GLU:HG3	2.15	0.46
1:A:412:ARG:C	1:A:413:ILE:HD13	2.40	0.46
1:A:683:ILE:HB	1:A:801:GLU:OE2	2.15	0.46
1:A:811:GLN:O	1:A:812:GLU:C	2.59	0.46
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	3.03	0.46
2:B:302:CYS:HB2	2:B:310:MET:HE3	1.98	0.46
2:B:308:TRP:NE1	9:I:52:ILE:CD1	2.78	0.46
2:B:619:ILE:HD13	9:I:65:ASP:CB	2.44	0.46
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.80	0.46
2:B:853:SER:OG	2:B:854:LEU:N	2.48	0.46
2:B:860:MET:HG3	2:B:965:LYS:HZ3	1.81	0.46
2:B:947:GLY:HA2	2:B:948:ILE:HD12	1.97	0.46
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.29	0.46
3:C:258:ILE:O	3:C:259:LEU:C	2.58	0.46
4:D:59:ILE:HG23	7:G:47:CYS:SG	2.56	0.46
5:E:98:ILE:HA	5:E:101:GLN:CB	2.45	0.46
11:K:10:PHE:CE1	11:K:11:LEU:HB2	2.50	0.46
1:A:49:LYS:CD	1:A:55:ASP:CB	2.88	0.46
1:A:118:HIS:O	1:A:119:ASN:CB	2.64	0.46
1:A:260:ASP:O	1:A:261:ASP:C	2.59	0.46
1:A:693:VAL:HG22	1:A:714:PHE:HE1	1.81	0.46
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.31	0.46
1:A:871:ASP:O	1:A:873:MET:HE2	2.16	0.46
1:A:1037:LEU:CD2	1:A:1042:PHE:HA	2.46	0.46
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.81	0.46
3:C:142:VAL:O	3:C:144:ILE:HG13	2.16	0.46
4:D:47:LEU:HD11	7:G:5:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:HA	6:F:100:GLN:OE1	2.16	0.46
6:F:132:LEU:HD23	6:F:132:LEU:HA	1.73	0.46
8:H:25:ARG:HA	8:H:41:ASP:HA	1.98	0.46
9:I:50:THR:O	9:I:51:ASN:OD1	2.34	0.46
1:A:450:LEU:HD11	1:A:1074:GLU:CG	2.41	0.45
1:A:1118:VAL:HG23	1:A:1327:ILE:HD12	1.98	0.45
2:B:129:PHE:CE1	2:B:166:PHE:HD1	2.34	0.45
2:B:459:TYR:HE2	2:B:470:LYS:HD3	1.80	0.45
2:B:533:CYS:C	2:B:535:LEU:N	2.74	0.45
2:B:995:ARG:HH11	11:K:6:ARG:NH2	2.13	0.45
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.16	0.45
3:C:114:TYR:HB3	3:C:140:ASN:O	2.17	0.45
4:D:27:LEU:HD21	4:D:173:HIS:CG	2.52	0.45
7:G:23:LYS:HG3	7:G:56:ILE:HD13	1.98	0.45
7:G:23:LYS:HG2	7:G:56:ILE:HG21	1.98	0.45
8:H:58:THR:HB	8:H:143:LEU:CD1	2.45	0.45
9:I:24:ARG:HH21	9:I:37:GLU:CB	2.29	0.45
10:J:1:MET:C	10:J:2:ILE:HG22	2.40	0.45
12:L:41:SER:O	12:L:42:ARG:O	2.34	0.45
1:A:56:PRO:C	1:A:57:ARG:HG3	2.41	0.45
1:A:107:CYS:C	1:A:109:HIS:H	2.25	0.45
1:A:847:ASP:OD2	1:A:859:SER:CB	2.64	0.45
1:A:911:SER:C	1:A:978:PRO:HB3	2.40	0.45
1:A:1133:LEU:O	1:A:1137:ALA:HB2	2.16	0.45
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.16	0.45
1:A:1365:TYR:O	1:A:1366:ARG:C	2.59	0.45
2:B:173:MET:CE	2:B:201:GLY:HA2	2.46	0.45
2:B:215:GLN:OE1	2:B:501:PRO:HG3	2.16	0.45
2:B:484:ASN:OD1	2:B:486:TYR:HD2	1.98	0.45
2:B:784:ASN:OD1	2:B:788:ARG:HD3	2.16	0.45
2:B:955:THR:O	2:B:963:PHE:N	2.50	0.45
2:B:1131:GLY:O	2:B:1132:GLU:C	2.60	0.45
2:B:1167:GLY:HA3	2:B:1215:ARG:HB3	1.99	0.45
3:C:35:ARG:HH21	11:K:41:THR:HG23	1.80	0.45
3:C:167:HIS:NE2	12:L:70:ARG:HA	2.31	0.45
5:E:12:LEU:CD1	5:E:55:ARG:HH21	2.29	0.45
7:G:96:GLN:HG2	7:G:121:PHE:CZ	2.51	0.45
8:H:15:VAL:HA	8:H:26:ILE:CD1	2.46	0.45
9:I:62:ILE:HD13	9:I:102:VAL:HG11	1.98	0.45
9:I:78:CYS:O	9:I:79:HIS:HB2	2.16	0.45
9:I:103:CYS:SG	9:I:106:CYS:SG	3.07	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:LYS:HZ1	11:K:38:GLU:HG2	1.81	0.45
1:A:23:SER:C	1:A:25:GLU:H	2.24	0.45
1:A:29:ALA:C	1:A:31:SER:N	2.74	0.45
1:A:148:CYS:O	1:A:149:GLU:CG	2.63	0.45
1:A:299:HIS:CA	1:A:302:THR:HG22	2.45	0.45
1:A:616:VAL:HG12	1:A:617:VAL:O	2.17	0.45
1:A:622:VAL:O	1:A:623:GLY:O	2.34	0.45
1:A:700:ASN:ND2	1:A:700:ASN:O	2.45	0.45
1:A:942:PHE:HE2	5:E:207:ARG:HH21	1.64	0.45
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.16	0.45
1:A:1220:PHE:O	1:A:1221:LYS:C	2.59	0.45
2:B:31:TRP:HE1	2:B:807:ARG:HG3	1.78	0.45
2:B:606:LYS:O	2:B:686:ASN:OD1	2.34	0.45
2:B:659:ALA:C	2:B:661:LEU:H	2.23	0.45
2:B:803:LEU:HB2	2:B:822:ASN:OD1	2.16	0.45
2:B:809:MET:O	2:B:810:GLU:C	2.60	0.45
2:B:846:ILE:C	2:B:846:ILE:CD1	2.87	0.45
2:B:976:ILE:HA	2:B:990:ILE:CG2	2.47	0.45
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.81	0.45
2:B:1128:LEU:HD23	2:B:1128:LEU:N	2.30	0.45
2:B:1222:ARG:O	2:B:1223:ASP:HB2	2.16	0.45
3:C:170:TRP:O	3:C:172:PRO:HD3	2.16	0.45
9:I:53:GLY:CA	9:I:56:ALA:HB2	2.46	0.45
11:K:19:LEU:N	11:K:19:LEU:CD1	2.78	0.45
11:K:58:PHE:O	11:K:75:ILE:HA	2.16	0.45
1:A:273:ASN:HA	1:A:296:LEU:HD22	1.97	0.45
1:A:388:LEU:HD13	1:A:432:VAL:CG1	2.47	0.45
1:A:412:ARG:HH22	2:B:1108:ARG:HD3	1.82	0.45
1:A:452:LYS:CG	2:B:1140:ALA:CB	2.95	0.45
1:A:899:VAL:HA	1:A:1029:ARG:HH21	1.82	0.45
1:A:950:GLY:CA	1:A:1298:TYR:CE2	3.00	0.45
1:A:1039:LYS:HD3	1:A:1039:LYS:C	2.41	0.45
3:C:37:MET:CE	3:C:232:VAL:CG1	2.90	0.45
3:C:153:LEU:HD11	3:C:155:LEU:CD2	2.44	0.45
5:E:112:TYR:HB3	5:E:116:ILE:HD11	1.98	0.45
5:E:197:LYS:HG2	5:E:197:LYS:O	2.17	0.45
9:I:42:LEU:C	9:I:42:LEU:CD2	2.89	0.45
10:J:18:TRP:O	10:J:21:TYR:N	2.47	0.45
1:A:135:PHE:HE1	1:A:222:LEU:HD11	1.81	0.45
1:A:392:VAL:C	1:A:394:ASN:N	2.71	0.45
1:A:396:PRO:HG3	1:A:402:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.47	0.45
1:A:1005:GLU:HG2	1:A:1009:ASN:HD21	1.78	0.45
1:A:1118:VAL:O	1:A:1305:VAL:HG23	2.17	0.45
1:A:1141:THR:CG2	1:A:1205:LYS:HD2	2.47	0.45
1:A:1372:VAL:O	1:A:1375:MET:N	2.42	0.45
1:A:1418:LEU:HD22	1:A:1418:LEU:HA	1.78	0.45
2:B:25:ILE:HG13	2:B:29:ASP:HB3	1.99	0.45
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.45
2:B:510:LYS:HD3	2:B:512:ARG:HG3	1.97	0.45
2:B:729:ILE:O	2:B:729:ILE:CG2	2.64	0.45
2:B:995:ARG:NH1	11:K:6:ARG:NH2	2.64	0.45
3:C:166:GLU:HG2	11:K:6:ARG:HB2	1.98	0.45
4:D:8:PHE:HD2	4:D:38:ILE:CG1	2.29	0.45
4:D:55:ALA:C	4:D:59:ILE:CD1	2.90	0.45
6:F:144:GLU:O	6:F:146:TRP:HD1	1.99	0.45
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.31	0.45
8:H:13:SER:HB3	8:H:27:GLU:C	2.39	0.45
1:A:172:PRO:HG2	1:A:174:ILE:CG1	2.47	0.45
1:A:182:VAL:HA	1:A:201:VAL:HA	1.97	0.45
1:A:230:ARG:HG3	1:A:233:TRP:CH2	2.52	0.45
1:A:243:PRO:HB2	1:A:244:PRO:CD	2.47	0.45
1:A:398:GLU:O	1:A:399:HIS:C	2.59	0.45
1:A:674:PRO:O	1:A:677:ARG:HB3	2.17	0.45
1:A:775:ILE:HD12	1:A:776:ALA:N	2.32	0.45
1:A:982:THR:H	1:A:985:ASP:CG	2.22	0.45
2:B:59:LEU:HD11	2:B:417:PHE:CE2	2.52	0.45
2:B:293:PRO:HD2	2:B:296:GLU:CB	2.47	0.45
2:B:493:SER:HB3	2:B:775:LYS:HE2	1.98	0.45
2:B:552:MET:HA	2:B:555:ILE:HG13	1.99	0.45
2:B:831:SER:OG	2:B:833:TYR:HD2	1.98	0.45
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.49	0.45
2:B:859:TYR:N	2:B:859:TYR:CD1	2.85	0.45
5:E:190:LEU:HA	5:E:194:GLU:OE1	2.17	0.45
7:G:31:LEU:HD22	7:G:48:VAL:HG11	1.99	0.45
9:I:85:PHE:HD1	9:I:99:LEU:HD11	1.82	0.45
1:A:39:GLU:HB3	1:A:42:ASP:CG	2.41	0.45
1:A:100:LYS:O	1:A:102:VAL:N	2.50	0.45
1:A:107:CYS:HA	1:A:171:GLN:CD	2.42	0.45
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.98	0.45
1:A:550:LEU:O	1:A:551:TYR:C	2.59	0.45
1:A:660:ASN:OD1	2:B:1082:MET:SD	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:VAL:HA	1:A:746:MET:HE3	1.99	0.45
1:A:794:PRO:HD2	1:A:795:GLU:OE1	2.17	0.45
1:A:864:ILE:C	1:A:865:GLN:HG3	2.41	0.45
1:A:1358:SER:OG	1:A:1359:ASP:N	2.50	0.45
1:A:1361:SER:O	1:A:1362:TYR:CB	2.65	0.45
2:B:48:LEU:CD1	2:B:173:MET:HE1	2.47	0.45
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.97	0.45
2:B:283:VAL:O	2:B:284:ILE:C	2.58	0.45
2:B:483:LEU:HD12	2:B:484:ASN:H	1.82	0.45
2:B:1146:PHE:CE1	2:B:1150:ARG:HD3	2.52	0.45
3:C:33:LEU:O	3:C:34:ARG:C	2.59	0.45
3:C:168:ALA:O	3:C:171:GLY:N	2.49	0.45
3:C:184:ASN:HB3	3:C:191:TYR:OH	2.17	0.45
4:D:27:LEU:CD2	4:D:173:HIS:CG	2.99	0.45
4:D:54:GLU:O	4:D:58:VAL:CG1	2.65	0.45
5:E:85:GLU:H	5:E:85:GLU:HG2	1.58	0.45
5:E:188:LEU:O	5:E:188:LEU:HD23	2.17	0.45
7:G:20:PRO:HB2	7:G:21:ARG:H	1.53	0.45
10:J:7:CYS:O	10:J:11:GLY:HA2	2.16	0.45
13:R:10:G:H1	14:T:19:DC:N4	2.15	0.45
1:A:149:GLU:OE1	1:A:152:VAL:HG23	2.15	0.45
1:A:415:LEU:CD1	1:A:415:LEU:H	2.27	0.45
1:A:569:LYS:HB3	8:H:46:LEU:HD13	1.99	0.45
1:A:666:ILE:CG2	2:B:1026:LEU:CB	2.93	0.45
1:A:780:VAL:HG22	2:B:699:GLU:OE1	2.16	0.45
1:A:1279:ILE:HD12	1:A:1279:ILE:N	2.32	0.45
1:A:1294:PRO:C	1:A:1296:GLY:N	2.75	0.45
1:A:1332:PHE:HE1	1:A:1381:LEU:HD23	1.80	0.45
2:B:225:VAL:O	2:B:226:PHE:CD1	2.69	0.45
2:B:705:MET:O	2:B:742:GLU:HB3	2.17	0.45
5:E:13:TRP:HZ2	5:E:38:PRO:HA	1.81	0.45
5:E:145:THR:HA	5:E:150:VAL:HG11	1.98	0.45
6:F:90:ARG:O	6:F:94:LEU:N	2.49	0.45
7:G:96:GLN:CG	7:G:121:PHE:CE2	3.00	0.45
9:I:50:THR:C	9:I:51:ASN:OD1	2.60	0.45
9:I:67:THR:OG1	9:I:68:LEU:HD12	2.17	0.45
1:A:236:LEU:CD2	1:A:304:MET:HE1	2.47	0.45
1:A:323:LYS:NZ	13:R:3:C:H4'	2.31	0.45
1:A:569:LYS:O	1:A:570:PRO:C	2.60	0.45
1:A:726:ARG:HD2	1:A:727:ASP:N	2.32	0.45
1:A:784:LEU:C	1:A:786:HIS:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:ALA:O	1:A:1052:GLN:C	2.60	0.45
1:A:1162:VAL:O	1:A:1163:ILE:C	2.60	0.45
1:A:1331:SER:C	1:A:1333:ILE:N	2.75	0.45
2:B:53:GLN:HG3	2:B:547:VAL:HG12	1.99	0.45
2:B:651:LEU:N	2:B:651:LEU:HD23	2.32	0.45
2:B:831:SER:OG	2:B:833:TYR:HB2	2.17	0.45
2:B:1036:ALA:O	2:B:1038:SER:N	2.50	0.45
2:B:1216:LEU:HD23	2:B:1216:LEU:HA	1.73	0.45
3:C:74:SER:O	3:C:77:ILE:HB	2.17	0.45
7:G:23:LYS:HE2	7:G:27:LYS:NZ	2.32	0.45
8:H:23:VAL:CG1	8:H:24:CYS:N	2.79	0.45
8:H:34:ASP:N	8:H:35:GLN:OE1	2.50	0.45
8:H:48:PRO:C	8:H:49:VAL:HG13	2.42	0.45
1:A:21:LEU:N	1:A:228:PHE:O	2.42	0.45
1:A:525:GLN:NE2	2:B:836:GLU:OE1	2.48	0.45
1:A:531:ILE:HD13	1:A:617:VAL:CG1	2.47	0.45
1:A:963:ILE:O	1:A:963:ILE:HG22	2.16	0.45
1:A:1004:ASN:ND2	5:E:167:ARG:HH11	2.15	0.45
1:A:1202:MET:HE2	1:A:1209:MET:SD	2.57	0.45
1:A:1390:ASN:HD21	1:A:1399:ARG:CB	2.30	0.45
1:A:1443:VAL:CG2	7:G:61:ILE:HB	2.42	0.45
2:B:119:LEU:HD12	2:B:119:LEU:N	2.31	0.45
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.52	0.45
2:B:659:ALA:C	2:B:661:LEU:N	2.75	0.45
2:B:893:LEU:CD2	2:B:898:LEU:O	2.65	0.45
2:B:1058:LEU:O	2:B:1059:LEU:C	2.60	0.45
4:D:144:THR:OG1	7:G:105:PRO:HG3	2.16	0.45
7:G:46:LEU:HD11	7:G:105:PRO:HG2	1.98	0.45
7:G:63:PRO:HB2	7:G:64:THR:H	1.66	0.45
8:H:44:VAL:HG23	8:H:48:PRO:HB3	1.98	0.45
8:H:95:TYR:HE1	8:H:97:MET:SD	2.40	0.45
10:J:48:ARG:HD2	10:J:48:ARG:C	2.42	0.45
10:J:59:LYS:O	10:J:63:TYR:HE1	1.99	0.45
1:A:463:ILE:HB	1:A:464:PRO:CD	2.44	0.44
1:A:911:SER:O	1:A:912:LEU:HD23	2.17	0.44
1:A:1089:VAL:HG23	1:A:1090:ALA:N	2.31	0.44
1:A:1301:GLU:HG3	1:A:1301:GLU:O	2.17	0.44
1:A:1425:SER:O	1:A:1429:ILE:HD13	2.17	0.44
2:B:179:CYS:SG	2:B:180:TYR:N	2.90	0.44
2:B:293:PRO:O	2:B:296:GLU:HB3	2.17	0.44
2:B:307:ASP:C	2:B:311:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ARG:CB	2:B:566:LEU:HD11	2.44	0.44
2:B:597:MET:SD	2:B:617:ARG:HB3	2.58	0.44
2:B:797:TYR:CD1	2:B:853:SER:O	2.70	0.44
2:B:834:ASN:HB2	2:B:838:SER:O	2.17	0.44
2:B:841:MET:HE3	2:B:990:ILE:HD13	1.98	0.44
2:B:941:LEU:CG	2:B:942:ARG:H	2.29	0.44
3:C:258:ILE:HD12	11:K:35:PHE:HE1	1.82	0.44
4:D:50:LEU:HD23	4:D:50:LEU:H	1.78	0.44
5:E:112:TYR:O	5:E:112:TYR:CD1	2.70	0.44
5:E:171:LYS:O	5:E:172:GLU:C	2.60	0.44
6:F:72:LYS:O	6:F:73:ALA:CB	2.65	0.44
8:H:11:GLN:CG	8:H:12:VAL:H	2.24	0.44
1:A:80:HIS:N	1:A:80:HIS:ND1	2.64	0.44
1:A:262:LEU:HD12	1:A:262:LEU:N	2.32	0.44
1:A:703:THR:O	1:A:703:THR:OG1	2.34	0.44
1:A:1004:ASN:ND2	5:E:167:ARG:NH1	2.64	0.44
1:A:1042:PHE:O	1:A:1045:VAL:N	2.50	0.44
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.18	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.98	0.44
1:A:1317:MET:HG2	5:E:142:VAL:HG11	2.00	0.44
1:A:1390:ASN:ND2	1:A:1399:ARG:HG2	2.33	0.44
2:B:90:ILE:HG13	2:B:90:ILE:O	2.16	0.44
2:B:293:PRO:HD2	2:B:296:GLU:CG	2.47	0.44
2:B:595:ARG:O	2:B:599:THR:CG2	2.65	0.44
2:B:803:LEU:HG	10:J:52:THR:CG2	2.47	0.44
2:B:805:THR:HG21	2:B:1041:GLU:CG	2.44	0.44
2:B:992:ILE:HD12	11:K:67:PHE:CE1	2.52	0.44
2:B:1202:LEU:C	2:B:1204:PHE:N	2.74	0.44
5:E:4:GLU:CA	5:E:6:GLU:OE1	2.63	0.44
6:F:123:LYS:O	6:F:124:GLU:C	2.60	0.44
7:G:142:ARG:HB2	7:G:171:ILE:HG21	1.99	0.44
7:G:160:ILE:N	7:G:160:ILE:CD1	2.75	0.44
9:I:62:ILE:HD13	9:I:102:VAL:CG1	2.46	0.44
9:I:89:GLN:O	9:I:89:GLN:CG	2.65	0.44
1:A:379:VAL:HG12	1:A:380:VAL:N	2.31	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.61	0.44
1:A:525:GLN:CB	2:B:1015:HIS:CD2	2.99	0.44
1:A:643:ALA:O	1:A:646:PHE:N	2.50	0.44
1:A:1198:ASP:C	1:A:1198:ASP:OD1	2.60	0.44
1:A:1261:LYS:O	1:A:1264:GLU:HB2	2.17	0.44
2:B:202:TYR:N	2:B:202:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ALA:O	2:B:462:ALA:N	2.50	0.44
2:B:703:ILE:HG23	2:B:741:CYS:CA	2.47	0.44
2:B:797:TYR:C	2:B:798:TYR:CD1	2.95	0.44
2:B:873:THR:O	2:B:915:THR:N	2.44	0.44
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.32	0.44
3:C:166:GLU:O	11:K:6:ARG:NH1	2.50	0.44
7:G:18:PHE:CD1	7:G:18:PHE:N	2.83	0.44
1:A:70:CYS:C	1:A:72:GLU:H	2.26	0.44
1:A:563:PRO:HD2	8:H:79:TRP:NE1	2.32	0.44
1:A:614:PHE:HB3	8:H:122:LEU:HD11	1.99	0.44
1:A:690:VAL:O	1:A:690:VAL:CG1	2.64	0.44
1:A:724:GLU:HB2	1:A:728:LYS:HD2	2.00	0.44
1:A:836:TYR:OH	1:A:1403:GLU:OE1	2.35	0.44
1:A:850:VAL:HG12	1:A:851:HIS:O	2.18	0.44
1:A:942:PHE:CD1	1:A:942:PHE:C	2.96	0.44
1:A:1128:GLN:H	1:A:1128:GLN:CD	2.26	0.44
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.50	0.44
1:A:1225:PHE:HB2	1:A:1243:VAL:HG23	1.99	0.44
2:B:97:VAL:HG22	2:B:128:LEU:HD23	2.00	0.44
2:B:115:GLN:HE22	2:B:118:ARG:NH1	2.15	0.44
2:B:254:LEU:HD22	2:B:381:MET:HE1	1.99	0.44
2:B:459:TYR:CE2	2:B:470:LYS:NZ	2.83	0.44
2:B:682:SER:HA	2:B:685:LEU:HG	1.99	0.44
2:B:702:LEU:HG	2:B:738:PHE:HD1	1.82	0.44
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.00	0.44
2:B:784:ASN:O	2:B:788:ARG:HB2	2.18	0.44
3:C:104:PHE:CD1	3:C:105:GLY:N	2.85	0.44
4:D:5:THR:O	7:G:42:PHE:HE2	1.99	0.44
4:D:53:SER:O	4:D:56:ARG:HB3	2.17	0.44
5:E:42:PHE:O	5:E:46:TYR:N	2.50	0.44
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.98	0.44
10:J:33:GLY:O	10:J:47:ARG:NH2	2.51	0.44
11:K:29:ASN:O	11:K:29:ASN:OD1	2.35	0.44
11:K:32:VAL:CG2	11:K:74:ARG:HG3	2.45	0.44
1:A:49:LYS:NZ	1:A:55:ASP:HB2	2.33	0.44
2:B:279:ASP:N	2:B:279:ASP:OD1	2.50	0.44
2:B:308:TRP:CZ2	9:I:52:ILE:CD1	3.00	0.44
2:B:373:ARG:CA	2:B:566:LEU:HD11	2.48	0.44
2:B:700:SER:O	2:B:701:ILE:CG2	2.66	0.44
2:B:954:VAL:HA	2:B:963:PHE:O	2.17	0.44
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:MET:CE	11:K:21:ILE:HG13	2.42	0.44
4:D:52:LEU:O	4:D:55:ALA:HB3	2.17	0.44
5:E:161:LYS:C	5:E:163:GLU:N	2.75	0.44
9:I:22:ASN:OD1	9:I:22:ASN:O	2.36	0.44
1:A:149:GLU:HB2	1:A:164:ARG:CZ	2.48	0.44
1:A:507:VAL:H	1:A:508:PRO:HD3	1.81	0.44
1:A:742:ASN:O	1:A:746:MET:N	2.50	0.44
1:A:808:LEU:HB3	1:A:812:GLU:HB2	1.99	0.44
1:A:849:MET:O	1:A:850:VAL:C	2.61	0.44
1:A:1152:ILE:HD12	9:I:44:TYR:CB	2.46	0.44
1:A:1368:MET:O	1:A:1371:LEU:N	2.50	0.44
1:A:1423:GLY:HA3	1:A:1426:GLU:OE1	2.17	0.44
2:B:173:MET:HB3	2:B:203:PHE:CE1	2.52	0.44
2:B:417:PHE:C	2:B:417:PHE:CD1	2.96	0.44
2:B:545:ILE:C	2:B:634:TYR:HE1	2.24	0.44
2:B:874:PHE:CE1	2:B:912:ILE:CG2	3.01	0.44
3:C:104:PHE:CD1	3:C:104:PHE:C	2.96	0.44
4:D:63:LEU:CD2	4:D:133:THR:OG1	2.66	0.44
7:G:1:MET:HE2	7:G:79:PHE:CE2	2.52	0.44
11:K:47:ARG:HG3	11:K:60:ALA:HA	1.99	0.44
12:L:39:SER:O	12:L:40:LEU:HB2	2.18	0.44
1:A:5:GLN:CD	2:B:1175:LEU:CD1	2.91	0.44
1:A:31:SER:HB2	1:A:82:GLY:HA2	1.99	0.44
1:A:325:ILE:O	1:A:326:ARG:C	2.58	0.44
1:A:337:ARG:HH12	2:B:1132:GLU:CG	2.31	0.44
1:A:664:THR:CG2	2:B:1014:PRO:HB3	2.48	0.44
1:A:667:GLY:C	3:C:192:TRP:HZ2	2.25	0.44
1:A:741:ASN:OD1	1:A:743:VAL:HG12	2.17	0.44
1:A:811:GLN:O	1:A:814:PHE:N	2.49	0.44
1:A:834:PRO:HA	1:A:837:ILE:CG1	2.48	0.44
1:A:955:PRO:O	1:A:956:LEU:HG	2.18	0.44
1:A:1340:GLY:N	5:E:183:PRO:HG2	2.33	0.44
2:B:103:ASN:OD1	2:B:109:THR:HA	2.18	0.44
2:B:313:MET:C	2:B:315:LYS:N	2.76	0.44
2:B:496:ARG:CD	2:B:751:VAL:HG21	2.32	0.44
2:B:654:ARG:O	2:B:656:GLY:N	2.50	0.44
2:B:980:PHE:CE1	2:B:1094:ARG:HG3	2.51	0.44
2:B:1116:ARG:HG2	2:B:1198:TYR:CE2	2.53	0.44
3:C:37:MET:HE1	3:C:232:VAL:CG2	2.47	0.44
3:C:148:ARG:O	3:C:150:GLY:N	2.51	0.44
3:C:193:TYR:HD2	3:C:196:ASP:C	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:HH12	4:D:155:ARG:HA	1.82	0.44
1:A:112:LYS:O	1:A:113:LEU:C	2.61	0.44
1:A:330:LYS:HG2	1:A:331:GLY:H	1.82	0.44
1:A:503:GLN:OE1	1:A:503:GLN:HA	2.17	0.44
1:A:514:PRO:O	1:A:515:GLN:C	2.61	0.44
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.43	0.44
1:A:683:ILE:O	1:A:687:LYS:HE3	2.18	0.44
1:A:858:ASN:ND2	1:A:860:LEU:HD12	2.33	0.44
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.81	0.44
1:A:1133:LEU:O	1:A:1137:ALA:N	2.51	0.44
2:B:588:GLY:O	2:B:589:VAL:HG22	2.18	0.44
2:B:618:ASP:O	2:B:619:ILE:C	2.60	0.44
3:C:246:ARG:HA	3:C:249:ASP:HB3	2.00	0.44
4:D:209:ARG:NH2	4:D:213:GLU:HG3	2.33	0.44
5:E:12:LEU:HD13	5:E:55:ARG:HE	1.83	0.44
5:E:39:LEU:HD23	5:E:39:LEU:H	1.83	0.44
7:G:59:GLY:HA3	7:G:70:PHE:CE1	2.53	0.44
12:L:46:VAL:O	12:L:47:ARG:CG	2.56	0.44
1:A:262:LEU:O	1:A:266:LEU:HG	2.18	0.44
1:A:541:ILE:HG21	1:A:549:MET:HE3	2.00	0.44
1:A:834:PRO:HG2	1:A:1077:THR:HA	1.98	0.44
1:A:1055:ARG:NH2	6:F:154:ASP:OD1	2.24	0.44
1:A:1149:ALA:HA	9:I:47:GLU:HA	2.00	0.44
2:B:121:ASN:ND2	2:B:965:LYS:HZ1	2.15	0.44
2:B:226:PHE:O	2:B:227:LYS:C	2.61	0.44
2:B:326:ASP:OD1	2:B:326:ASP:C	2.61	0.44
2:B:415:GLN:O	2:B:419:THR:OG1	2.29	0.44
2:B:637:LEU:CD2	2:B:703:ILE:HG12	2.45	0.44
2:B:831:SER:CB	2:B:833:TYR:HD2	2.31	0.44
2:B:853:SER:O	2:B:971:THR:HG23	2.17	0.44
2:B:860:MET:HE1	2:B:862:GLN:NE2	2.32	0.44
2:B:1168:LEU:HD13	2:B:1170:THR:HG21	2.00	0.44
3:C:84:ARG:HE	11:K:11:LEU:HD22	1.82	0.44
3:C:236:GLY:O	3:C:237:SER:C	2.60	0.44
6:F:109:VAL:HG13	6:F:123:LYS:HD3	1.98	0.44
7:G:112:LYS:C	7:G:112:LYS:CD	2.89	0.44
7:G:112:LYS:HD3	7:G:112:LYS:O	2.17	0.44
1:A:69:THR:HG22	1:A:70:CYS:N	2.33	0.43
1:A:145:LYS:HE3	1:A:147:VAL:HG23	2.00	0.43
1:A:640:GLN:CD	1:A:640:GLN:N	2.73	0.43
1:A:954:TRP:HB3	1:A:955:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:LEU:HD11	5:E:147:HIS:CD2	2.53	0.43
2:B:46:GLN:HG2	2:B:47:GLN:N	2.33	0.43
2:B:95:ILE:C	2:B:96:TYR:CD1	2.96	0.43
2:B:122:LEU:HD21	2:B:958:GLN:N	2.33	0.43
2:B:580:VAL:O	2:B:586:TRP:HD1	2.00	0.43
2:B:1106:ARG:NH2	2:B:1111:MET:HE2	2.33	0.43
3:C:238:ILE:HD11	3:C:246:ARG:HH21	1.82	0.43
5:E:155:ARG:HD2	5:E:188:LEU:CD2	2.48	0.43
5:E:182:ASP:O	5:E:183:PRO:C	2.61	0.43
7:G:159:ALA:C	7:G:160:ILE:HD12	2.43	0.43
8:H:44:VAL:O	8:H:44:VAL:HG22	2.18	0.43
10:J:16:ASP:CG	10:J:17:LYS:N	2.76	0.43
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.44	0.43
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.00	0.43
11:K:47:ARG:O	11:K:50:LEU:N	2.51	0.43
11:K:90:ALA:O	11:K:94:ILE:HG13	2.17	0.43
1:A:675:THR:O	1:A:676:MET:C	2.59	0.43
1:A:782:ARG:NH2	2:B:699:GLU:O	2.48	0.43
1:A:833:GLU:HB3	1:A:834:PRO:CD	2.44	0.43
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.43
1:A:1195:LEU:HD23	1:A:1267:MET:CE	2.46	0.43
1:A:1209:MET:SD	1:A:1236:LEU:HD13	2.58	0.43
2:B:198:ASP:OD1	2:B:199:MET:N	2.51	0.43
2:B:916:THR:O	2:B:935:ARG:HB2	2.18	0.43
2:B:956:THR:HB	2:B:960:GLY:HA2	1.99	0.43
3:C:8:VAL:HG21	11:K:101:LEU:HD12	2.00	0.43
4:D:27:LEU:HD21	4:D:173:HIS:CB	2.48	0.43
7:G:9:LEU:HG	7:G:11:ILE:HG13	2.00	0.43
9:I:65:ASP:OD1	9:I:67:THR:CG2	2.66	0.43
9:I:65:ASP:HB3	9:I:68:LEU:HD12	2.00	0.43
10:J:6:ARG:H	10:J:15:GLY:H	1.65	0.43
1:A:183:GLY:N	1:A:200:ARG:O	2.46	0.43
1:A:486:GLU:O	1:A:487:MET:HG3	2.19	0.43
1:A:532:ARG:HG2	1:A:749:ALA:HB2	2.01	0.43
1:A:902:LEU:N	1:A:902:LEU:HD12	2.34	0.43
1:A:960:ILE:C	1:A:962:ARG:N	2.76	0.43
2:B:781:PHE:HE2	2:B:793:ALA:HB1	1.82	0.43
2:B:800:GLN:OE1	2:B:821:GLN:HB3	2.18	0.43
3:C:35:ARG:HH21	11:K:41:THR:H	1.66	0.43
3:C:36:VAL:HG11	3:C:251:LEU:CD1	2.49	0.43
3:C:74:SER:O	3:C:75:MET:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG11	6:F:123:LYS:HD3	2.00	0.43
6:F:127:GLU:O	6:F:128:LYS:C	2.61	0.43
8:H:12:VAL:HG21	8:H:50:ALA:N	2.33	0.43
10:J:25:LEU:O	10:J:29:GLU:HA	2.19	0.43
1:A:423:ASP:CG	1:A:424:ILE:H	2.17	0.43
1:A:440:ASP:HB2	1:A:460:VAL:CG2	2.48	0.43
1:A:452:LYS:O	1:A:454:SER:N	2.51	0.43
1:A:587:HIS:CD2	1:A:608:ILE:HG23	2.54	0.43
1:A:663:SER:HB2	2:B:827:ILE:O	2.19	0.43
2:B:223:VAL:HG13	2:B:240:ILE:HD13	2.01	0.43
2:B:294:ASP:HB2	2:B:318:VAL:HG13	1.99	0.43
2:B:367:LEU:N	2:B:367:LEU:CD2	2.68	0.43
2:B:401:PHE:CE2	2:B:521:LEU:HD12	2.53	0.43
2:B:496:ARG:NE	2:B:751:VAL:HG22	2.33	0.43
2:B:753:ALA:O	2:B:755:ILE:N	2.50	0.43
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.43
2:B:973:ILE:O	2:B:975:GLN:N	2.52	0.43
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.31	0.43
2:B:1065:GLN:OE1	3:C:201:TRP:HA	2.18	0.43
2:B:1222:ARG:O	2:B:1223:ASP:CB	2.66	0.43
3:C:198:ALA:C	3:C:200:GLU:H	2.26	0.43
4:D:48:ILE:CG2	7:G:4:ILE:HG13	2.49	0.43
6:F:110:ASP:OD1	6:F:110:ASP:C	2.60	0.43
9:I:24:ARG:NH2	9:I:37:GLU:HG3	2.33	0.43
9:I:94:ASP:O	9:I:95:THR:C	2.62	0.43
11:K:87:LEU:O	11:K:88:LYS:C	2.62	0.43
1:A:673:GLY:C	1:A:675:THR:N	2.76	0.43
1:A:843:LYS:NZ	1:A:846:GLU:OE2	2.52	0.43
1:A:964:ILE:HG13	1:A:965:GLN:H	1.83	0.43
1:A:1155:ASP:C	1:A:1155:ASP:OD1	2.60	0.43
1:A:1349:TYR:O	1:A:1350:LYS:C	2.61	0.43
2:B:234:ILE:HG21	2:B:237:VAL:CG2	2.49	0.43
2:B:350:GLN:C	2:B:352:ALA:N	2.76	0.43
2:B:657:HIS:HA	2:B:660:LYS:HB3	1.99	0.43
2:B:662:MET:HE3	2:B:662:MET:HB3	1.61	0.43
2:B:689:LEU:C	2:B:690:VAL:HG13	2.44	0.43
2:B:986:GLN:HG2	2:B:1025:HIS:CD2	2.54	0.43
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.43
2:B:1169:MET:H	2:B:1169:MET:HG2	1.64	0.43
3:C:137:LYS:C	3:C:139:GLY:H	2.26	0.43
3:C:242:GLN:O	3:C:246:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.98	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.17	0.43
10:J:41:LEU:N	10:J:41:LEU:HD12	2.33	0.43
1:A:243:PRO:CB	1:A:244:PRO:CD	2.96	0.43
1:A:417:TYR:O	1:A:418:SER:C	2.60	0.43
1:A:836:TYR:OH	1:A:1403:GLU:CD	2.61	0.43
1:A:903:ASN:O	1:A:907:THR:OG1	2.36	0.43
1:A:962:ARG:CA	1:A:965:GLN:OE1	2.63	0.43
1:A:1133:LEU:O	1:A:1137:ALA:CB	2.67	0.43
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.53	0.43
2:B:803:LEU:HD12	2:B:822:ASN:OD1	2.19	0.43
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.31	0.43
2:B:1202:LEU:O	2:B:1205:GLN:N	2.52	0.43
3:C:44:LEU:HG	3:C:45:ALA:N	2.34	0.43
4:D:138:ASN:HD21	4:D:141:LEU:HB2	1.83	0.43
7:G:22:MET:HG2	7:G:26:LEU:HD11	2.00	0.43
10:J:53:HIS:CD2	10:J:53:HIS:C	2.95	0.43
1:A:75:ASN:O	1:A:76:GLU:CB	2.67	0.43
1:A:361:LEU:HG	1:A:507:VAL:CG1	2.48	0.43
1:A:556:TRP:CG	1:A:558:GLY:H	2.37	0.43
1:A:738:LYS:HD3	1:A:739:ASP:H	1.78	0.43
1:A:970:THR:CG2	1:A:971:PHE:CD1	2.99	0.43
1:A:1011:GLN:HE22	1:A:1015:VAL:HG13	1.82	0.43
1:A:1042:PHE:CE2	1:A:1046:LEU:CD1	3.02	0.43
1:A:1048:ASN:O	1:A:1049:ILE:C	2.59	0.43
1:A:1444:MET:N	6:F:133:VAL:O	2.48	0.43
1:A:1453:TYR:CE1	6:F:129:LYS:HA	2.53	0.43
2:B:30:SER:O	2:B:33:VAL:HB	2.18	0.43
2:B:34:ILE:HG12	2:B:542:MET:HE1	2.01	0.43
2:B:216:GLU:HA	2:B:406:LEU:CA	2.46	0.43
2:B:309:GLN:HA	2:B:312:GLU:HG2	2.00	0.43
2:B:451:LYS:HE2	2:B:451:LYS:HB3	1.89	0.43
2:B:522:VAL:CG1	2:B:523:CYS:H	2.31	0.43
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.53	0.43
2:B:583:ASN:HD21	2:B:628:THR:HG1	1.66	0.43
2:B:702:LEU:H	2:B:739:THR:HG23	1.84	0.43
2:B:759:PRO:HB3	2:B:767:ASN:HD21	1.81	0.43
5:E:63:ASN:CB	5:E:64:PRO:HD2	2.49	0.43
10:J:5:VAL:C	10:J:6:ARG:HG2	2.44	0.43
10:J:26:GLN:O	10:J:29:GLU:HG2	2.18	0.43
1:A:41:MET:CB	1:A:49:LYS:HA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:O	1:A:94:GLY:N	2.52	0.43
1:A:95:PHE:O	1:A:99:ILE:HG13	2.19	0.43
1:A:403:LYS:C	1:A:415:LEU:HD13	2.44	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.54	0.43
1:A:1061:GLY:O	1:A:1062:GLU:C	2.62	0.43
2:B:237:VAL:HG12	2:B:238:ALA:N	2.33	0.43
2:B:309:GLN:HG3	2:B:390:LEU:HD13	2.01	0.43
2:B:375:ALA:C	2:B:377:PHE:H	2.27	0.43
2:B:652:LYS:HG2	2:B:689:LEU:HD23	2.01	0.43
2:B:710:LEU:HB3	2:B:733:HIS:HB3	2.01	0.43
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.19	0.43
5:E:52:ARG:O	5:E:53:PRO:C	2.61	0.43
7:G:93:SER:HB2	7:G:100:GLU:HB2	2.01	0.43
10:J:45:CYS:SG	10:J:46:CYS:N	2.92	0.43
11:K:63:VAL:C	11:K:65:HIS:N	2.77	0.43
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.52	0.43
1:A:794:PRO:HG2	1:A:795:GLU:CD	2.44	0.43
1:A:836:TYR:O	1:A:840:ARG:HG3	2.19	0.43
1:A:1389:PHE:HZ	1:A:1402:PHE:CE2	2.37	0.43
3:C:238:ILE:HG13	3:C:239:PRO:CD	2.49	0.43
4:D:58:VAL:O	4:D:58:VAL:CG2	2.67	0.43
4:D:138:ASN:OD1	4:D:141:LEU:N	2.39	0.43
5:E:83:CYS:HB2	5:E:110:PHE:HZ	1.82	0.43
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.54	0.43
9:I:15:TYR:HE1	9:I:30:ARG:HB2	1.84	0.43
11:K:109:TRP:C	11:K:111:LEU:H	2.26	0.43
12:L:58:LYS:O	12:L:59:ALA:O	2.37	0.43
1:A:106:VAL:CG2	1:A:107:CYS:N	2.82	0.43
1:A:341:MET:CE	1:A:1401:SER:OG	2.67	0.43
1:A:366:VAL:HG21	1:A:489:LEU:HD11	2.01	0.43
1:A:443:LEU:HD23	2:B:1146:PHE:CZ	2.54	0.43
1:A:538:ASP:OD1	8:H:22:LYS:CB	2.66	0.43
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.67	0.43
1:A:981:LEU:HD13	1:A:1032:LEU:HD21	2.01	0.43
1:A:1146:VAL:HG13	1:A:1201:ALA:HB1	2.00	0.43
1:A:1443:VAL:HG22	6:F:92:ARG:HH21	1.83	0.43
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.54	0.43
2:B:814:PHE:C	2:B:816:GLU:N	2.77	0.43
2:B:849:GLY:HA2	2:B:852:ARG:HE	1.84	0.43
2:B:953:LEU:HD11	12:L:55:ILE:HG13	1.99	0.43
4:D:156:ASP:O	4:D:159:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:VAL:HG23	4:D:161:GLY:N	2.33	0.43
7:G:112:LYS:HD2	7:G:113:HIS:ND1	2.32	0.43
1:A:545:GLN:NE2	1:A:549:MET:HE2	2.33	0.42
1:A:597:LEU:HD21	8:H:103:LYS:HB3	2.00	0.42
1:A:680:THR:C	1:A:683:ILE:HG12	2.44	0.42
1:A:775:ILE:HG12	1:A:797:LYS:CA	2.49	0.42
1:A:854:ASN:O	1:A:866:PHE:O	2.37	0.42
1:A:981:LEU:HD12	1:A:981:LEU:N	2.34	0.42
1:A:1017:LEU:CD1	5:E:204:THR:O	2.67	0.42
2:B:31:TRP:CZ3	2:B:34:ILE:CD1	3.02	0.42
2:B:114:PRO:O	2:B:115:GLN:C	2.60	0.42
2:B:729:ILE:O	2:B:729:ILE:HG23	2.17	0.42
3:C:21:ILE:O	3:C:21:ILE:CG1	2.67	0.42
5:E:157:SER:N	5:E:160:GLU:HB2	2.34	0.42
10:J:61:LEU:N	10:J:61:LEU:HD23	2.34	0.42
1:A:39:GLU:HB3	1:A:42:ASP:OD1	2.19	0.42
1:A:49:LYS:HD2	1:A:55:ASP:CB	2.41	0.42
1:A:248:PRO:O	1:A:260:ASP:HB2	2.19	0.42
1:A:308:ILE:HD12	1:A:311:GLN:HG2	2.01	0.42
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.32	0.42
1:A:549:MET:O	1:A:550:LEU:C	2.60	0.42
1:A:681:GLU:O	1:A:684:ALA:N	2.52	0.42
1:A:721:PHE:O	1:A:725:ALA:HB2	2.20	0.42
1:A:754:SER:OG	1:A:755:PHE:N	2.52	0.42
1:A:1017:LEU:O	1:A:1018:PHE:C	2.61	0.42
1:A:1044:TRP:O	1:A:1045:VAL:C	2.62	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.54	0.42
2:B:122:LEU:HD22	2:B:958:GLN:HB3	2.00	0.42
2:B:752:ALA:C	2:B:754:SER:N	2.77	0.42
2:B:844:SER:HA	2:B:847:ASP:HB2	2.01	0.42
2:B:1059:LEU:HD12	2:B:1059:LEU:HA	1.80	0.42
2:B:1103:ILE:O	2:B:1122:ARG:HD2	2.19	0.42
6:F:152:ILE:O	6:F:153:VAL:CG2	2.66	0.42
7:G:99:PHE:HD2	7:G:115:MET:HE2	1.77	0.42
8:H:48:PRO:O	8:H:49:VAL:HG13	2.19	0.42
9:I:46:HIS:NE2	9:I:48:LEU:HD21	2.33	0.42
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.83	0.42
1:A:121:LEU:HB3	1:A:141:LEU:HD12	2.00	0.42
1:A:353:ILE:HG21	1:A:487:MET:CB	2.42	0.42
1:A:359:LEU:HD22	1:A:363:GLN:CG	2.45	0.42
1:A:606:LEU:O	1:A:613:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLY:HA2	1:A:763:ALA:HB2	2.00	0.42
1:A:897:TYR:HE1	1:A:1024:SER:O	2.02	0.42
1:A:1143:LEU:HD23	1:A:1268:LEU:HA	2.01	0.42
1:A:1332:PHE:CE1	1:A:1381:LEU:CD2	3.01	0.42
1:A:1452:LYS:HB2	1:A:1452:LYS:HE3	1.75	0.42
2:B:658:ILE:HG22	2:B:659:ALA:H	1.84	0.42
2:B:702:LEU:H	2:B:739:THR:CG2	2.33	0.42
2:B:876:LYS:HD2	2:B:895:ASP:HA	2.01	0.42
2:B:1103:ILE:HG13	2:B:1104:HIS:N	2.35	0.42
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.50	0.42
4:D:27:LEU:CD1	4:D:197:SER:CB	2.96	0.42
6:F:103:MET:O	6:F:104:ASN:HB2	2.19	0.42
6:F:127:GLU:CB	6:F:129:LYS:HG3	2.48	0.42
11:K:24:ASP:HB3	11:K:30:ALA:HB3	2.00	0.42
13:R:8:G:H2'	13:R:9:G:C8	2.54	0.42
1:A:356:ASP:HB3	1:A:359:LEU:HB2	2.01	0.42
1:A:586:ILE:CD1	1:A:633:VAL:HG12	2.49	0.42
1:A:900:ASP:O	1:A:907:THR:OG1	2.30	0.42
1:A:1004:ASN:HD22	5:E:167:ARG:NH1	2.17	0.42
1:A:1099:PRO:O	1:A:1102:LYS:N	2.52	0.42
2:B:515:HIS:ND1	2:B:517:THR:N	2.60	0.42
2:B:754:SER:OG	2:B:808:ALA:HB1	2.18	0.42
2:B:834:ASN:HB3	2:B:840:ILE:HG23	2.01	0.42
2:B:976:ILE:HD13	2:B:992:ILE:HA	2.01	0.42
2:B:995:ARG:NH1	11:K:9:LEU:CD1	2.78	0.42
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.50	0.42
3:C:251:LEU:HD12	3:C:251:LEU:HA	1.84	0.42
4:D:178:ALA:O	4:D:180:LEU:N	2.52	0.42
5:E:198:ILE:HD11	5:E:212:ARG:HB2	2.00	0.42
8:H:130:ARG:O	8:H:130:ARG:HG2	2.19	0.42
9:I:15:TYR:CD1	9:I:30:ARG:HG3	2.53	0.42
9:I:19:ASP:CG	9:I:24:ARG:HG2	2.44	0.42
11:K:18:LYS:C	11:K:19:LEU:HD12	2.45	0.42
11:K:43:GLY:O	11:K:44:ASN:C	2.63	0.42
1:A:178:GLY:O	1:A:180:LYS:N	2.52	0.42
1:A:443:LEU:HD23	2:B:1146:PHE:HZ	1.85	0.42
1:A:446:ARG:NH1	1:A:446:ARG:HG3	2.34	0.42
1:A:617:VAL:CG1	1:A:622:VAL:HB	2.50	0.42
1:A:960:ILE:HG12	1:A:1021:LEU:HD21	2.01	0.42
1:A:1390:ASN:HD21	1:A:1399:ARG:HB3	1.84	0.42
1:A:1409:LEU:HD12	1:A:1409:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:O	2:B:365:THR:CB	2.63	0.42
2:B:544:CYS:SG	2:B:545:ILE:N	2.88	0.42
2:B:680:THR:HG22	2:B:683:SER:H	1.84	0.42
2:B:781:PHE:CD1	2:B:781:PHE:C	2.97	0.42
3:C:178:PHE:C	3:C:178:PHE:CD1	2.98	0.42
3:C:186:LEU:HB2	3:C:188:HIS:HD2	1.85	0.42
3:C:252:GLN:HE22	11:K:102:LYS:HD2	1.85	0.42
4:D:59:ILE:HB	4:D:145:MET:SD	2.59	0.42
4:D:153:ARG:NH1	4:D:184:ALA:HA	2.34	0.42
5:E:14:ARG:HH21	5:E:141:VAL:HG22	1.84	0.42
5:E:66:GLU:HA	5:E:69:ILE:CG1	2.50	0.42
1:A:107:CYS:O	1:A:109:HIS:N	2.52	0.42
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.54	0.42
1:A:330:LYS:CG	1:A:331:GLY:N	2.83	0.42
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.00	0.42
1:A:525:GLN:CA	2:B:1015:HIS:HD2	2.31	0.42
1:A:692:ASP:C	1:A:694:THR:N	2.77	0.42
1:A:919:ILE:HD11	1:A:925:LEU:HD23	2.01	0.42
2:B:256:VAL:HG22	2:B:271:ALA:CB	2.48	0.42
2:B:299:GLU:HB3	2:B:572:HIS:NE2	2.34	0.42
2:B:326:ASP:OD2	2:B:329:THR:HG23	2.19	0.42
2:B:384:ARG:NH2	2:B:623:GLU:OE1	2.53	0.42
2:B:583:ASN:ND2	2:B:628:THR:OG1	2.47	0.42
2:B:595:ARG:O	2:B:595:ARG:HG3	2.19	0.42
2:B:609:ILE:HG22	2:B:610:ASN:N	2.34	0.42
2:B:778:MET:HG3	2:B:794:ASN:HB3	2.01	0.42
2:B:789:MET:CE	2:B:967:ARG:HB2	2.48	0.42
2:B:873:THR:O	2:B:914:LYS:HA	2.19	0.42
2:B:1017:ILE:CG1	2:B:1018:PRO:HD3	2.44	0.42
2:B:1168:LEU:HD13	2:B:1170:THR:CG2	2.49	0.42
3:C:197:SER:O	3:C:198:ALA:C	2.62	0.42
4:D:50:LEU:N	4:D:50:LEU:CD2	2.77	0.42
4:D:51:ASN:CB	4:D:181:GLY:O	2.66	0.42
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.19	0.42
10:J:26:GLN:O	10:J:29:GLU:N	2.53	0.42
1:A:40:THR:HG21	1:A:259:GLU:CG	2.46	0.42
1:A:70:CYS:O	1:A:70:CYS:SG	2.78	0.42
1:A:440:ASP:H	1:A:460:VAL:H	1.66	0.42
1:A:446:ARG:CG	1:A:447:GLN:H	2.32	0.42
1:A:542:GLU:CG	1:A:543:LEU:N	2.81	0.42
1:A:571:LEU:HD12	1:A:571:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:PRO:HG2	1:A:640:GLN:CD	2.44	0.42
1:A:846:GLU:C	1:A:848:ILE:H	2.28	0.42
1:A:960:ILE:C	1:A:962:ARG:H	2.28	0.42
1:A:1294:PRO:O	1:A:1296:GLY:N	2.53	0.42
1:A:1339:LEU:HD22	5:E:147:HIS:CD2	2.54	0.42
2:B:128:LEU:HB3	2:B:167:ILE:HB	2.01	0.42
2:B:221:ASN:ND2	2:B:243:ALA:O	2.53	0.42
2:B:893:LEU:HD23	2:B:899:ILE:CG2	2.50	0.42
2:B:969:ARG:HG2	2:B:969:ARG:HH11	1.85	0.42
2:B:995:ARG:O	2:B:996:ARG:C	2.62	0.42
2:B:1039:GLY:HA3	10:J:33:GLY:CA	2.49	0.42
3:C:58:LEU:HD21	10:J:57:ILE:HD12	2.02	0.42
4:D:37:GLN:HE21	4:D:47:LEU:CD1	2.23	0.42
4:D:48:ILE:HG21	7:G:4:ILE:CB	2.49	0.42
7:G:87:VAL:HG23	7:G:145:VAL:CG2	2.50	0.42
7:G:114:LEU:N	7:G:114:LEU:CD2	2.81	0.42
8:H:143:LEU:O	8:H:144:ILE:CD1	2.68	0.42
9:I:28:GLU:HG2	9:I:29:CYS:N	2.34	0.42
1:A:46:THR:C	1:A:48:ALA:N	2.77	0.42
1:A:95:PHE:CZ	1:A:1414:ALA:HB2	2.54	0.42
1:A:114:LEU:O	1:A:164:ARG:NH2	2.53	0.42
1:A:120:GLU:HA	1:A:123:ARG:NE	2.33	0.42
1:A:366:VAL:CG2	1:A:489:LEU:HD11	2.49	0.42
1:A:405:VAL:O	1:A:405:VAL:HG13	2.19	0.42
1:A:423:ASP:O	1:A:424:ILE:HG22	2.20	0.42
1:A:457:ALA:CB	1:A:505:CYS:O	2.68	0.42
1:A:569:LYS:HB3	8:H:46:LEU:CD1	2.50	0.42
1:A:699:ALA:C	1:A:701:LEU:H	2.28	0.42
1:A:1262:LYS:HB3	1:A:1263:ILE:HD12	2.02	0.42
1:A:1268:LEU:CD1	9:I:48:LEU:HD11	2.50	0.42
1:A:1397:LEU:HD13	1:A:1429:ILE:HG21	2.00	0.42
2:B:33:VAL:O	2:B:34:ILE:C	2.63	0.42
2:B:283:VAL:CG2	2:B:284:ILE:N	2.83	0.42
2:B:370:PHE:C	2:B:372:SER:H	2.28	0.42
2:B:546:SER:N	2:B:634:TYR:HE1	2.18	0.42
2:B:846:ILE:HB	2:B:974:PRO:HG2	2.00	0.42
2:B:1024:ALA:O	2:B:1028:GLU:HB2	2.20	0.42
2:B:1027:ILE:O	2:B:1030:LEU:N	2.53	0.42
2:B:1029:CYS:HB3	2:B:1086:PHE:HZ	1.84	0.42
2:B:1199:ALA:O	2:B:1202:LEU:HB3	2.19	0.42
5:E:142:VAL:HG13	5:E:142:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ARG:HB2	8:H:41:ASP:OD1	2.20	0.42
8:H:30:SER:HB3	8:H:33:GLN:O	2.20	0.42
8:H:102:TYR:N	8:H:102:TYR:CD1	2.88	0.42
8:H:124:ARG:CZ	8:H:126:GLU:OE2	2.67	0.42
1:A:142:CYS:C	1:A:144:THR:N	2.78	0.42
1:A:460:VAL:HG12	1:A:461:LYS:N	2.35	0.42
1:A:513:SER:O	1:A:517:ASN:HA	2.20	0.42
1:A:563:PRO:C	1:A:576:GLN:HE22	2.28	0.42
1:A:733:ALA:C	1:A:735:VAL:N	2.76	0.42
1:A:1311:VAL:O	1:A:1311:VAL:HG12	2.20	0.42
1:A:1323:ASP:O	1:A:1324:PRO:C	2.62	0.42
2:B:113:TYR:HB3	2:B:114:PRO:HD2	2.01	0.42
2:B:956:THR:HG22	2:B:961:LEU:O	2.20	0.42
2:B:1031:LEU:HD23	2:B:1031:LEU:C	2.44	0.42
5:E:123:LEU:HD23	5:E:123:LEU:H	1.84	0.42
9:I:34:TYR:O	9:I:35:VAL:CG2	2.68	0.42
9:I:58:VAL:O	9:I:58:VAL:CG2	2.67	0.42
10:J:6:ARG:CB	10:J:12:LYS:C	2.93	0.42
11:K:50:LEU:HD13	11:K:75:ILE:CD1	2.50	0.42
1:A:76:GLU:OE1	2:B:1159:ARG:NH2	2.53	0.42
1:A:848:ILE:O	1:A:1065:GLY:N	2.33	0.42
1:A:989:GLY:O	1:A:990:VAL:C	2.62	0.42
1:A:1054:LEU:O	1:A:1057:VAL:CG1	2.68	0.42
1:A:1339:LEU:HD21	5:E:147:HIS:CD2	2.55	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.50	0.42
2:B:218:SER:O	2:B:219:ALA:C	2.63	0.42
2:B:282:ILE:O	2:B:286:PHE:HD2	2.02	0.42
2:B:446:LEU:O	2:B:447:ALA:CB	2.64	0.42
2:B:818:PRO:HD2	10:J:54:VAL:HG11	2.02	0.42
3:C:214:ASN:O	3:C:215:GLU:C	2.62	0.42
4:D:202:ILE:O	4:D:202:ILE:CG2	2.68	0.42
6:F:81:THR:O	6:F:82:THR:C	2.62	0.42
7:G:171:ILE:O	7:G:171:ILE:CG2	2.67	0.42
10:J:40:GLY:C	10:J:41:LEU:HD12	2.45	0.42
1:A:102:VAL:HG23	1:A:211:PHE:CE1	2.54	0.41
1:A:524:VAL:O	1:A:525:GLN:C	2.63	0.41
1:A:667:GLY:C	3:C:192:TRP:CZ2	2.98	0.41
1:A:1188:GLN:HA	1:A:1243:VAL:HA	2.02	0.41
2:B:31:TRP:O	2:B:32:ALA:C	2.63	0.41
2:B:333:PHE:O	2:B:333:PHE:CD1	2.73	0.41
2:B:373:ARG:HB3	2:B:566:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:HIS:ND1	2:B:517:THR:HG21	2.35	0.41
2:B:846:ILE:HD13	2:B:974:PRO:HD2	2.02	0.41
2:B:1188:LYS:HA	2:B:1191:ILE:HD11	2.01	0.41
4:D:23:ASN:HB2	4:D:28:GLN:O	2.20	0.41
4:D:39:ASN:ND2	4:D:45:GLU:OE2	2.53	0.41
4:D:155:ARG:C	4:D:155:ARG:HD2	2.45	0.41
4:D:208:GLU:HA	4:D:211:LEU:HB2	2.01	0.41
5:E:26:ARG:O	5:E:75:MET:CE	2.64	0.41
7:G:30:LEU:HD13	7:G:72:VAL:HG11	2.02	0.41
11:K:100:ALA:O	11:K:104:ASN:ND2	2.53	0.41
1:A:106:VAL:O	1:A:171:GLN:NE2	2.54	0.41
1:A:335:ARG:HD2	2:B:1202:LEU:HD23	2.02	0.41
1:A:474:VAL:O	1:A:478:TYR:CD2	2.66	0.41
1:A:840:ARG:O	1:A:844:ALA:HB2	2.20	0.41
1:A:1109:LYS:O	1:A:1111:MET:N	2.50	0.41
2:B:381:MET:HE3	2:B:381:MET:HB3	1.91	0.41
2:B:832:GLY:CA	2:B:835:GLN:CG	2.98	0.41
5:E:84:ASP:OD1	5:E:85:GLU:N	2.52	0.41
7:G:109:PHE:O	7:G:160:ILE:HA	2.20	0.41
8:H:9:ILE:HG13	8:H:56:THR:HG23	2.02	0.41
12:L:34:CYS:SG	12:L:35:SER:N	2.92	0.41
1:A:56:PRO:HD2	1:A:58:LEU:HG	2.02	0.41
1:A:345:VAL:HG12	2:B:1150:ARG:O	2.21	0.41
1:A:446:ARG:HH12	1:A:480:ALA:HA	1.84	0.41
1:A:579:SER:HA	1:A:582:ILE:HD12	2.02	0.41
1:A:818:MET:HA	2:B:514:LEU:HB3	2.02	0.41
1:A:886:ILE:HD12	1:A:943:LEU:HB3	2.02	0.41
1:A:946:VAL:HG13	5:E:201:LYS:HB2	2.02	0.41
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.55	0.41
2:B:358:LYS:O	2:B:366:GLN:OE1	2.38	0.41
2:B:540:SER:HB2	2:B:749:LEU:O	2.20	0.41
2:B:1156:ASP:OD1	2:B:1198:TYR:HB3	2.20	0.41
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.35	0.41
5:E:55:ARG:O	5:E:58:MET:HG2	2.21	0.41
6:F:109:VAL:HG21	6:F:123:LYS:HE3	2.00	0.41
7:G:47:CYS:N	7:G:77:VAL:HG12	2.36	0.41
11:K:42:LEU:O	11:K:43:GLY:C	2.63	0.41
11:K:57:LEU:N	11:K:76:GLN:O	2.44	0.41
12:L:28:LYS:HB2	12:L:39:SER:HA	2.01	0.41
1:A:108:MET:HG3	1:A:210:ILE:HG13	2.02	0.41
1:A:420:ARG:O	1:A:421:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:MET:CE	2:B:1134:GLU:CG	2.98	0.41
1:A:590:ARG:HH12	1:A:621:THR:HG23	1.86	0.41
1:A:919:ILE:O	1:A:922:ASP:HB2	2.21	0.41
1:A:923:LEU:HD23	1:A:923:LEU:N	2.35	0.41
1:A:1004:ASN:CB	5:E:167:ARG:CZ	2.98	0.41
1:A:1393:ASN:O	1:A:1394:THR:O	2.38	0.41
2:B:60:GLN:C	2:B:62:ILE:H	2.28	0.41
2:B:286:PHE:CD2	2:B:297:ILE:HG21	2.56	0.41
2:B:326:ASP:OD1	2:B:329:THR:N	2.49	0.41
2:B:600:LEU:HB3	2:B:615:MET:SD	2.61	0.41
2:B:776:GLN:OE1	13:R:9:G:OP1	2.38	0.41
2:B:797:TYR:CE2	2:B:852:ARG:HD2	2.55	0.41
2:B:809:MET:HE1	2:B:983:ARG:HH22	1.85	0.41
2:B:904:ARG:HH11	12:L:67:PHE:HD1	1.67	0.41
2:B:1098:MET:HE2	2:B:1098:MET:HB2	1.67	0.41
2:B:1117:GLN:HB3	2:B:1118:PRO:CD	2.50	0.41
2:B:1208:MET:HE2	2:B:1208:MET:HB3	1.96	0.41
3:C:80:LEU:HD11	3:C:95:CYS:N	2.34	0.41
4:D:40:HIS:C	4:D:41:GLN:OE1	2.63	0.41
5:E:16:PHE:CZ	5:E:20:LYS:HD3	2.55	0.41
6:F:83:PRO:HA	6:F:146:TRP:CH2	2.55	0.41
8:H:16:ASP:OD1	8:H:17:PRO:C	2.64	0.41
11:K:44:ASN:HA	11:K:61:TYR:HE1	1.81	0.41
12:L:32:ALA:C	12:L:34:CYS:H	2.28	0.41
1:A:204:THR:HG23	1:A:205:GLU:N	2.36	0.41
1:A:283:GLY:O	1:A:285:PRO:HD3	2.21	0.41
1:A:345:VAL:HA	2:B:1154:ALA:O	2.20	0.41
1:A:391:LEU:C	1:A:394:ASN:H	2.28	0.41
1:A:663:SER:OG	1:A:664:THR:N	2.53	0.41
1:A:742:ASN:O	1:A:745:GLN:N	2.53	0.41
1:A:815:PHE:O	1:A:816:HIS:C	2.63	0.41
1:A:886:ILE:HB	1:A:943:LEU:HD12	2.02	0.41
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.79	0.41
1:A:1331:SER:C	1:A:1333:ILE:H	2.28	0.41
1:A:1434:ALA:HA	1:A:1435:PRO:HD2	1.90	0.41
2:B:51:PHE:CG	2:B:173:MET:HG2	2.55	0.41
2:B:276:ILE:HD13	2:B:276:ILE:HA	1.95	0.41
2:B:453:ILE:HD12	2:B:453:ILE:N	2.33	0.41
2:B:459:TYR:CD2	2:B:470:LYS:NZ	2.83	0.41
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.88	0.41
2:B:604:ARG:NH2	2:B:691:GLU:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1155:SER:O	2:B:1156:ASP:O	2.38	0.41
4:D:3:VAL:HG11	7:G:10:ASN:O	2.19	0.41
4:D:31:GLN:O	4:D:34:GLN:HB3	2.20	0.41
4:D:37:GLN:NE2	4:D:47:LEU:HD13	2.33	0.41
5:E:201:LYS:O	5:E:201:LYS:HG3	2.21	0.41
7:G:121:PHE:HB2	7:G:130:TYR:CE1	2.55	0.41
11:K:83:PRO:O	11:K:86:ALA:N	2.52	0.41
1:A:27:VAL:O	1:A:29:ALA:N	2.53	0.41
1:A:304:MET:CG	2:B:1210:MET:HG2	2.50	0.41
1:A:311:GLN:OE1	1:A:311:GLN:N	2.53	0.41
1:A:334:GLY:O	1:A:335:ARG:HB2	2.21	0.41
1:A:374:LEU:HA	1:A:374:LEU:HD23	1.56	0.41
1:A:439:ASN:OD1	1:A:459:ARG:HB3	2.21	0.41
1:A:447:GLN:OE1	1:A:447:GLN:HA	2.21	0.41
1:A:577:ILE:O	1:A:577:ILE:HD12	2.21	0.41
1:A:645:LEU:O	1:A:646:PHE:C	2.62	0.41
1:A:1083:THR:HB	1:A:1092:LYS:CB	2.51	0.41
1:A:1399:ARG:C	1:A:1401:SER:N	2.69	0.41
1:A:1447:GLU:CD	7:G:23:LYS:HG3	2.46	0.41
2:B:34:ILE:O	2:B:35:SER:C	2.63	0.41
2:B:132:VAL:HG12	2:B:165:VAL:HG12	2.01	0.41
2:B:203:PHE:CD2	2:B:461:LEU:CD1	3.03	0.41
2:B:629:ASP:CB	2:B:632:ARG:HE	2.34	0.41
2:B:855:PHE:CD1	2:B:856:PHE:N	2.88	0.41
2:B:1117:GLN:HB3	2:B:1118:PRO:HD2	2.01	0.41
3:C:70:ILE:CG2	3:C:71:PRO:HD2	2.48	0.41
3:C:113:VAL:HG23	3:C:144:ILE:HB	2.02	0.41
3:C:264:GLN:HE21	3:C:264:GLN:HB3	1.64	0.41
4:D:8:PHE:O	4:D:38:ILE:CD1	2.68	0.41
4:D:23:ASN:OD1	4:D:23:ASN:O	2.39	0.41
4:D:170:THR:HG23	4:D:170:THR:H	1.45	0.41
5:E:22:MET:O	5:E:22:MET:CG	2.68	0.41
9:I:10:CYS:SG	9:I:31:THR:HG22	2.61	0.41
1:A:74:MET:HE2	1:A:74:MET:HB3	1.93	0.41
1:A:100:LYS:O	1:A:103:CYS:N	2.54	0.41
1:A:151:ASP:CG	1:A:163:SER:N	2.78	0.41
1:A:274:ILE:O	1:A:275:SER:C	2.62	0.41
1:A:494:SER:O	1:A:498:ARG:HD2	2.20	0.41
1:A:698:GLN:HB2	9:I:97:MET:O	2.21	0.41
1:A:710:LEU:HD13	9:I:96:SER:HB2	2.02	0.41
1:A:1292:PRO:HA	1:A:1298:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1396:ALA:N	1:A:1419:ASP:OD2	2.54	0.41
2:B:26:THR:HG23	2:B:29:ASP:H	1.85	0.41
2:B:792:MET:O	2:B:793:ALA:CB	2.68	0.41
2:B:792:MET:HE2	2:B:792:MET:HB3	1.91	0.41
2:B:912:ILE:O	2:B:938:SER:HB2	2.20	0.41
2:B:1076:HIS:CG	11:K:40:HIS:CD2	3.08	0.41
2:B:1209:ALA:O	2:B:1211:ASN:N	2.54	0.41
3:C:204:SER:C	3:C:206:ASN:H	2.28	0.41
4:D:56:ARG:N	4:D:148:LEU:HD13	2.32	0.41
4:D:202:ILE:HG12	4:D:203:SER:O	2.20	0.41
5:E:155:ARG:HD2	5:E:188:LEU:HD22	2.02	0.41
9:I:35:VAL:CG1	9:I:36:GLU:H	2.33	0.41
10:J:26:GLN:O	10:J:27:GLU:C	2.64	0.41
11:K:58:PHE:CD1	11:K:58:PHE:C	2.98	0.41
12:L:61:THR:O	12:L:63:ARG:N	2.53	0.41
1:A:22:PHE:CD1	1:A:27:VAL:HG22	2.55	0.41
1:A:114:LEU:CD2	1:A:171:GLN:HG3	2.48	0.41
1:A:135:PHE:O	1:A:136:ALA:C	2.62	0.41
1:A:224:PHE:CZ	1:A:231:PRO:HB3	2.56	0.41
1:A:229:SER:CB	1:A:1414:ALA:O	2.69	0.41
1:A:451:HIS:HA	1:A:1070:GLN:OE1	2.21	0.41
1:A:871:ASP:CG	1:A:873:MET:HB2	2.46	0.41
1:A:1042:PHE:O	1:A:1044:TRP:N	2.54	0.41
1:A:1326:ARG:O	1:A:1327:ILE:C	2.63	0.41
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.20	0.41
2:B:113:TYR:HE2	2:B:192:LEU:HD13	1.86	0.41
2:B:408:LEU:O	2:B:409:ALA:C	2.62	0.41
2:B:412:LEU:O	2:B:466:TRP:HZ2	2.04	0.41
2:B:814:PHE:O	2:B:815:ARG:C	2.63	0.41
3:C:83:SER:HA	3:C:95:CYS:HB2	2.03	0.41
4:D:27:LEU:CD1	4:D:197:SER:OG	2.69	0.41
6:F:136:ARG:O	6:F:143:PHE:HA	2.20	0.41
8:H:55:LEU:O	8:H:56:THR:O	2.38	0.41
10:J:31:ASP:OD1	10:J:31:ASP:C	2.64	0.41
1:A:15:LYS:O	1:A:1421:CYS:SG	2.79	0.41
1:A:337:ARG:NH1	2:B:1132:GLU:HG3	2.36	0.41
1:A:347:PHE:CD1	1:A:347:PHE:N	2.89	0.41
1:A:395:GLY:O	1:A:401:GLY:HA3	2.20	0.41
1:A:477:PRO:HG3	1:A:521:MET:SD	2.61	0.41
1:A:496:GLU:HG3	1:A:497:THR:N	2.36	0.41
1:A:543:LEU:O	1:A:544:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ALA:HA	1:A:702:LEU:HB2	2.03	0.41
1:A:929:LEU:HA	1:A:929:LEU:HD22	1.87	0.41
1:A:1015:VAL:O	1:A:1016:THR:C	2.63	0.41
1:A:1016:THR:O	1:A:1017:LEU:C	2.64	0.41
1:A:1288:ASP:N	1:A:1288:ASP:OD1	2.53	0.41
1:A:1293:SER:O	1:A:1294:PRO:C	2.64	0.41
1:A:1412:ALA:O	1:A:1413:GLY:C	2.63	0.41
1:A:1418:LEU:HD13	1:A:1418:LEU:C	2.45	0.41
2:B:27:ALA:C	2:B:29:ASP:N	2.77	0.41
2:B:281:PRO:C	2:B:283:VAL:N	2.78	0.41
2:B:308:TRP:CE2	9:I:52:ILE:CD1	3.04	0.41
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.83	0.41
2:B:528:PRO:O	2:B:533:CYS:HA	2.21	0.41
2:B:549:THR:CG2	2:B:550:ASP:N	2.82	0.41
2:B:778:MET:HE1	2:B:853:SER:HB2	2.03	0.41
2:B:803:LEU:CB	2:B:822:ASN:OD1	2.69	0.41
2:B:832:GLY:HA2	2:B:835:GLN:CG	2.51	0.41
2:B:834:ASN:HB3	2:B:840:ILE:H	1.86	0.41
2:B:845:SER:HA	2:B:848:ARG:HH11	1.85	0.41
2:B:867:GLY:O	2:B:869:SER:N	2.46	0.41
2:B:992:ILE:CG2	2:B:994:TYR:CE1	3.04	0.41
2:B:1034:VAL:O	2:B:1035:ALA:C	2.64	0.41
2:B:1223:ASP:O	2:B:1224:PHE:C	2.64	0.41
3:C:51:VAL:HG11	12:L:60:ARG:HH22	1.85	0.41
4:D:212:LYS:O	4:D:215:SER:HB2	2.21	0.41
7:G:157:ILE:O	7:G:157:ILE:HG12	2.21	0.41
10:J:60:PHE:O	10:J:61:LEU:C	2.64	0.41
1:A:27:VAL:C	1:A:29:ALA:N	2.80	0.41
1:A:34:LYS:HB2	1:A:36:ARG:NH1	2.36	0.41
1:A:538:ASP:CG	8:H:22:LYS:HB2	2.46	0.41
1:A:565:ILE:HG21	8:H:46:LEU:CD1	2.50	0.41
1:A:747:VAL:HG22	1:A:752:LYS:O	2.21	0.41
1:A:825:ILE:CD1	2:B:512:ARG:HB2	2.49	0.41
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.20	0.41
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.21	0.41
2:B:185:THR:O	2:B:186:GLU:C	2.64	0.41
2:B:431:TYR:CZ	2:B:446:LEU:O	2.74	0.41
2:B:487:THR:C	19:B:2601:HOH:O	2.63	0.41
2:B:661:LEU:O	2:B:664:THR:HG22	2.20	0.41
2:B:780:VAL:HG21	10:J:56:LEU:CD1	2.50	0.41
2:B:827:ILE:O	2:B:828:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ARG:CZ	2:B:942:ARG:HD3	2.51	0.41
2:B:1043:ASP:OD2	2:B:1045:SER:OG	2.39	0.41
3:C:82:TYR:CD1	3:C:84:ARG:NH1	2.89	0.41
7:G:54:ILE:HG22	7:G:55:ASP:O	2.21	0.41
8:H:125:LEU:CD1	8:H:130:ARG:NH1	2.84	0.41
8:H:137:GLN:HB2	8:H:139:ASN:HB2	2.03	0.41
9:I:37:GLU:O	9:I:37:GLU:HG2	2.19	0.41
9:I:46:HIS:NE2	9:I:48:LEU:CD2	2.83	0.41
1:A:43:GLU:OE2	1:A:46:THR:HB	2.22	0.40
1:A:239:LEU:HD23	1:A:240:PRO:O	2.21	0.40
1:A:393:ARG:HB3	1:A:393:ARG:HH11	1.85	0.40
1:A:475:THR:HG22	1:A:476:SER:N	2.35	0.40
1:A:517:ASN:O	1:A:517:ASN:CG	2.64	0.40
1:A:671:ALA:C	1:A:673:GLY:N	2.78	0.40
1:A:728:LYS:H	1:A:728:LYS:HG3	1.71	0.40
1:A:802:ASN:ND2	2:B:729:ILE:HG22	2.36	0.40
1:A:893:PHE:CE1	1:A:937:VAL:HG22	2.56	0.40
1:A:899:VAL:HG11	1:A:908:LEU:HD11	2.03	0.40
1:A:983:ILE:O	1:A:987:VAL:HG22	2.20	0.40
1:A:1143:LEU:HD23	1:A:1267:MET:C	2.46	0.40
2:B:48:LEU:HD12	2:B:48:LEU:N	2.36	0.40
2:B:331:LEU:HA	2:B:334:ILE:HG13	2.02	0.40
2:B:521:LEU:HD13	2:B:633:VAL:CG1	2.51	0.40
2:B:700:SER:O	2:B:701:ILE:HG23	2.21	0.40
2:B:987:LYS:HB2	2:B:988:GLY:H	1.63	0.40
4:D:33:PHE:N	4:D:33:PHE:HD1	2.19	0.40
5:E:55:ARG:C	5:E:57:MET:H	2.30	0.40
5:E:58:MET:HE2	5:E:58:MET:HB3	1.94	0.40
5:E:103:LYS:HA	5:E:103:LYS:HD2	1.82	0.40
1:A:29:ALA:O	1:A:31:SER:N	2.55	0.40
1:A:440:ASP:O	1:A:442:VAL:HG13	2.19	0.40
1:A:800:VAL:HG13	1:A:812:GLU:OE1	2.20	0.40
1:A:1381:LEU:H	1:A:1381:LEU:CD1	2.31	0.40
1:A:1444:MET:CA	7:G:59:GLY:O	2.65	0.40
2:B:105:SER:O	2:B:106:ASP:HB2	2.20	0.40
2:B:399:ASP:O	2:B:515:HIS:CD2	2.73	0.40
2:B:527:THR:HG23	2:B:528:PRO:N	2.37	0.40
2:B:735:ALA:O	2:B:737:THR:N	2.40	0.40
2:B:802:PRO:HG3	2:B:814:PHE:CE2	2.54	0.40
2:B:892:LYS:HD3	2:B:903:VAL:CG1	2.51	0.40
2:B:1004:GLU:HB2	2:B:1006:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:CD1	3:C:94:LYS:O	2.69	0.40
5:E:110:PHE:CD1	5:E:110:PHE:C	2.99	0.40
5:E:195:VAL:HA	5:E:213:ILE:HA	2.03	0.40
7:G:1:MET:CE	7:G:80:LYS:H	2.33	0.40
8:H:124:ARG:NH2	8:H:126:GLU:OE2	2.54	0.40
8:H:129:TYR:C	8:H:131:ASN:H	2.29	0.40
11:K:91:CYS:O	11:K:94:ILE:HB	2.21	0.40
1:A:679:ILE:O	1:A:679:ILE:CG2	2.68	0.40
1:A:932:GLU:C	1:A:934:LYS:N	2.79	0.40
1:A:964:ILE:HD12	1:A:965:GLN:N	2.36	0.40
1:A:971:PHE:O	1:A:972:HIS:HB2	2.21	0.40
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.21	0.40
2:B:706:GLN:HE21	2:B:707:PRO:HG2	1.87	0.40
2:B:752:ALA:O	2:B:753:ALA:C	2.64	0.40
2:B:872:GLU:O	2:B:873:THR:CB	2.69	0.40
2:B:1032:SER:HA	2:B:1035:ALA:HB3	2.04	0.40
3:C:97:VAL:CG2	3:C:129:ILE:CG2	2.99	0.40
3:C:241:ASP:HB3	11:K:109:TRP:CZ2	2.56	0.40
6:F:94:LEU:O	6:F:95:GLY:C	2.62	0.40
9:I:15:TYR:HA	9:I:16:PRO:HD2	1.96	0.40
9:I:85:PHE:HB2	9:I:99:LEU:CD2	2.40	0.40
10:J:2:ILE:C	10:J:53:HIS:HE1	2.30	0.40
12:L:31:CYS:SG	12:L:48:CYS:HB2	2.62	0.40
1:A:23:SER:C	1:A:25:GLU:N	2.79	0.40
1:A:119:ASN:H	1:A:123:ARG:NH1	2.19	0.40
1:A:390:GLN:O	1:A:390:GLN:HG3	2.21	0.40
1:A:476:SER:HB2	1:A:477:PRO:HD3	2.02	0.40
1:A:666:ILE:HD12	1:A:667:GLY:CA	2.48	0.40
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.02	0.40
1:A:1407:GLU:O	1:A:1410:PHE:HB2	2.21	0.40
2:B:123:THR:HG21	2:B:458:LYS:HG3	2.03	0.40
2:B:375:ALA:O	2:B:377:PHE:N	2.55	0.40
2:B:500:THR:HB	2:B:535:LEU:O	2.21	0.40
2:B:1202:LEU:HG	2:B:1206:GLU:CD	2.46	0.40
3:C:35:ARG:NH2	11:K:41:THR:HG23	2.36	0.40
3:C:58:LEU:N	3:C:58:LEU:HD23	2.36	0.40
3:C:178:PHE:HD1	3:C:178:PHE:C	2.28	0.40
4:D:27:LEU:HD21	4:D:173:HIS:HB2	2.02	0.40
6:F:127:GLU:C	6:F:129:LYS:N	2.78	0.40
7:G:99:PHE:O	7:G:99:PHE:CG	2.74	0.40
7:G:126:ASN:HA	7:G:127:PRO:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:O	8:H:59:ILE:HG13	2.21	0.40
9:I:17:ARG:O	9:I:26:LEU:CD2	2.69	0.40
11:K:82:ASP:HB3	11:K:85:ASP:HB2	2.02	0.40
1:A:337:ARG:NH1	2:B:1132:GLU:CD	2.79	0.40
1:A:341:MET:HE1	1:A:1429:ILE:CD1	2.48	0.40
1:A:528:LEU:HA	1:A:531:ILE:CG2	2.52	0.40
1:A:670:ILE:O	1:A:670:ILE:CG1	2.69	0.40
1:A:747:VAL:HG22	1:A:753:GLY:HA3	2.04	0.40
1:A:827:THR:HG21	1:A:1084:PHE:CD2	2.55	0.40
1:A:955:PRO:C	1:A:956:LEU:HG	2.46	0.40
1:A:993:LEU:HD23	1:A:1022:LEU:CD2	2.50	0.40
1:A:1066:VAL:HG22	1:A:1066:VAL:O	2.22	0.40
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.46	0.40
1:A:1443:VAL:HG22	6:F:92:ARG:NH2	2.36	0.40
1:A:1447:GLU:OE1	7:G:23:LYS:CD	2.70	0.40
2:B:114:PRO:O	2:B:117:ALA:N	2.49	0.40
2:B:185:THR:H	2:B:188:ASP:HB2	1.85	0.40
2:B:308:TRP:NE1	9:I:52:ILE:HD13	2.35	0.40
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.37	0.40
2:B:751:VAL:O	2:B:812:LEU:CD2	2.70	0.40
2:B:958:GLN:HG3	2:B:958:GLN:H	1.78	0.40
3:C:37:MET:HE3	3:C:37:MET:HB3	1.73	0.40
3:C:88:CYS:SG	3:C:90:ASP:O	2.80	0.40
3:C:184:ASN:HD21	3:C:189:THR:H	1.69	0.40
6:F:109:VAL:HG23	6:F:127:GLU:CD	2.46	0.40
7:G:11:ILE:HG22	7:G:12:THR:N	2.37	0.40
7:G:12:THR:HA	7:G:68:ALA:O	2.22	0.40
7:G:14:HIS:O	7:G:15:PRO:C	2.64	0.40
7:G:112:LYS:CD	7:G:113:HIS:ND1	2.85	0.40
9:I:76:PRO:HD2	9:I:108:HIS:HE1	1.85	0.40
11:K:12:LEU:HD21	11:K:18:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1380/1733 (80%)	959 (70%)	290 (21%)	131 (10%)	0	2
2	B	1036/1224 (85%)	726 (70%)	220 (21%)	90 (9%)	0	2
3	C	264/318 (83%)	205 (78%)	48 (18%)	11 (4%)	2	10
4	D	156/221 (71%)	113 (72%)	29 (19%)	14 (9%)	0	2
5	E	202/215 (94%)	164 (81%)	29 (14%)	9 (4%)	2	9
6	F	82/155 (53%)	56 (68%)	24 (29%)	2 (2%)	4	18
7	G	169/171 (99%)	132 (78%)	27 (16%)	10 (6%)	1	6
8	H	107/146 (73%)	73 (68%)	26 (24%)	8 (8%)	1	3
9	I	117/122 (96%)	82 (70%)	24 (20%)	11 (9%)	0	2
10	J	63/70 (90%)	51 (81%)	6 (10%)	6 (10%)	0	2
11	K	113/120 (94%)	77 (68%)	27 (24%)	9 (8%)	1	3
12	L	41/70 (59%)	15 (37%)	10 (24%)	16 (39%)	0	0
All	All	3730/4565 (82%)	2653 (71%)	760 (20%)	317 (8%)	0	3

All (317) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	57	ARG
1	A	76	GLU
1	A	119	ASN
1	A	128	ILE
1	A	178	GLY
1	A	232	GLU
1	A	376	TYR
1	A	525	GLN
1	A	567	LYS
1	A	569	LYS
1	A	584	ASN
1	A	672	ASP
1	A	774	ARG
1	A	847	ASP
1	A	915	SER
1	A	961	ARG
1	A	979	SER
1	A	986	ILE

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Mol	Chain	Res	Type
1	A	997	LEU
1	A	999	VAL
1	A	1091	SER
1	A	1096	SER
1	A	1108	ALA
1	A	1139	GLU
1	A	1162	VAL
1	A	1314	SER
1	A	1365	TYR
1	A	1381	LEU
1	A	1392	SER
1	A	1394	THR
1	A	1435	PRO
1	A	1437	GLY
2	B	45	SER
2	B	46	GLN
2	B	250	PHE
2	B	278	GLN
2	B	365	THR
2	B	422	LYS
2	B	466	TRP
2	B	594	ALA
2	B	749	LEU
2	B	792	MET
2	B	818	PRO
2	B	865	LYS
2	B	970	THR
2	B	1036	ALA
2	B	1108	ARG
2	B	1143	ALA
2	B	1156	ASP
2	B	1177	HIS
2	B	1210	MET
2	B	1219	ASP
3	C	75	MET
3	C	149	LYS
3	C	198	ALA
4	D	55	ALA
4	D	56	ARG
4	D	119	ARG
4	D	178	ALA
5	E	3	GLN

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Mol	Chain	Res	Type
5	E	117	THR
6	F	73	ALA
7	G	63	PRO
7	G	157	ILE
7	G	170	ALA
8	H	17	PRO
8	H	56	THR
8	H	62	SER
8	H	140	ALA
9	I	7	CYS
9	I	58	VAL
9	I	60	GLN
10	J	2	ILE
10	J	6	ARG
10	J	64	ASN
11	K	44	ASN
11	K	54	ARG
12	L	33	GLU
12	L	42	ARG
12	L	44	ASP
12	L	59	ALA
1	A	74	MET
1	A	130	ASP
1	A	131	SER
1	A	140	THR
1	A	151	ASP
1	A	309	ALA
1	A	392	VAL
1	A	393	ARG
1	A	416	ARG
1	A	423	ASP
1	A	517	ASN
1	A	623	GLY
1	A	911	SER
1	A	949	ASP
1	A	985	ASP
1	A	1016	THR
1	A	1087	ALA
1	A	1107	VAL
1	A	1120	LEU
1	A	1140	HIS
1	A	1171	GLN

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Mol	Chain	Res	Type
1	A	1331	SER
1	A	1360	GLY
1	A	1386	ARG
1	A	1388	GLY
1	A	1400	CYS
2	B	24	PRO
2	B	56	ASP
2	B	61	ASP
2	B	108	VAL
2	B	111	ALA
2	B	267	ARG
2	B	277	LYS
2	B	305	VAL
2	B	351	TYR
2	B	369	GLY
2	B	391	ASP
2	B	534	GLY
2	B	660	LYS
2	B	734	HIS
2	B	753	ALA
2	B	754	SER
2	B	854	LEU
2	B	873	THR
2	B	935	ARG
2	B	1017	ILE
2	B	1046	PRO
2	B	1123	SER
2	B	1125	ASP
2	B	1174	LYS
2	B	1223	ASP
3	C	6	PRO
3	C	89	GLU
3	C	184	ASN
4	D	36	LYS
4	D	44	GLU
4	D	46	GLU
4	D	137	ASN
4	D	170	THR
4	D	199	ASN
5	E	12	LEU
5	E	198	ILE
6	F	128	LYS

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Mol	Chain	Res	Type
7	G	20	PRO
7	G	154	VAL
9	I	57	GLY
9	I	59	VAL
9	I	67	THR
10	J	13	VAL
10	J	62	ARG
11	K	43	GLY
11	K	64	GLU
11	K	81	TYR
12	L	32	ALA
12	L	40	LEU
12	L	43	THR
12	L	52	GLY
12	L	54	ARG
1	A	108	MET
1	A	179	LEU
1	A	282	ASN
1	A	346	ASP
1	A	453	MET
1	A	455	MET
1	A	475	THR
1	A	704	ALA
1	A	706	HIS
1	A	727	ASP
1	A	775	ILE
1	A	785	PRO
1	A	846	GLU
1	A	903	ASN
1	A	922	ASP
1	A	1057	VAL
1	A	1089	VAL
1	A	1123	GLY
1	A	1295	THR
1	A	1361	SER
1	A	1367	HIS
1	A	1368	MET
1	A	1369	ALA
1	A	1377	THR
1	A	1421	CYS
2	B	27	ALA
2	B	28	GLU

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Mol	Chain	Res	Type
2	B	106	ASP
2	B	114	PRO
2	B	247	GLY
2	B	260	GLY
2	B	421	PHE
2	B	531	GLN
2	B	711	GLU
2	B	736	THR
2	B	793	ALA
2	B	891	ASP
2	B	1132	GLU
2	B	1133	MET
2	B	1169	MET
3	C	4	GLU
4	D	182	SER
4	D	198	LEU
5	E	210	SER
8	H	77	ARG
10	J	29	GLU
11	K	10	PHE
11	K	88	LYS
12	L	30	ILE
12	L	41	SER
12	L	58	LYS
1	A	32	VAL
1	A	47	ARG
1	A	424	ILE
1	A	449	SER
1	A	643	ALA
1	A	771	GLU
1	A	794	PRO
1	A	1128	GLN
1	A	1362	TYR
1	A	1452	LYS
2	B	48	LEU
2	B	58	THR
2	B	107	GLY
2	B	364	ILE
2	B	447	ALA
2	B	459	TYR
2	B	575	PRO
2	B	638	PHE

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Mol	Chain	Res	Type
2	B	664	THR
2	B	868	MET
2	B	888	GLY
2	B	1203	LEU
3	C	109	SER
3	C	138	GLU
3	C	199	LYS
4	D	120	GLU
5	E	53	PRO
5	E	129	PRO
7	G	16	SER
8	H	61	SER
8	H	78	SER
9	I	28	GLU
9	I	47	GLU
12	L	31	CYS
12	L	56	LEU
1	A	135	PHE
1	A	152	VAL
1	A	169	ASN
1	A	173	THR
1	A	223	GLY
1	A	285	PRO
1	A	433	GLU
1	A	441	PRO
1	A	585	GLY
1	A	664	THR
1	A	703	THR
1	A	850	VAL
1	A	958	VAL
1	A	1042	PHE
1	A	1060	PRO
1	A	1062	GLU
1	A	1115	SER
1	A	1359	ASP
2	B	294	ASP
2	B	658	ILE
2	B	694	ASP
2	B	770	GLN
2	B	815	ARG
2	B	842	ASN
2	B	853	SER

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Mol	Chain	Res	Type
2	B	872	GLU
2	B	943	SER
2	B	1015	HIS
2	B	1202	LEU
3	C	205	LYS
5	E	118	PRO
5	E	207	ARG
7	G	2	PHE
9	I	65	ASP
9	I	69	PRO
11	K	37	LYS
12	L	35	SER
12	L	62	LYS
1	A	71	GLN
1	A	143	LYS
1	A	544	ASP
1	A	562	THR
1	A	568	PRO
1	A	693	VAL
1	A	1302	PRO
2	B	350	GLN
2	B	1089	PRO
4	D	30	GLY
7	G	118	ASP
9	I	86	PHE
1	A	793	SER
2	B	55	VAL
2	B	410	GLY
2	B	976	ILE
1	A	52	GLY
1	A	422	GLY
1	A	1322	ILE
1	A	1372	VAL
2	B	1165	ILE
8	H	57	VAL
1	A	1066	VAL
1	A	1122	PRO
1	A	1163	ILE
1	A	1327	ILE
2	B	282	ILE
11	K	94	ILE
1	A	756	ILE

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Mol	Chain	Res	Type
7	G	136	VAL
1	A	308	ILE
1	A	325	ILE
7	G	139	ILE

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	1218/1520 (80%)	1214 (100%)	4 (0%)	86	85
2	B	917/1061 (86%)	913 (100%)	4 (0%)	84	84
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	144/200 (72%)	144 (100%)	0	100	100
5	E	192/197 (98%)	192 (100%)	0	100	100
6	F	74/137 (54%)	74 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	104/128 (81%)	103 (99%)	1 (1%)	68	77
9	I	113/116 (97%)	112 (99%)	1 (1%)	70	78
10	J	59/65 (91%)	59 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
All	All	3344/4009 (83%)	3334 (100%)	10 (0%)	86	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	LYS
1	A	524	VAL
1	A	575	LYS
1	A	658	LEU
2	B	527	THR
2	B	566	LEU

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Mol	Chain	Res	Type
2	B	996	ARG
2	B	1106	ARG
8	H	97	MET
9	I	74	GLU

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	273	ASN
1	A	282	ASN
1	A	299	HIS
1	A	445	ASN
1	A	545	GLN
1	A	626	ASN
1	A	736	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	935	GLN
1	A	972	HIS
1	A	1004	ASN
1	A	1009	ASN
1	A	1011	GLN
1	A	1078	GLN
1	A	1211	GLN
1	A	1218	GLN
1	A	1270	ASN
1	A	1312	ASN
1	A	1390	ASN
2	B	46	GLN
2	B	121	ASN
2	B	306	ASN
2	B	325	GLN
2	B	366	GLN
2	B	538	ASN
2	B	706	GLN
2	B	762	ASN
2	B	763	GLN
2	B	767	ASN
2	B	786	ASN
2	B	842	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	986	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1076	HIS
2	B	1084	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1195	HIS
3	C	73	GLN
3	C	188	HIS
3	C	203	GLN
3	C	206	ASN
3	C	264	GLN
4	D	31	GLN
5	E	99	HIS
5	E	143	ASN
5	E	146	HIS
5	E	147	HIS
6	F	104	ASN
7	G	96	GLN
7	G	102	GLN
7	G	122	ASN
8	H	128	ASN
8	H	131	ASN
8	H	137	GLN
9	I	22	ASN
9	I	23	ASN
10	J	53	HIS
10	J	64	ASN
11	K	40	HIS
11	K	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 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	$\# Z > 2$
17	ATP	B	2501	16	32,33,33	0.86	2 (6%)	48,52,52	1.44	4 (8%)
18	GOL	E	301	-	5,5,5	1.38	0	5,5,5	1.02	0

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
17	ATP	B	2501	16	-	2/22/38/38	0/3/3/3
18	GOL	E	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	2501	ATP	PG-O2G	-2.81	1.44	1.54
17	B	2501	ATP	PB-O2B	-2.25	1.44	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	2501	ATP	O2G-PG-O3B	-5.73	85.43	104.64
17	B	2501	ATP	O2B-PB-O3B	-5.62	92.07	107.27
17	B	2501	ATP	O3G-PG-O3B	2.71	113.72	104.64
17	B	2501	ATP	O3A-PA-O1A	-2.09	104.42	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

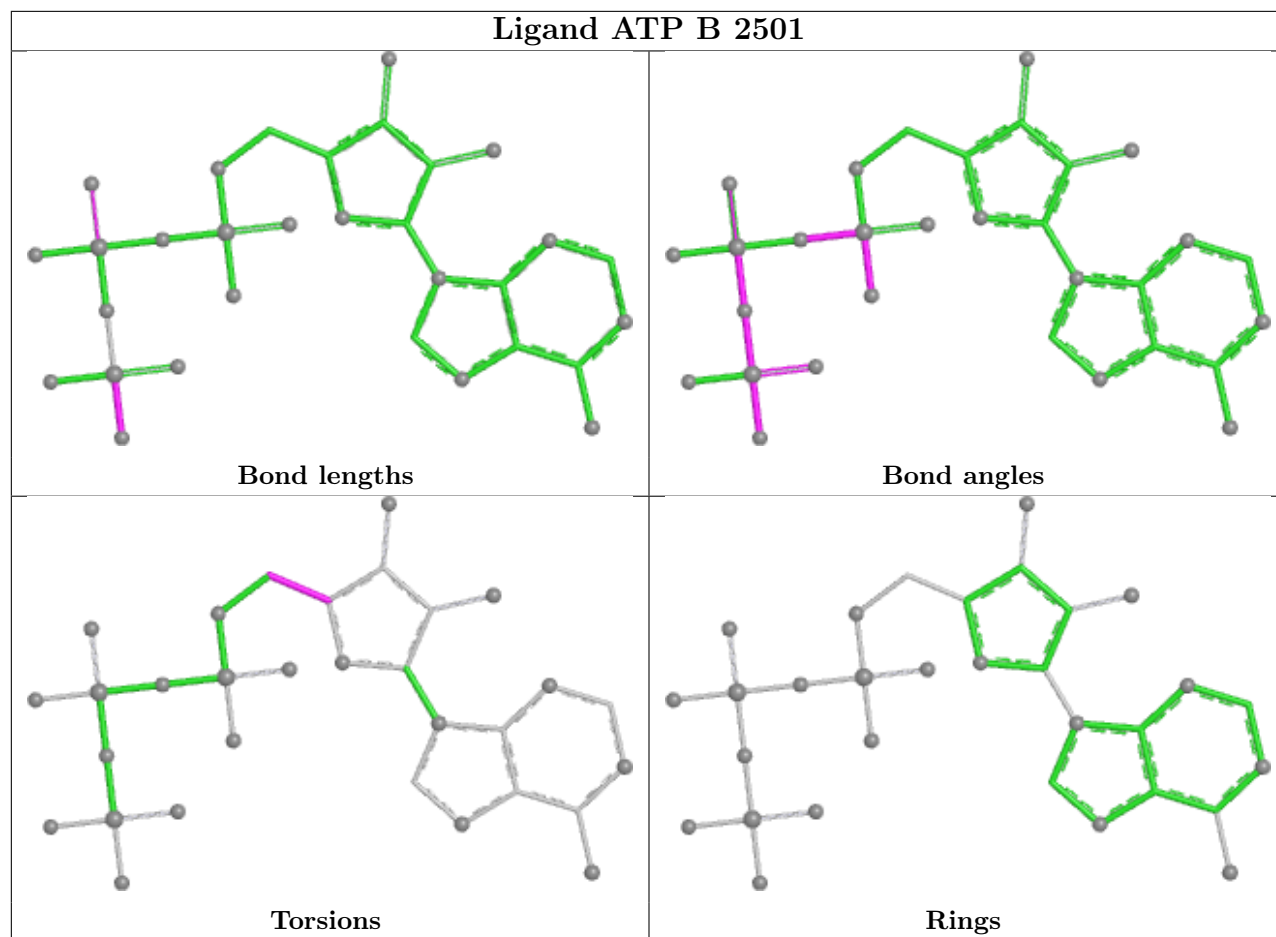
Mol	Chain	Res	Type	Atoms
17	B	2501	ATP	O4'-C4'-C5'-O5'
18	E	301	GOL	O1-C1-C2-C3
17	B	2501	ATP	C3'-C4'-C5'-O5'
18	E	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	2501	ATP	3	0
18	E	301	GOL	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	1398/1733 (80%)	-0.12	33 (2%) 59 37	38, 100, 164, 286	0
2	B	1060/1224 (86%)	-0.10	15 (1%) 73 51	40, 103, 172, 273	0
3	C	266/318 (83%)	-0.20	1 (0%) 88 75	50, 102, 153, 197	0
4	D	162/221 (73%)	-0.06	4 (2%) 58 35	73, 118, 163, 198	0
5	E	208/215 (96%)	0.03	4 (1%) 66 43	59, 132, 186, 293	0
6	F	84/155 (54%)	-0.17	0 100 100	44, 77, 116, 167	0
7	G	171/171 (100%)	0.28	12 (7%) 22 11	61, 103, 153, 189	0
8	H	117/146 (80%)	0.28	6 (5%) 33 17	93, 133, 189, 235	0
9	I	119/122 (97%)	0.19	6 (5%) 34 17	92, 147, 208, 248	0
10	J	65/70 (92%)	-0.14	0 100 100	68, 106, 148, 186	0
11	K	115/120 (95%)	-0.33	0 100 100	54, 95, 154, 175	0
12	L	43/70 (61%)	0.35	1 (2%) 61 38	78, 120, 181, 202	0
13	R	10/10 (100%)	0.07	0 100 100	117, 161, 213, 218	0
14	T	13/13 (100%)	0.44	0 100 100	128, 140, 169, 212	0
All	All	3831/4588 (83%)	-0.07	82 (2%) 63 40	38, 106, 173, 293	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	95	SER	6.8
2	B	728	ARG	5.4
7	G	5	LYS	5.2
7	G	153	GLN	5.2
1	A	1084	PHE	5.1
1	A	1080	THR	4.8
2	B	1065	GLN	3.8
1	A	303	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	525	ALA	3.6
5	E	139	ALA	3.5
9	I	69	PRO	3.5
12	L	55	ILE	3.5
1	A	1321	GLY	3.2
2	B	710	LEU	3.1
8	H	31	THR	3.1
1	A	1091	SER	3.0
9	I	104	LEU	3.0
1	A	56	PRO	2.9
3	C	191	TYR	2.9
4	D	40	HIS	2.9
2	B	1224	PHE	2.8
1	A	258	GLY	2.7
7	G	169	GLY	2.7
2	B	735	ALA	2.6
7	G	37	SER	2.6
1	A	1170	ILE	2.6
8	H	90	ALA	2.6
9	I	105	SER	2.5
5	E	44	ALA	2.5
1	A	1081	LEU	2.5
7	G	117	GLN	2.5
1	A	587	HIS	2.5
8	H	36	CYS	2.5
1	A	569	LYS	2.5
7	G	97	HIS	2.5
7	G	6	ASP	2.4
1	A	31	SER	2.4
1	A	1096	SER	2.4
7	G	94	CYS	2.4
1	A	323	LYS	2.4
1	A	42	ASP	2.4
1	A	179	LEU	2.4
1	A	34	LYS	2.4
2	B	246	LYS	2.4
1	A	49	LYS	2.3
2	B	349	ILE	2.3
1	A	453	MET	2.3
1	A	1386	ARG	2.3
7	G	33	GLU	2.3
1	A	1086	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	113	GLN	2.3
4	D	123	LEU	2.3
1	A	1205	LYS	2.3
2	B	617	ARG	2.3
1	A	1161	THR	2.3
1	A	33	ALA	2.2
4	D	167	LEU	2.2
4	D	122	GLU	2.2
2	B	1015	HIS	2.2
1	A	1094	VAL	2.2
7	G	19	GLY	2.2
8	H	50	ALA	2.2
1	A	618	GLU	2.2
2	B	731	VAL	2.2
1	A	766	GLY	2.2
1	A	1236	LEU	2.1
2	B	615	MET	2.1
1	A	570	PRO	2.1
2	B	1126	GLY	2.1
7	G	137	ILE	2.1
9	I	52	ILE	2.1
9	I	99	LEU	2.1
1	A	59	GLY	2.1
1	A	32	VAL	2.1
1	A	678	GLU	2.1
1	A	1327	ILE	2.0
9	I	13	MET	2.0
5	E	131	THR	2.0
8	H	11	GLN	2.0
8	H	136	LYS	2.0
2	B	836	GLU	2.0
2	B	1067	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

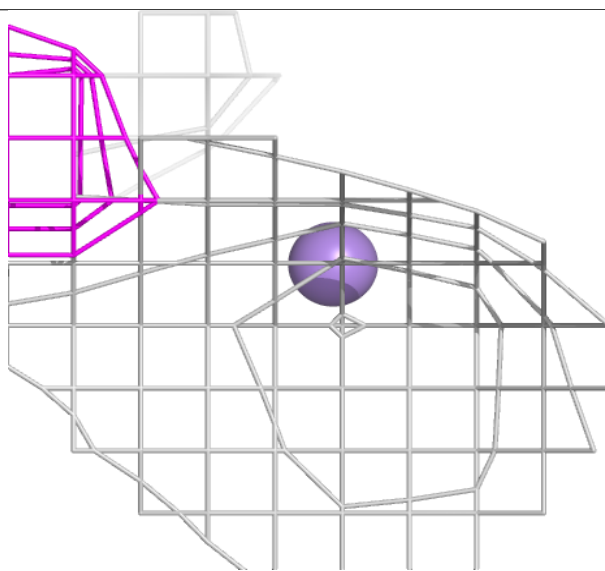
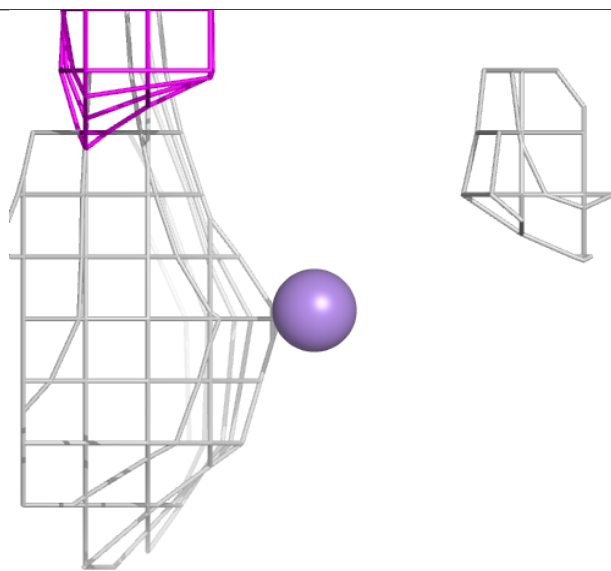
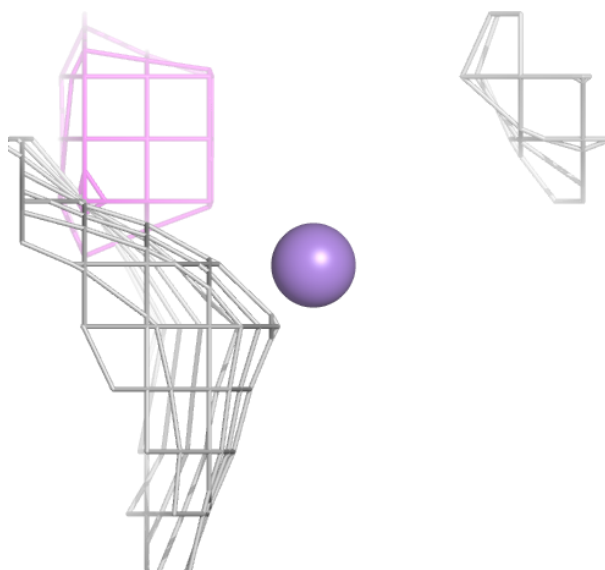
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	MN	B	2503	1/1	0.85	0.17	138,138,138,138	1
18	GOL	E	301	6/6	0.89	0.16	113,136,158,158	0
15	ZN	L	101	1/1	0.91	0.06	153,153,153,153	0
17	ATP	B	2501	31/31	0.94	0.11	117,141,170,172	0
15	ZN	I	202	1/1	0.97	0.03	182,182,182,182	0
15	ZN	A	1801	1/1	0.98	0.06	139,139,139,139	0
15	ZN	B	2502	1/1	0.99	0.02	77,77,77,77	0
16	MN	A	1803	1/1	0.99	0.04	69,69,69,69	0
16	MN	A	1804	1/1	0.99	0.05	78,78,78,78	0
15	ZN	C	401	1/1	0.99	0.04	69,69,69,69	0
15	ZN	I	201	1/1	0.99	0.05	119,119,119,119	0
15	ZN	A	1802	1/1	0.99	0.05	65,65,65,65	0
15	ZN	J	101	1/1	1.00	0.04	85,85,85,85	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.

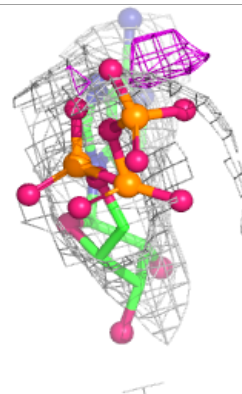
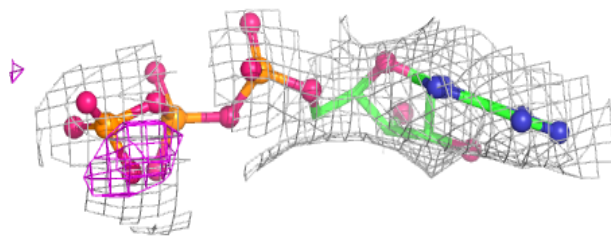
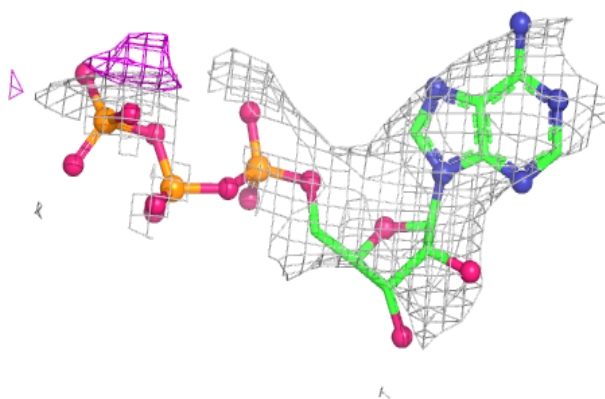
Electron density around MN B 2503:

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



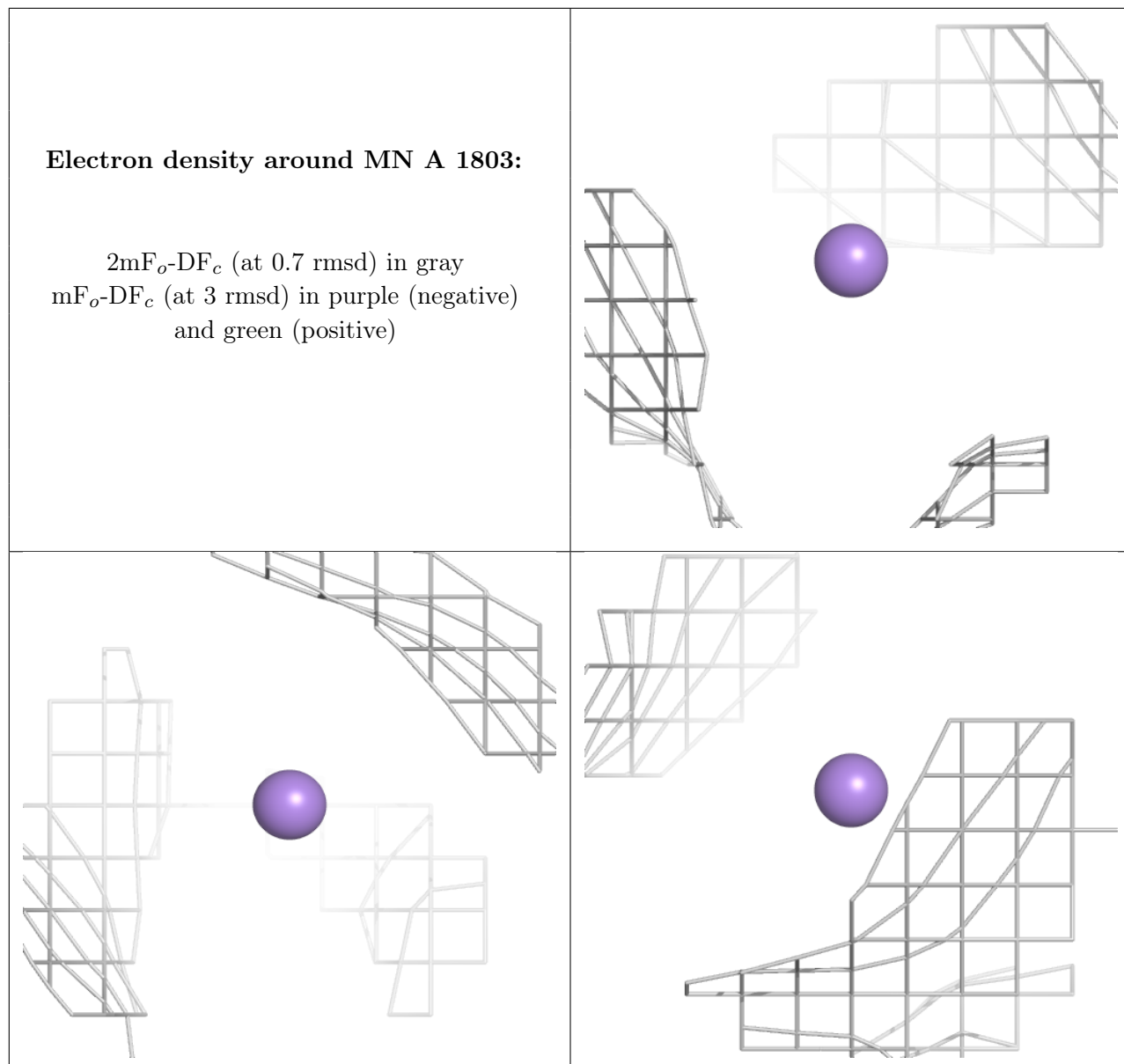
Electron density around ATP B 2501:

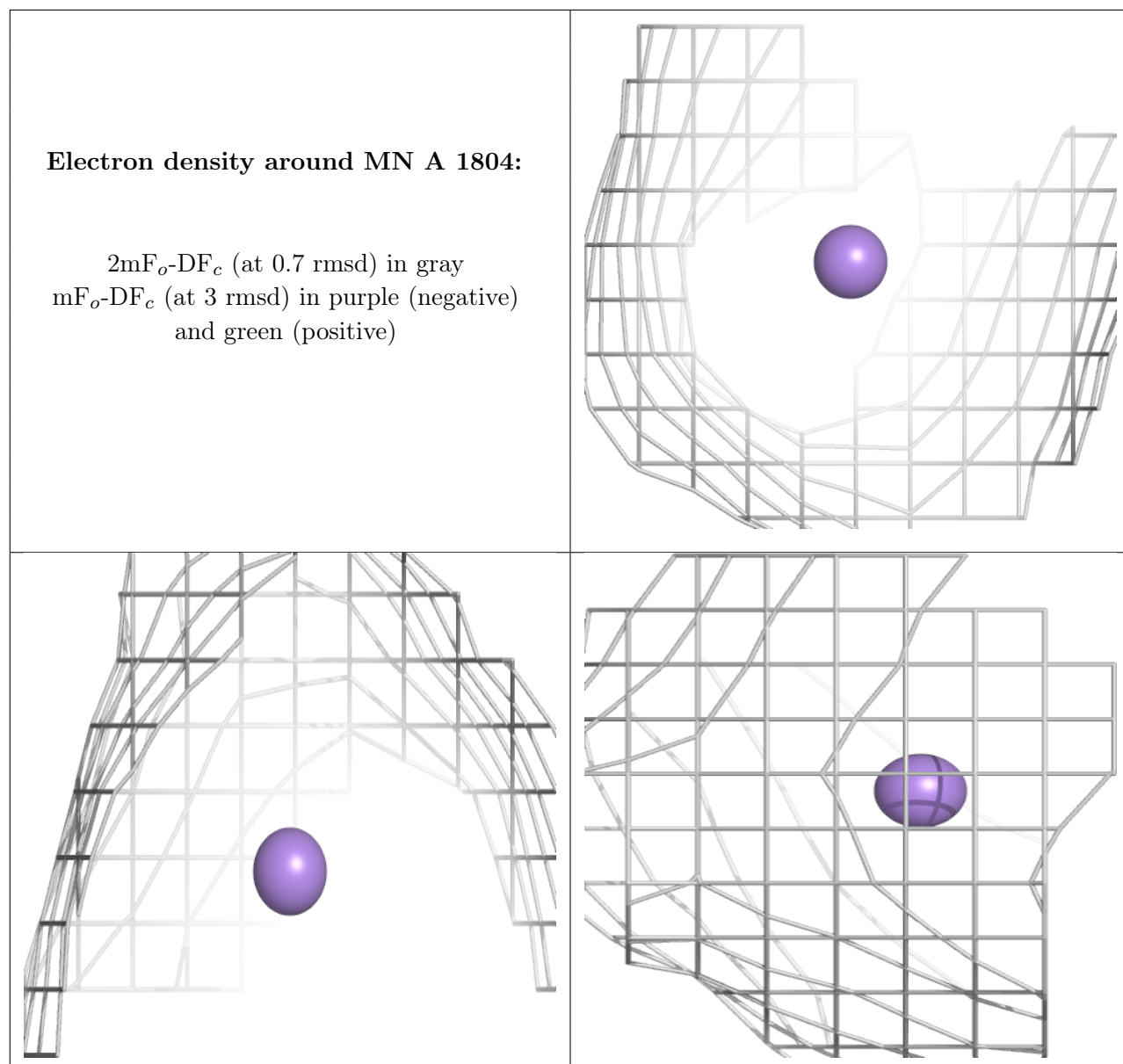
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 1803:

$2mF_o-DF_c$ (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.