



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:52 PM UTC

PDB ID : 3GTK / pdb_00003gtk
Title : Backtracked RNA polymerase II complex with 18mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

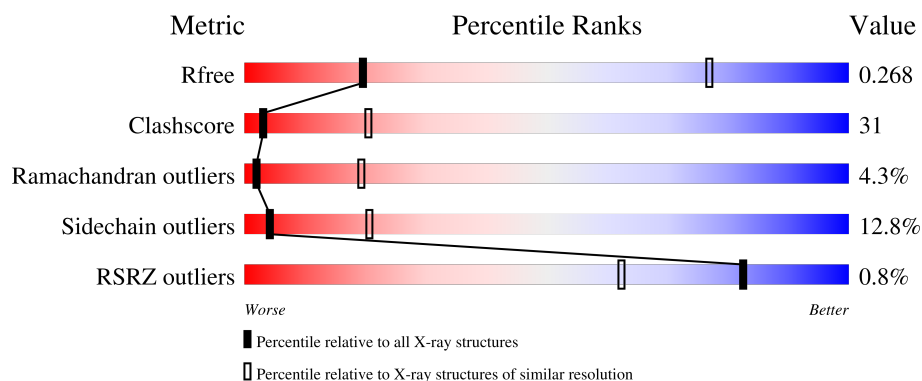
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	B	1224	
3	C	318	
4	E	215	
5	F	155	

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	18	
12	T	29	
13	N	14	

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
14	ZN	A	1734	-	-	X	-
14	ZN	C	319	-	-	X	-
14	ZN	J	101	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1442	Total	C	N	O	S	0	0	0
			11332	7133	1982	2156	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1153	Total	C	N	O	S	0	0	0
			9168	5795	1604	1713	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2135	1344	355	423	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1757	1114	310	322	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			684	437	116	128	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	136	Total	C	N	O	S	0	0	0
			1087	684	183	215	5			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is DNA/RNA hybrid called DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	14	Total	C	N	O	P	0	0	0
			284	126	55	90	13			

- Molecule 12 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	29	Total	C	N	O	P	0	0	0
			587	281	109	169	28			

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

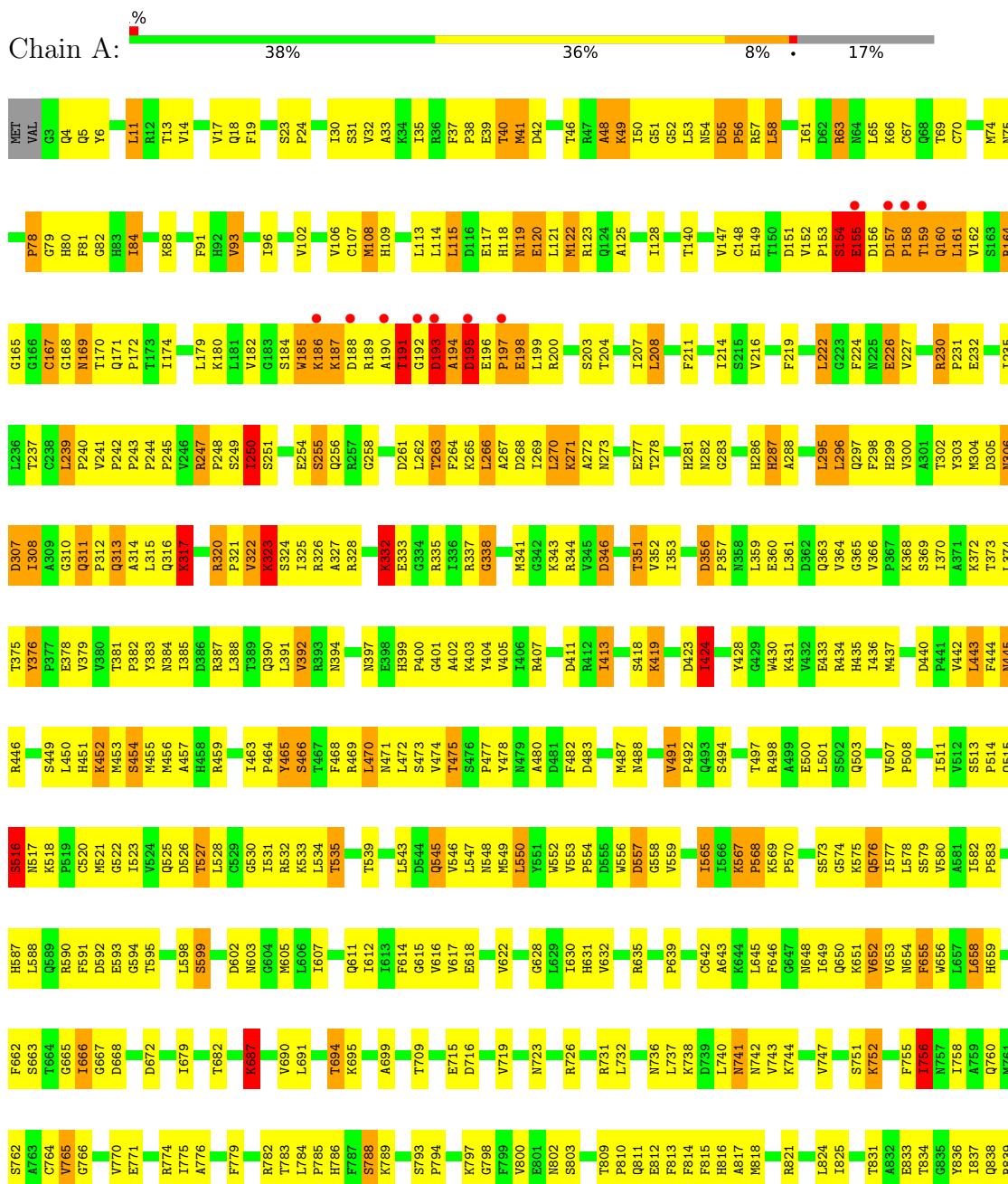
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

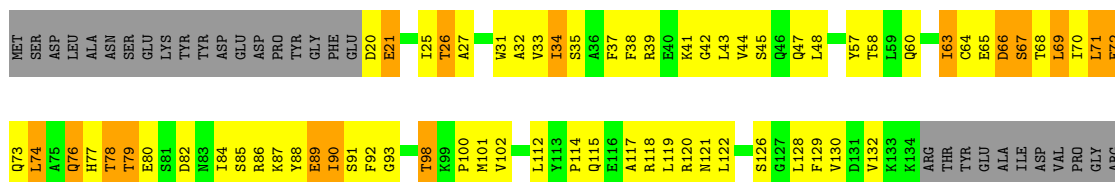
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total 2	Zn 2	0	0
14	B	1	Total 1	Zn 1	0	0
14	C	1	Total 1	Zn 1	0	0
14	I	2	Total 2	Zn 2	0	0
14	J	1	Total 1	Zn 1	0	0
14	L	1	Total 1	Zn 1	0	0

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.

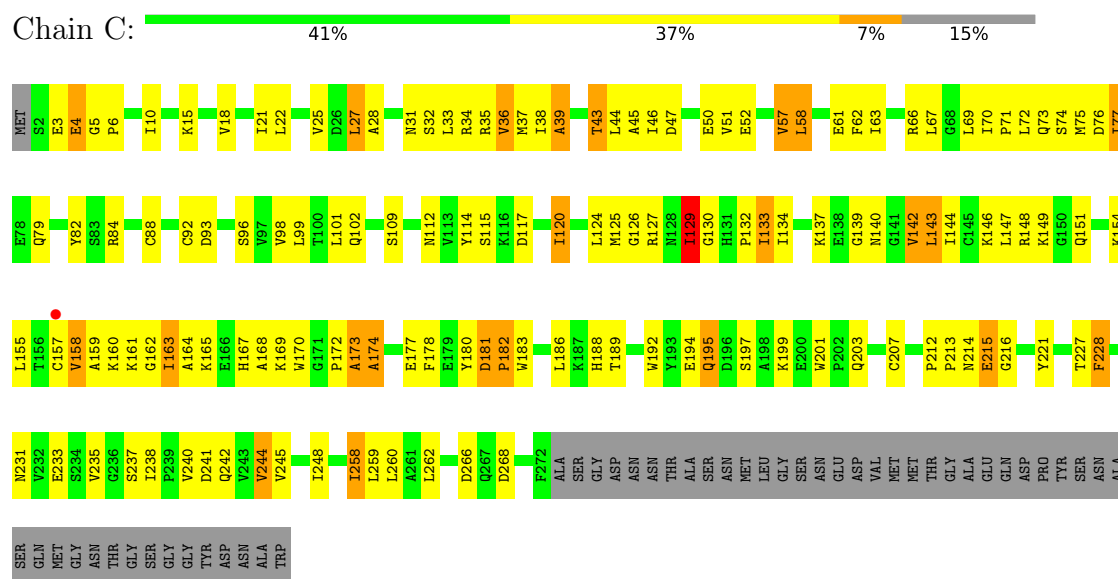
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



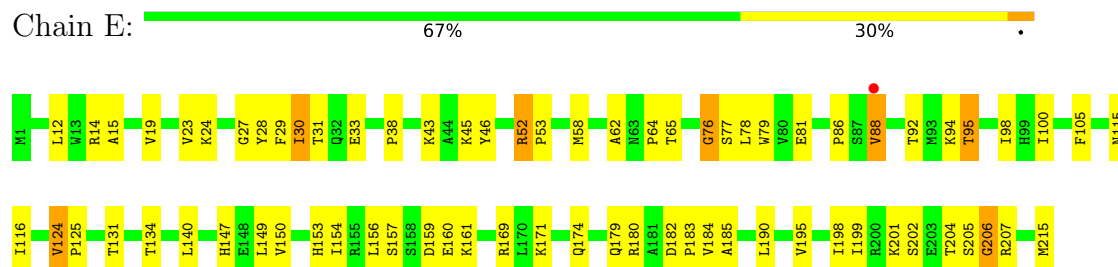


R1215	L1216	Y1217	S145	F1146	L1147	K1148	E1149	R1150	L1151	M1152	E1153	D1156	R1159	V1160	H1161	I1162	C1163	G1164	I1165	C1166	G1167	L1168	I1172	A1173	L1174	M1176	Q1179	F1180	E1181	M1187	K1188	I1189	D1190	Q1193	I1194	H1195	I1196	P1197	Y1198	A1199	A1200	K1201	L1202	L1203	F1204	Q1205	M1208	A1209	M1210	N1211	I1212	H1213	P1214	Q215	S218	N221	L222	V223	Q224	V225	S232	S235	H236	E239	L240	R241	S242	L244	E245	K246	Q255	V256	G260	R261	R267	T268	L273	P274	Y275	I276	K277	D282	V283	L284	E285	F286	R287	G290	I291	I292	P293	D294	E296	L298	I301	C302	V305	L308	N309	L311	L312	L313	L314	M315	L316	I324	R327	A330	I334	G335	R336	R337	G338	T339	A340	L341	C342	I343	K344	Q345	E346	K347	R348	K353	D354	I355	K358	E359	F360	L361	P362	H363	I364	T365	Q366	F370	E371	K374	F377	L378	G379	I382	N383	L386	K469	K470	K471	A472	K473	S474	S475	R476	A477	G478	V479	S480	O481	V482	L483	N484	R485	Y486	T487	Y488	S489	S490	T491	L492	L495	R496	R497	T498	F502	GLY	ARG	ASP	GLY	LYS	LEU	A509	R512	Q513	L514	L515	H516	T517	H518	W519	C523	T527	C530	Q531	L535	V536	K537	L541	H542	I545	S546	V547	G548	T549	D550	P551	N552	E553	I554	J555	L558	S559	E560	V561	E567	V570	I568	L561	M562	K563	L564	K565	I568	M569	A569	V576	E577	E578	Y579	F580	F581	N592	P593	L596	N597	E598	T599	L600	L603	R604	L609	E612	V613	S614	N615	L616	R620	E623	L626	T628	O631	R632	V633	Y634	R635	P636	L637	F638	D642	D643	E644	S645	G646	H648	L651	K652	K653	R654	K655	I658	M661	M662	L663	A663	T664	V676	E677	E678	Y679	T680	S683	L689	V690	E691	Y692	I693	D694	A695	E696	E697	E698	I701	L702	I703	A704	T705	P706	P707	L710	E711	P712	A713	E714	A715	N716	E717	E718	N719	L720	D721	D722	V723	R728	L729	R730	T731	H732	S733	H740	T743	H744	P745	S746	M747	L748	L749	V751	I756	F757	F758	P759	D760	H761	N762	R766	N767	T768	Y769	Q770	S771	K775	Q776	A777	M778	G779	V780	F781	L782	T783	Y784	Y785	R788	M789	D790	T791	M792	A793	N794	I795	L796	Y797	Y798	K801	P802	L803	G804	R805	T806	R807	N808	T809	T810	M811	L812	R815	E816	L817	P818	Q821	N822	V825	A826	I827	C828	S829	Y830	S831	G832	Y833	N834	Q835	E836	D837	S838	M839	I840	M841	N842	Q843	S844	S845	I846	F851	Y856	Y859	M860	Q861	Q862	S863	K864	K865	S869	I870	T871	E872	T873	F874	E875	K876	R877	Q878	R879	T880	T881	T882	M885	K886	I889	P890	V895	S896	V897	D898	F899	G900	P901	V905	S906	I907	D908	I909	P910	Q911	I912	G913	K914	T915	T916	P917	I918	S919	PRO	ASP	GLU	GLU	GLU	LEU	GLY	GLN	ARG	THR	ALA	TYR	HIS	S933	K934	S938	L941	R942	T943	T944	E945	N946	D950	Q951	V952	T955	T956	N957	Q959	I961	K962	F963	V964	K965	V966	R967	V968	R969	T970	T971	K972	P973	P974	Q975	S976	G977	D978	K979	F980	A981	S982	R983	H984	Q985	Q986	Q987	G988	T989	I990	G991	I992	T993	Y994	R995	Y996	E997	D998	N999	P1000	F1001	T1002	A1003	E1004	L1081	M1082	A1083	Q1084	I1085	L1086	F1087	G1088	P1089	T1090	Y1091	Q1092	Q1093	R1094	L1095	R1096	H1097	M1098	V1099	D1100	D1101	K1102	C1103	H1104	A1105	R1106	A1107	R1108	G1109	P1110	M1111	Q1112	L1113	T1114	L1115	R1116	Q1117	P1118	V1119	E1120	G1121	L1122	R1123	S1124	D1125	A1126	G1127	L1128	R1129	F1130	G1131	E1132	M1133	E1134	R1135	I1136	A1140	H1141	G1142	L1215	L1216	Y1217	S145	F1146	L1147	K1148	E1149	R1150	L1151	M1152	E1153	D1156	R1159	V1160	H1161	I1162	C1163	G1164	I1165	C1166	G1167	L1168	I1172	A1173	L1174	M1176	Q1179	F1180	E1181	M1187	K1188	I1189	D1190	Q1193	I1194	H1195	I1196	P1197	Y1198	A1199	A1200	K1201	L1202	L1203	F1204	Q1205	M1208	A1209	M1210	N1211	I1212	H1213	P1214	Q215	S218	N221	L222	V223	Q224	V225	S232	S235	H236	E239	L240	R241	S242	L244	E245	K246	Q255	V256	G260	R261	R267	T268	L273	P274	Y275	I276	K277	D282	V283	L284	E285	F286	R287	G290	I291	I292	P293	D294	E296	L298	I301	C302	V305	L308	N309	L311	L312	L313	L314	M315	L316	I324	R327	A330	I334	G335	R336	R337	G338	T339	A340	L341	C342	I343	K344	Q345	E346	K347	R348	K353	D354	I355	K358	E359	F360	L361	P362	H363	I364	T365	Q366	F370	E371	K374	F377	L378	G379	I382	N383	L386	K469	K470	K471	A472	K473	S474	S475	R476	A477	G478	V479	S480	O481	V482	L483	N484	R485	Y486	T487	Y488	S489	S490	T491	L492	L495	R496	R497	T498	F502	GLY	ARG	ASP	GLY	LYS	LEU	A509	R512	Q513	L514	L515	H516	T517	H518	W519	C523	T527	C530	Q531	L535	V536	K537	L541	H542	I545	S546	V547	G548	T549	D550	P551	N552	E553	I554	J555	L558	S559	E560	V561	E567	V570	I568	L561	M562	K563	L564	K565	I568	M569	A569	V576	E577	E578	Y579	F580	F581	N592	P593	L596	N597	E598	T599	L600	L603	R604	L609	E612	V613	S614	N615	L616	R620	E623	L626	T628	O631	R632	V633	Y634	R635	P636	L637	F638	D642	D643	E644	S645	G646	H648	L651	K652	K653	R654	K655	I658	M661	M662	L663	A663	T664	V676	E677	E678	Y679	T680	S683	L689	V690	E691	Y692	I693	D694	A695	E696	E697	E698	I701	L702	I703	A704	T705	P706	P707	L710	E711	P712	A713	E714	A715	N716	E717	E718	N719	L720	D721	D722	V723	R728	L729	R730	T731	H732	S733	H740	T743	H744	P745	S746	M747	L748	L749	V751	I756	F757	F758	P759	D760	H761	N762	R766	N767	T768	Y769	Q770	S771	K775	Q776	A777	M778	G779	V780	F781	L782	T783	Y784	Y785	R788	M789	D790	T791	M792	A793	N794	I795	L796	Y797	Y798	K801	P802	L803	G804	R805	T806	R807	N808	T809	T810	M811	L812	R815	E816	L817	P818	Q821	N822	V825	A826	I827	C828	S829	Y830	S831	G832	Y833	N834	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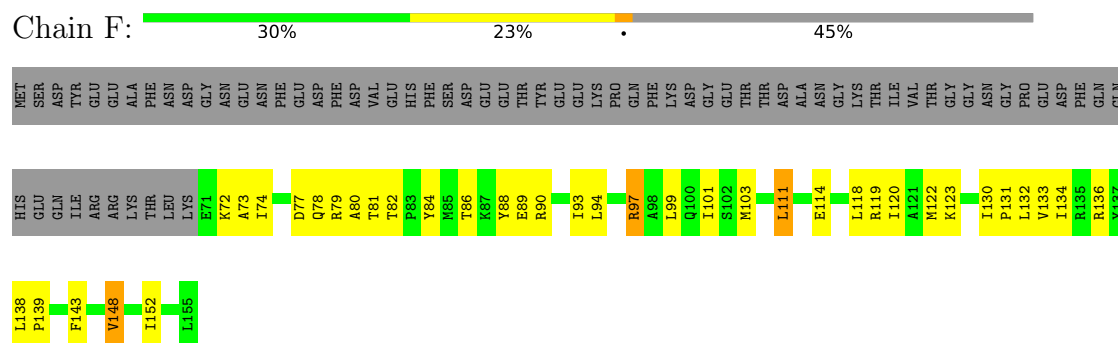
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



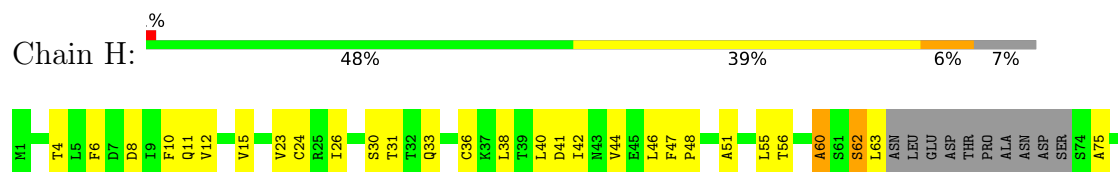
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

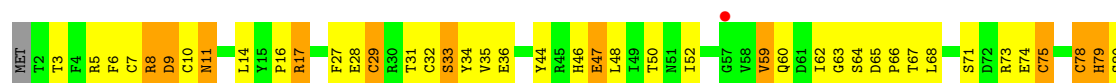
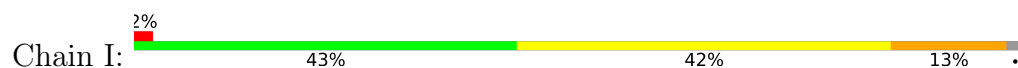


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

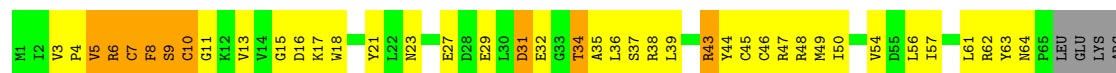




- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

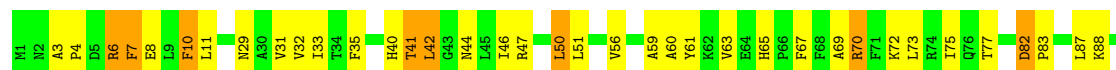


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

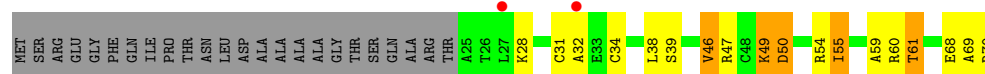


ASP

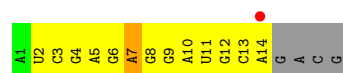
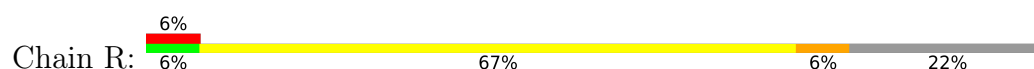
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



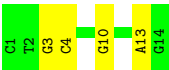
- Molecule 11: DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3')



● Molecule 12: DNA (29-MER)



● Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.45Å 222.29Å 195.09Å 90.00° 101.72° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 97.5 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.278 0.240 , 0.268	Depositor DCC
R_{free} test set	3444 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	116.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 104.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30111	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/11536	1.03	47/15605 (0.3%)
2	B	0.77	1/9348 (0.0%)	1.04	36/12611 (0.3%)
3	C	0.77	0/2174	1.03	8/2946 (0.3%)
4	E	0.63	0/1793	0.92	4/2413 (0.2%)
5	F	0.67	0/696	1.01	5/940 (0.5%)
6	H	0.67	0/1105	0.90	5/1495 (0.3%)
7	I	0.69	0/989	0.95	1/1331 (0.1%)
8	J	0.74	0/541	1.00	0/727
9	K	0.70	0/937	0.98	2/1265 (0.2%)
10	L	0.81	0/365	1.10	1/485 (0.2%)
11	R	0.86	1/318 (0.3%)	1.41	4/496 (0.8%)
12	T	0.47	0/658	1.13	0/1012
13	N	0.63	0/317	1.24	1/488 (0.2%)
All	All	0.72	2/30777 (0.0%)	1.03	114/41814 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	830	TYR	N-CA	5.91	1.53	1.46
11	R	11	U	C1'-N1	5.37	1.56	1.48

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	N-CA-C	10.18	125.85	113.12
3	C	39	ALA	N-CA-C	9.83	122.01	110.41
2	B	344	LYS	N-CA-C	9.50	123.30	112.57
2	B	1156	ASP	N-CA-C	9.44	124.93	113.41
1	A	885	THR	N-CA-C	-9.01	103.39	114.75
1	A	516	SER	N-CA-C	-8.99	94.24	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1167	GLU	N-CA-C	-8.64	99.77	111.96
2	B	344	LYS	N-CA-CB	-8.64	97.26	110.91
2	B	343	ILE	CB-CA-C	8.58	125.46	112.16
1	A	41	MET	N-CA-CB	8.22	124.47	110.50
2	B	976	ILE	N-CA-C	8.07	126.12	109.34
5	F	103	MET	N-CA-C	7.96	120.68	110.65
1	A	516	SER	CB-CA-C	7.84	124.06	109.71
1	A	397	ASN	N-CA-CB	-7.80	99.83	110.67
1	A	356	ASP	CA-C-N	7.78	127.50	119.56
1	A	356	ASP	C-N-CA	7.78	127.50	119.56
10	L	50	ASP	N-CA-C	7.56	126.90	110.80
1	A	88	LYS	CA-C-N	7.54	127.59	119.90
1	A	88	LYS	C-N-CA	7.54	127.59	119.90
1	A	397	ASN	N-CA-C	7.52	123.59	113.97
2	B	474	SER	CB-CA-C	-7.34	96.16	110.10
3	C	195	GLN	N-CA-C	7.27	126.28	110.80
1	A	250	ILE	N-CA-CB	7.18	123.08	111.23
2	B	361	LEU	CA-C-N	6.91	126.61	119.56
2	B	361	LEU	C-N-CA	6.91	126.61	119.56
2	B	635	ARG	CA-C-N	6.83	128.37	119.84
2	B	635	ARG	C-N-CA	6.83	128.37	119.84
1	A	122	MET	N-CA-C	-6.71	106.97	114.62
11	R	7	A	C4'-C3'-O3'	-6.71	102.93	113.00
1	A	328	ARG	N-CA-C	-6.71	103.78	112.23
1	A	226	GLU	N-CA-CB	-6.57	99.38	110.49
1	A	40	THR	CB-CA-C	-6.56	98.74	109.56
2	B	342	GLY	N-CA-C	-6.53	106.26	114.16
3	C	181	ASP	CA-C-N	6.42	127.86	119.84
3	C	181	ASP	C-N-CA	6.42	127.86	119.84
11	R	10	A	O5'-C5'-C4'	6.34	121.01	111.50
2	B	715	ALA	CB-CA-C	6.32	122.99	110.42
1	A	93	VAL	N-CA-C	6.15	116.81	110.36
4	E	52	ARG	CA-C-N	6.11	127.48	119.84
4	E	52	ARG	C-N-CA	6.11	127.48	119.84
2	B	715	ALA	N-CA-C	-6.03	97.95	110.80
1	A	977	LYS	CA-C-N	5.99	125.95	119.78
1	A	977	LYS	C-N-CA	5.99	125.95	119.78
2	B	308	TRP	N-CA-C	5.97	117.46	111.07
1	A	864	ILE	N-CA-C	-5.91	106.48	111.56
2	B	716	ASN	N-CA-CB	-5.89	100.48	110.50
13	N	10	DG	P-O3'-C3'	5.87	129.01	120.20
2	B	798	TYR	CA-C-N	5.85	125.76	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	798	TYR	C-N-CA	5.85	125.76	119.85
3	C	173	ALA	N-CA-C	5.85	120.43	113.12
1	A	296	LEU	N-CA-C	-5.83	107.41	114.75
2	B	1055	ILE	N-CA-C	-5.80	104.97	110.42
1	A	1124	HIS	CB-CA-C	-5.76	97.99	109.33
2	B	801	LYS	CA-C-N	5.74	125.74	119.89
2	B	801	LYS	C-N-CA	5.74	125.74	119.89
6	H	80	ARG	CA-C-N	5.73	126.28	120.38
6	H	80	ARG	C-N-CA	5.73	126.28	120.38
7	I	85	PHE	N-CA-C	5.67	116.57	108.74
2	B	790	ASP	CB-CA-C	5.66	118.99	109.48
1	A	366	VAL	CB-CA-C	-5.65	105.72	111.08
1	A	1125	ALA	N-CA-CB	-5.62	101.00	110.49
2	B	716	ASN	N-CA-C	5.61	126.71	111.00
2	B	341	LEU	N-CA-C	-5.54	99.00	110.80
1	A	687	LYS	N-CA-C	-5.54	106.57	113.38
5	F	74	ILE	CA-C-N	5.54	125.54	119.89
5	F	74	ILE	C-N-CA	5.54	125.54	119.89
2	B	869	SER	CB-CA-C	5.54	121.44	110.42
4	E	95	THR	N-CA-C	5.52	116.98	111.07
5	F	138	LEU	CA-C-N	5.52	126.74	119.84
5	F	138	LEU	C-N-CA	5.52	126.74	119.84
2	B	875	GLU	N-CA-C	5.52	115.53	108.24
3	C	149	LYS	N-CA-C	5.51	122.55	110.80
2	B	1047	PHE	N-CA-C	-5.50	99.77	108.73
2	B	861	ASP	N-CA-C	5.49	116.75	108.46
1	A	491	VAL	CA-C-N	5.47	125.42	119.78
1	A	491	VAL	C-N-CA	5.47	125.42	119.78
2	B	830	TYR	N-CA-C	5.47	122.44	110.80
1	A	1075	PRO	N-CA-C	-5.45	107.05	113.86
11	R	2	U	C4'-C3'-C2'	-5.44	97.16	102.60
6	H	128	ASN	N-CA-CB	-5.42	103.24	111.15
1	A	776	ALA	N-CA-C	5.32	116.78	110.19
1	A	317	LYS	CB-CA-C	5.32	120.09	111.26
1	A	204	THR	N-CA-CB	-5.30	102.31	110.42
1	A	247	ARG	CA-C-N	5.30	126.47	119.84
1	A	247	ARG	C-N-CA	5.30	126.47	119.84
1	A	655	PHE	N-CA-C	-5.29	105.20	110.97
2	B	535	LEU	N-CA-C	-5.27	106.80	113.18
1	A	230	ARG	CA-C-N	5.26	125.06	119.28
1	A	230	ARG	C-N-CA	5.26	125.06	119.28
1	A	1222	ASN	N-CA-C	5.25	118.84	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	11	U	N1-C1'-C2'	5.24	119.86	112.00
1	A	204	THR	N-CA-C	5.22	119.65	113.12
1	A	532	ARG	N-CA-C	-5.21	104.61	111.96
3	C	174	ALA	CB-CA-C	-5.21	110.15	117.23
1	A	594	GLY	N-CA-C	-5.20	100.85	113.18
1	A	317	LYS	N-CA-C	-5.17	105.19	112.12
2	B	1064	TYR	N-CA-C	5.16	117.04	109.24
6	H	91	ASP	N-CA-C	5.15	117.81	108.69
2	B	78	THR	CA-C-N	5.15	130.97	121.70
2	B	78	THR	C-N-CA	5.15	130.97	121.70
1	A	376	TYR	CA-C-N	5.15	126.28	119.84
1	A	376	TYR	C-N-CA	5.15	126.28	119.84
2	B	829	CYS	CB-CA-C	5.14	119.33	110.86
3	C	133	ILE	N-CA-C	5.13	115.70	108.36
2	B	648	HIS	CB-CA-C	-5.10	110.68	116.54
2	B	648	HIS	N-CA-C	5.10	116.06	108.31
1	A	283	GLY	N-CA-C	-5.09	104.84	112.89
6	H	126	GLU	N-CA-C	5.05	116.65	108.26
2	B	1123	SER	N-CA-C	-5.04	107.28	112.93
4	E	115	ASN	N-CA-C	5.04	115.80	108.14
1	A	1188	GLN	N-CA-CB	5.02	119.04	110.50
1	A	115	LEU	CB-CA-C	5.01	118.40	109.38
9	K	82	ASP	CA-C-N	5.01	124.61	119.05
9	K	82	ASP	C-N-CA	5.01	124.61	119.05

There are no chirality outliers.

There are no planarity outliers.

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	11332	0	11391	860	0
2	B	9168	0	9179	649	0
3	C	2135	0	2091	150	0
4	E	1757	0	1781	49	0
5	F	684	0	703	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1087	0	1062	61	0
7	I	971	0	930	65	0
8	J	532	0	544	50	0
9	K	919	0	929	56	0
10	L	363	0	389	13	0
11	R	284	0	142	18	0
12	T	587	0	327	24	0
13	N	284	0	161	3	0
14	A	2	0	0	2	0
14	B	1	0	0	0	0
14	C	1	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	0	0
All	All	30111	0	29629	1866	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 31.

All (1866) 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)
2:B:438:GLU:HB3	2:B:440:HIS:CD2	1.53	1.43
1:A:1168:GLU:CA	1:A:1171:GLN:HB2	1.51	1.41
1:A:1172:LEU:O	1:A:1174:PHE:N	1.56	1.34
2:B:439:ALA:CB	2:B:440:HIS:HA	1.56	1.29
1:A:1169:ILE:CB	1:A:1170:ILE:HB	1.60	1.29
1:A:1169:ILE:CG2	1:A:1170:ILE:HG13	1.64	1.26
1:A:1169:ILE:HB	1:A:1170:ILE:CB	1.67	1.23
2:B:444:MET:HE3	2:B:446:LEU:CD1	1.70	1.21
1:A:1168:GLU:O	1:A:1169:ILE:HD12	1.38	1.21
1:A:1169:ILE:CA	1:A:1170:ILE:HB	1.72	1.20
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.70	1.20
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.72	1.19
2:B:472:ALA:HB1	2:B:476:ARG:CG	1.72	1.18
1:A:157:ASP:CA	1:A:159:THR:HB	1.73	1.17
2:B:445:LYS:CA	2:B:446:LEU:HB3	1.74	1.17
1:A:1169:ILE:CG2	1:A:1170:ILE:CG1	2.23	1.15
2:B:444:MET:HE3	2:B:446:LEU:HD13	1.27	1.14
1:A:1169:ILE:N	1:A:1170:ILE:HB	1.60	1.13
2:B:438:GLU:CB	2:B:440:HIS:CD2	2.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:ILE:CB	1:A:1170:ILE:HD12	1.79	1.12
1:A:1169:ILE:H	1:A:1170:ILE:C	1.55	1.12
2:B:78:THR:H	2:B:79:THR:HB	1.02	1.12
2:B:445:LYS:HA	2:B:446:LEU:CB	1.76	1.12
1:A:156:ASP:C	1:A:158:PRO:HD3	1.74	1.11
2:B:444:MET:HG2	2:B:446:LEU:HD22	1.26	1.11
1:A:1168:GLU:HA	1:A:1171:GLN:CB	1.78	1.11
1:A:1168:GLU:HB2	1:A:1171:GLN:HG3	1.33	1.11
1:A:1178:ASP:CB	1:A:1179:GLU:HA	1.74	1.11
1:A:1169:ILE:HB	1:A:1170:ILE:HB	1.11	1.09
1:A:1168:GLU:CB	1:A:1171:GLN:CB	2.30	1.09
1:A:157:ASP:HA	1:A:159:THR:HB	1.13	1.09
1:A:1178:ASP:CG	1:A:1179:GLU:HA	1.77	1.08
1:A:419:LYS:NZ	1:A:419:LYS:HB3	1.66	1.08
1:A:1166:ASP:HB3	1:A:1170:ILE:CD1	1.84	1.07
3:C:32:SER:O	3:C:36:VAL:HG12	1.54	1.07
1:A:313:GLN:HG2	1:A:314:ALA:HB2	1.10	1.06
1:A:1169:ILE:HB	1:A:1170:ILE:CD1	1.85	1.06
1:A:1169:ILE:HG22	1:A:1170:ILE:CG1	1.81	1.06
1:A:1179:GLU:HG3	1:A:1179:GLU:O	1.52	1.06
1:A:1166:ASP:CB	1:A:1170:ILE:HD13	1.84	1.05
1:A:310:GLY:CA	1:A:311:GLN:HB3	1.86	1.05
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.85	1.05
2:B:472:ALA:HB1	2:B:476:ARG:HG2	1.06	1.05
1:A:1168:GLU:HB2	1:A:1171:GLN:CB	1.87	1.05
1:A:1169:ILE:HB	1:A:1170:ILE:CG1	1.87	1.05
1:A:1173:HIS:NE2	1:A:1175:SER:HB3	1.72	1.04
1:A:1168:GLU:HB2	1:A:1171:GLN:CG	1.85	1.04
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.38	1.04
1:A:313:GLN:HG2	1:A:314:ALA:CB	1.89	1.03
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.24	1.03
1:A:1166:ASP:HB3	1:A:1170:ILE:HD13	1.09	1.03
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.24	1.03
1:A:775:ILE:HB	1:A:797:LYS:O	1.59	1.02
1:A:1168:GLU:CA	1:A:1171:GLN:CB	2.35	1.02
1:A:154:SER:O	1:A:155:GLU:HB2	1.55	1.02
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.42	1.01
1:A:1168:GLU:HG3	1:A:1171:GLN:HB3	1.43	1.01
3:C:142:VAL:HG22	3:C:143:LEU:H	1.24	1.00
1:A:1169:ILE:CB	1:A:1170:ILE:CB	2.30	1.00
1:A:1167:GLU:O	1:A:1170:ILE:HG22	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HD3	1:A:188:ASP:N	1.76	0.99
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.92	0.99
2:B:444:MET:C	2:B:445:LYS:HG3	1.86	0.99
1:A:567:LYS:CB	1:A:568:PRO:CD	2.41	0.99
1:A:1169:ILE:CB	1:A:1170:ILE:CG1	2.40	0.99
2:B:955:THR:HG22	2:B:956:THR:H	1.28	0.98
1:A:1169:ILE:CG2	1:A:1170:ILE:CD1	2.40	0.97
1:A:157:ASP:C	1:A:159:THR:HB	1.88	0.97
1:A:118:HIS:CE1	1:A:155:GLU:HG2	1.98	0.97
1:A:192:GLY:O	1:A:193:ASP:HB3	1.63	0.97
1:A:172:PRO:HG3	1:A:185:TRP:NE1	1.79	0.96
1:A:1178:ASP:OD2	1:A:1179:GLU:HA	1.64	0.96
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.01	0.95
2:B:1020:ARG:O	2:B:1021:MET:HB2	1.64	0.95
1:A:187:LYS:HZ2	1:A:188:ASP:H	1.01	0.95
1:A:249:SER:O	1:A:250:ILE:HG13	1.66	0.95
2:B:472:ALA:CB	2:B:476:ARG:CG	2.44	0.95
1:A:158:PRO:N	1:A:159:THR:CB	2.30	0.94
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.31	0.94
1:A:1169:ILE:HG22	1:A:1170:ILE:HG13	0.94	0.94
1:A:187:LYS:O	1:A:189:ARG:HG3	1.67	0.94
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.97	0.94
1:A:1169:ILE:N	1:A:1170:ILE:CB	2.30	0.94
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.50	0.94
1:A:157:ASP:HA	1:A:159:THR:CB	1.97	0.93
1:A:1169:ILE:H	1:A:1171:GLN:N	1.64	0.93
2:B:445:LYS:HA	2:B:446:LEU:HB3	0.96	0.93
1:A:310:GLY:N	1:A:311:GLN:HB3	1.82	0.93
2:B:1056:SER:HB3	2:B:1066:SER:O	1.68	0.93
2:B:472:ALA:CB	2:B:476:ARG:HG2	1.99	0.92
3:C:167:HIS:HD2	3:C:169:LYS:H	1.08	0.92
11:R:6:G:H2'	11:R:7:A:H8	1.32	0.92
2:B:444:MET:CE	2:B:446:LEU:HD13	1.99	0.92
2:B:843:GLN:HG2	2:B:993:THR:HB	1.50	0.92
1:A:1169:ILE:HG21	1:A:1170:ILE:CD1	1.98	0.92
6:H:109:LYS:HB3	6:H:111:LEU:H	1.33	0.91
1:A:310:GLY:HA2	1:A:311:GLN:HB3	1.50	0.91
1:A:313:GLN:CG	1:A:314:ALA:HB2	2.00	0.91
1:A:1168:GLU:CG	1:A:1171:GLN:HB3	2.01	0.91
1:A:49:LYS:HB3	1:A:55:ASP:OD2	1.71	0.91
1:A:419:LYS:HB3	1:A:419:LYS:HZ2	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.53	0.90
1:A:1169:ILE:CB	1:A:1170:ILE:CD1	2.43	0.90
4:E:94:LYS:HE2	4:E:94:LYS:HA	1.51	0.90
2:B:78:THR:H	2:B:79:THR:CB	1.84	0.90
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.54	0.90
2:B:710:LEU:HD13	2:B:733:HIS:HB3	1.53	0.90
1:A:203:SER:O	1:A:207:ILE:CD1	2.20	0.89
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.54	0.89
1:A:157:ASP:C	1:A:159:THR:CG2	2.45	0.89
1:A:1168:GLU:CB	1:A:1171:GLN:HB3	2.03	0.89
1:A:1168:GLU:CB	1:A:1171:GLN:HB2	1.98	0.89
1:A:158:PRO:N	1:A:159:THR:CA	2.33	0.89
2:B:438:GLU:HB3	2:B:440:HIS:CG	2.07	0.89
2:B:444:MET:HE3	2:B:446:LEU:HD11	1.54	0.89
1:A:1169:ILE:HB	1:A:1170:ILE:HD12	1.44	0.88
3:C:88:CYS:HG	14:C:319:ZN:ZN	0.84	0.88
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.39	0.88
2:B:444:MET:CG	2:B:446:LEU:HD22	2.02	0.88
2:B:85:SER:H	2:B:86:ARG:HB3	1.39	0.88
2:B:77:HIS:HB3	2:B:78:THR:HB	1.56	0.88
1:A:158:PRO:N	1:A:159:THR:HB	1.89	0.87
1:A:310:GLY:H	1:A:311:GLN:HB3	1.37	0.87
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.73	0.87
2:B:759:PRO:HB3	2:B:767:ASN:HD21	1.39	0.87
2:B:636:PRO:CB	2:B:637:LEU:HA	2.03	0.87
1:A:161:LEU:HD22	1:A:162:VAL:N	1.90	0.87
2:B:78:THR:N	2:B:79:THR:HB	1.87	0.87
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.38	0.87
1:A:157:ASP:C	1:A:159:THR:CB	2.47	0.87
1:A:1178:ASP:CB	1:A:1179:GLU:CA	2.52	0.87
1:A:1169:ILE:CG2	1:A:1170:ILE:HD12	2.02	0.86
1:A:1178:ASP:HB2	1:A:1179:GLU:HA	1.57	0.86
2:B:863:GLU:HA	2:B:864:LYS:HB2	1.58	0.86
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.24	0.86
1:A:157:ASP:N	1:A:158:PRO:HD3	1.85	0.85
1:A:1178:ASP:HB2	1:A:1179:GLU:CA	2.07	0.85
1:A:1172:LEU:HD23	1:A:1173:HIS:H	1.42	0.85
2:B:863:GLU:HA	2:B:864:LYS:CB	2.07	0.85
1:A:286:HIS:HB3	1:A:287:HIS:HB2	1.59	0.85
1:A:157:ASP:C	1:A:159:THR:HG22	2.01	0.85
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:C	1:A:158:PRO:CD	2.50	0.85
2:B:766:ARG:NH2	2:B:1020:ARG:NH1	2.25	0.84
1:A:158:PRO:N	1:A:159:THR:HA	1.93	0.84
1:A:160:GLN:CD	1:A:160:GLN:N	2.36	0.84
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.41	0.84
1:A:752:LYS:HG3	2:B:1019:SER:HB2	1.60	0.84
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.58	0.84
3:C:167:HIS:CD2	3:C:169:LYS:H	1.95	0.83
2:B:470:LYS:HE2	2:B:470:LYS:HA	1.59	0.83
6:H:109:LYS:HA	6:H:110:ASP:HB3	1.60	0.83
1:A:40:THR:N	1:A:41:MET:HB2	1.93	0.83
1:A:567:LYS:CG	1:A:568:PRO:CD	2.55	0.83
1:A:310:GLY:H	1:A:311:GLN:CB	1.91	0.83
2:B:759:PRO:HB3	2:B:767:ASN:ND2	1.94	0.83
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.59	0.83
7:I:34:TYR:OH	7:I:36:GLU:HB3	1.77	0.83
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.42	0.82
2:B:715:ALA:HB3	2:B:716:ASN:HA	1.58	0.82
8:J:10:CYS:HG	14:J:101:ZN:ZN	0.51	0.82
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.62	0.82
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.09	0.82
1:A:1168:GLU:HA	1:A:1171:GLN:HB2	0.82	0.82
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.60	0.82
2:B:444:MET:O	2:B:445:LYS:HG3	1.80	0.82
12:T:15:DA:H2''	12:T:16:DC:H5''	1.61	0.82
1:A:666:ILE:CD1	2:B:1026:LEU:HB3	2.09	0.82
1:A:335:ARG:HD2	2:B:1202:LEU:HD12	1.62	0.81
1:A:1082:ASN:HA	1:A:1083:THR:C	2.05	0.81
2:B:827:ILE:HD11	2:B:1086:PHE:HD2	1.44	0.81
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.62	0.81
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.98	0.81
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.96	0.81
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.62	0.81
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.62	0.81
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.61	0.81
1:A:148:CYS:HG	14:A:1734:ZN:ZN	0.92	0.81
1:A:573:SER:H	1:A:576:GLN:HG3	1.46	0.81
11:R:6:G:H2'	11:R:7:A:C8	2.15	0.81
1:A:457:ALA:O	1:A:507:VAL:HG23	1.81	0.80
4:E:15:ALA:O	4:E:19:VAL:HG23	1.79	0.80
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:878:GLN:HG2	2:B:879:ARG:H	1.47	0.80
1:A:1167:GLU:C	1:A:1170:ILE:HG22	2.05	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.62	0.80
1:A:185:TRP:O	1:A:186:LYS:HB2	1.81	0.80
3:C:57:VAL:HG21	8:J:57:ILE:HD11	1.64	0.80
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.16	0.80
11:R:4:G:H2'	11:R:5:A:H8	1.45	0.80
1:A:1169:ILE:H	1:A:1170:ILE:CA	1.95	0.80
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.79
7:I:98:VAL:HG11	7:I:113:ASP:HB2	1.64	0.79
1:A:118:HIS:HB2	1:A:123:ARG:HG2	1.64	0.79
2:B:716:ASN:O	2:B:717:GLU:CG	2.30	0.79
1:A:466:SER:O	2:B:1103:ILE:HD11	1.82	0.79
1:A:190:ALA:O	1:A:191:THR:HG23	1.83	0.79
1:A:470:LEU:HD21	1:A:487:MET:CE	2.13	0.79
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.63	0.79
2:B:168:GLY:H	2:B:450:ALA:HB1	1.48	0.78
2:B:472:ALA:CB	2:B:476:ARG:HD3	2.13	0.78
12:T:10:DA:H2''	12:T:11:DG:H5''	1.65	0.78
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.65	0.78
1:A:148:CYS:SG	14:A:1734:ZN:ZN	1.72	0.78
2:B:716:ASN:O	2:B:717:GLU:CB	2.32	0.78
1:A:40:THR:H	1:A:41:MET:HB2	1.49	0.78
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.66	0.78
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.66	0.78
2:B:803:LEU:N	2:B:822:ASN:HD21	1.81	0.78
7:I:78:CYS:O	7:I:79:HIS:HB2	1.83	0.78
11:R:5:A:H2'	11:R:6:G:C8	2.18	0.78
2:B:863:GLU:CA	2:B:864:LYS:HB2	2.14	0.78
1:A:172:PRO:CG	1:A:185:TRP:NE1	2.46	0.77
2:B:65:GLU:CG	2:B:66:ASP:H	1.94	0.77
2:B:716:ASN:O	2:B:717:GLU:HG3	1.84	0.77
1:A:41:MET:HG3	1:A:42:ASP:H	1.48	0.77
2:B:176:SER:O	2:B:182:SER:HB3	1.85	0.77
3:C:148:ARG:HH22	8:J:64:ASN:HD22	1.30	0.77
1:A:1172:LEU:C	1:A:1174:PHE:N	2.43	0.77
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.66	0.77
2:B:976:ILE:O	2:B:990:ILE:HB	1.85	0.76
2:B:906:SER:HA	2:B:946:ASN:HB2	1.65	0.76
2:B:65:GLU:HG2	2:B:66:ASP:N	1.98	0.76
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HB3	1:A:321:PRO:CD	2.16	0.76
1:A:185:TRP:HH2	1:A:200:ARG:HD2	1.50	0.76
7:I:103:CYS:HB3	7:I:108:HIS:HB3	1.67	0.76
2:B:864:LYS:HG3	2:B:872:GLU:HB2	1.68	0.76
1:A:472:LEU:O	1:A:475:THR:HB	1.86	0.76
2:B:864:LYS:HE2	2:B:864:LYS:HA	1.67	0.76
6:H:109:LYS:HB3	6:H:111:LEU:N	2.01	0.76
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.51	0.76
1:A:158:PRO:CD	1:A:159:THR:HA	2.17	0.75
1:A:1178:ASP:OD2	1:A:1179:GLU:CA	2.34	0.75
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.66	0.75
1:A:161:LEU:HD22	1:A:162:VAL:H	1.50	0.75
2:B:445:LYS:CA	2:B:446:LEU:CB	2.49	0.75
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	1.98	0.75
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.67	0.75
1:A:156:ASP:O	1:A:158:PRO:HD2	1.86	0.75
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.67	0.75
2:B:438:GLU:HG2	2:B:440:HIS:NE2	2.01	0.75
6:H:38:LEU:HD11	6:H:123:MET:HE2	1.68	0.75
1:A:419:LYS:HB3	1:A:419:LYS:HZ3	1.47	0.75
1:A:666:ILE:HD12	1:A:666:ILE:N	2.01	0.75
2:B:839:MET:HE3	2:B:1010:LEU:HD12	1.68	0.75
3:C:148:ARG:HH22	8:J:64:ASN:ND2	1.84	0.75
8:J:9:SER:OG	8:J:45:CYS:HB2	1.85	0.75
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.27	0.75
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.69	0.74
5:F:111:LEU:HD22	5:F:111:LEU:H	1.51	0.74
1:A:508:PRO:O	1:A:511:ILE:HG13	1.86	0.74
1:A:193:ASP:O	1:A:194:ALA:CB	2.35	0.74
1:A:809:THR:HB	1:A:810:PRO:HD2	1.68	0.74
1:A:445:ASN:CB	1:A:455:MET:HG2	2.18	0.74
1:A:567:LYS:HD3	1:A:568:PRO:HD2	1.70	0.74
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.02	0.74
2:B:906:SER:HA	2:B:946:ASN:CB	2.17	0.74
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.53	0.73
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.69	0.73
1:A:156:ASP:O	1:A:158:PRO:CD	2.36	0.73
2:B:515:HIS:HD2	2:B:517:THR:H	1.37	0.73
2:B:766:ARG:NH2	2:B:1020:ARG:HH12	1.85	0.73
1:A:482:PHE:O	2:B:989:THR:HG23	1.87	0.73
2:B:85:SER:N	2:B:86:ARG:HB3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:GLU:O	1:A:1179:GLU:CG	2.31	0.73
1:A:1173:HIS:CD2	1:A:1175:SER:CB	2.72	0.73
2:B:66:ASP:CG	2:B:66:ASP:O	2.30	0.73
1:A:858:ASN:C	1:A:858:ASN:HD22	1.95	0.73
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.70	0.73
1:A:1169:ILE:HG21	1:A:1170:ILE:HD12	1.65	0.73
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.70	0.73
3:C:142:VAL:HG21	8:J:5:VAL:HG13	1.70	0.73
8:J:43:ARG:HB3	8:J:43:ARG:HH11	1.52	0.73
1:A:310:GLY:CA	1:A:311:GLN:CB	2.67	0.73
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.54	0.73
1:A:192:GLY:O	1:A:193:ASP:CB	2.37	0.72
2:B:956:THR:HA	2:B:961:LEU:O	1.88	0.72
1:A:91:PHE:H	1:A:297:GLN:HE22	1.34	0.72
2:B:759:PRO:CB	2:B:767:ASN:HD21	2.02	0.72
2:B:472:ALA:HB2	2:B:476:ARG:HD3	1.69	0.72
2:B:515:HIS:H	2:B:518:HIS:CD2	2.07	0.72
2:B:338:GLY:HA3	2:B:341:LEU:HG	1.71	0.72
1:A:401:GLY:C	1:A:435:HIS:CD2	2.68	0.72
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	1.89	0.72
6:H:112:ILE:HG22	6:H:127:GLY:O	1.89	0.72
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.05	0.72
2:B:445:LYS:HB3	2:B:447:ALA:H	1.55	0.72
1:A:187:LYS:HB2	1:A:187:LYS:NZ	2.03	0.71
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.25	0.71
4:E:24:LYS:HB3	4:E:30:ILE:HD12	1.70	0.71
1:A:630:ILE:H	1:A:630:ILE:HD12	1.55	0.71
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.70	0.71
2:B:438:GLU:O	2:B:439:ALA:C	2.34	0.71
1:A:264:PHE:CE2	12:T:29:DA:H3'	2.26	0.71
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.70	0.71
1:A:1169:ILE:N	1:A:1170:ILE:CA	2.53	0.71
3:C:124:LEU:O	3:C:127:ARG:HG2	1.89	0.71
2:B:64:CYS:SG	2:B:65:GLU:N	2.61	0.71
2:B:440:HIS:C	2:B:442:PHE:H	1.98	0.71
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.72	0.71
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.73	0.71
1:A:672:ASP:H	1:A:736:ASN:HD21	1.36	0.71
1:A:203:SER:O	1:A:207:ILE:HD12	1.89	0.71
1:A:1169:ILE:N	1:A:1171:GLN:N	2.39	0.71
2:B:463:THR:CG2	2:B:465:ASN:HD21	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	1.90	0.71
1:A:193:ASP:O	1:A:194:ALA:HB3	1.88	0.71
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.56	0.71
1:A:1169:ILE:N	1:A:1170:ILE:C	2.40	0.71
1:A:1269:GLU:O	1:A:1270:ASN:HB2	1.90	0.71
2:B:472:ALA:CB	2:B:476:ARG:CD	2.69	0.71
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.71	0.71
2:B:1166:CYS:O	2:B:1215:ARG:HD2	1.91	0.71
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.06	0.70
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.56	0.70
1:A:185:TRP:O	1:A:186:LYS:CB	2.38	0.70
1:A:310:GLY:N	1:A:311:GLN:CB	2.50	0.70
1:A:1168:GLU:O	1:A:1169:ILE:CD1	2.30	0.70
3:C:182:PRO:HB3	3:C:207:CYS:SG	2.31	0.70
1:A:1177:LEU:O	1:A:1177:LEU:CD1	2.39	0.70
2:B:636:PRO:CB	2:B:637:LEU:CA	2.69	0.70
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.74	0.70
1:A:821:ARG:O	1:A:825:ILE:HG12	1.92	0.70
2:B:65:GLU:HG2	2:B:66:ASP:H	1.54	0.70
2:B:439:ALA:HB3	2:B:440:HIS:HA	0.76	0.70
2:B:445:LYS:CA	2:B:447:ALA:H	2.05	0.70
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.70
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.56	0.70
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.73	0.70
1:A:172:PRO:HG3	1:A:185:TRP:CE2	2.27	0.70
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.22	0.70
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.73	0.70
1:A:157:ASP:CA	1:A:159:THR:CB	2.59	0.69
1:A:187:LYS:CD	1:A:188:ASP:N	2.54	0.69
1:A:1169:ILE:CG1	1:A:1170:ILE:HD12	2.21	0.69
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.73	0.69
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.56	0.69
2:B:438:GLU:CG	2:B:440:HIS:CD2	2.75	0.69
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.69
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.23	0.69
2:B:715:ALA:HB3	2:B:716:ASN:C	2.17	0.69
8:J:7:CYS:SG	14:J:101:ZN:ZN	1.81	0.69
1:A:187:LYS:NZ	1:A:188:ASP:H	1.85	0.69
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.73	0.69
1:A:154:SER:O	1:A:155:GLU:CB	2.37	0.69
1:A:1173:HIS:HD2	1:A:1175:SER:OG	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:H	2:B:518:HIS:HD2	1.38	0.69
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.23	0.69
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.75	0.69
2:B:744:HIS:HD2	2:B:746:SER:OG	1.76	0.69
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.27	0.69
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.22	0.69
2:B:717:GLU:O	2:B:720:ASP:N	2.26	0.69
9:K:46:ILE:O	9:K:50:LEU:HB2	1.91	0.69
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.91	0.68
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.57	0.68
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.93	0.68
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.75	0.68
3:C:133:ILE:HD11	3:C:237:SER:HA	1.74	0.68
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	1.74	0.68
2:B:65:GLU:CG	2:B:66:ASP:N	2.56	0.68
2:B:334:ILE:HG22	2:B:334:ILE:O	1.94	0.68
2:B:339:THR:O	2:B:340:ALA:HB3	1.93	0.68
2:B:717:GLU:O	2:B:718:GLU:C	2.36	0.68
2:B:872:GLU:HG2	2:B:916:THR:HB	1.75	0.68
1:A:889:SER:HB2	1:A:892:ALA:H	1.59	0.68
3:C:88:CYS:SG	14:C:319:ZN:ZN	1.83	0.68
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.75	0.68
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.82	0.68
1:A:55:ASP:H	1:A:56:PRO:HD2	1.60	0.67
1:A:255:SER:HA	1:A:256:GLN:C	2.19	0.67
1:A:834:THR:HG21	1:A:1077:THR:HA	1.75	0.67
1:A:320:ARG:HA	1:A:320:ARG:HE	1.58	0.67
1:A:382:PRO:HG3	1:A:428:TYR:CE2	2.29	0.67
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.76	0.67
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.77	0.67
1:A:264:PHE:HE2	12:T:29:DA:H3'	1.59	0.67
2:B:87:LYS:NZ	2:B:436:VAL:HG11	2.09	0.67
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.76	0.67
9:K:102:LYS:O	9:K:106:GLU:HG2	1.93	0.67
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.76	0.67
2:B:516:ASN:HD22	2:B:516:ASN:H	1.41	0.67
1:A:1173:HIS:CD2	1:A:1175:SER:HB3	2.29	0.67
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.77	0.67
2:B:784:ASN:OD1	2:B:788:ARG:HD2	1.95	0.67
5:F:132:LEU:O	5:F:148:VAL:HG23	1.95	0.67
9:K:63:VAL:HG23	9:K:63:VAL:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:GLY:H	11:R:12:G:H22	1.41	0.67
1:A:172:PRO:HG3	1:A:185:TRP:HE1	1.58	0.67
3:C:102:GLN:HG2	3:C:154:LYS:HD2	1.77	0.67
3:C:142:VAL:HG22	3:C:143:LEU:N	2.01	0.67
6:H:62:SER:O	6:H:63:LEU:O	2.12	0.67
2:B:655:LYS:O	2:B:658:ILE:HG22	1.95	0.66
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	2.74	0.66
12:T:2:DT:H2"	12:T:3:DA:C8	2.31	0.66
1:A:599:SER:HB2	1:A:603:ASN:H	1.60	0.66
2:B:438:GLU:CB	2:B:440:HIS:HD2	1.99	0.66
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.77	0.66
2:B:976:ILE:HG23	2:B:977:GLY:H	1.61	0.66
7:I:105:SER:O	7:I:106:CYS:HB3	1.95	0.66
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.77	0.66
6:H:4:THR:HA	6:H:60:ALA:HB2	1.77	0.66
2:B:716:ASN:O	2:B:717:GLU:HB2	1.95	0.66
2:B:715:ALA:N	2:B:716:ASN:HA	2.10	0.66
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.60	0.66
4:E:94:LYS:HE2	4:E:94:LYS:CA	2.26	0.66
1:A:873:MET:C	1:A:1058:VAL:HG23	2.20	0.66
1:A:1173:HIS:CD2	1:A:1175:SER:OG	2.49	0.66
6:H:12:VAL:HG13	6:H:26:ILE:HD11	1.77	0.66
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.78	0.66
1:A:809:THR:HB	1:A:810:PRO:CD	2.26	0.66
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.31	0.66
1:A:917:SER:O	1:A:918:GLU:HG3	1.96	0.66
3:C:133:ILE:CD1	3:C:237:SER:HA	2.25	0.66
6:H:109:LYS:HA	6:H:110:ASP:CB	2.25	0.66
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.25	0.66
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.77	0.66
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.31	0.66
2:B:445:LYS:CB	2:B:447:ALA:H	2.08	0.66
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.78	0.65
2:B:463:THR:HG22	2:B:465:ASN:HD21	1.61	0.65
2:B:706:GLN:O	2:B:710:LEU:HB2	1.96	0.65
1:A:118:HIS:NE2	1:A:155:GLU:HG2	2.11	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.65
2:B:637:LEU:HD11	2:B:740:HIS:HB3	1.78	0.65
2:B:994:TYR:HB2	2:B:999:MET:CE	2.26	0.65
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.77	0.65
5:F:114:GLU:OE2	5:F:119:ARG:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:5:A:H2'	11:R:6:G:H8	1.60	0.65
1:A:1386:ARG:NH2	12:T:15:DA:H8	1.94	0.65
2:B:715:ALA:HB3	2:B:716:ASN:CA	2.25	0.65
3:C:43:THR:CG2	3:C:44:LEU:N	2.59	0.65
1:A:320:ARG:HB3	1:A:321:PRO:HD2	1.76	0.65
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.62	0.65
2:B:715:ALA:CB	2:B:716:ASN:HA	2.20	0.65
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.08	0.65
1:A:1177:LEU:O	1:A:1177:LEU:HD12	1.94	0.65
1:A:118:HIS:NE2	1:A:155:GLU:CG	2.59	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.65
1:A:741:ASN:ND2	1:A:744:LYS:H	1.94	0.65
1:A:779:PHE:CZ	2:B:517:THR:HA	2.32	0.65
1:A:1030:ARG:HG2	1:A:1034:GLU:CD	2.22	0.65
2:B:463:THR:CG2	2:B:465:ASN:ND2	2.60	0.65
7:I:78:CYS:O	7:I:79:HIS:CB	2.45	0.65
2:B:459:TYR:C	2:B:459:TYR:CD2	2.76	0.64
1:A:1269:GLU:O	1:A:1270:ASN:CB	2.44	0.64
2:B:439:ALA:CB	2:B:440:HIS:CA	2.43	0.64
1:A:535:THR:O	1:A:575:LYS:HE2	1.97	0.64
1:A:775:ILE:HB	1:A:797:LYS:C	2.22	0.64
1:A:883:LEU:O	1:A:885:THR:N	2.30	0.64
1:A:1173:HIS:NE2	1:A:1175:SER:CB	2.55	0.64
2:B:291:ILE:HD12	2:B:291:ILE:N	2.12	0.64
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.32	0.64
2:B:986:GLN:HE21	2:B:1022:THR:CG2	2.07	0.64
1:A:503:GLN:HE22	5:F:90:ARG:HH21	1.45	0.64
1:A:109:HIS:HB2	1:A:167:CYS:SG	2.38	0.64
8:J:43:ARG:HB3	8:J:43:ARG:NH1	2.12	0.64
1:A:151:ASP:HB2	1:A:162:VAL:O	1.98	0.64
6:H:26:ILE:HG22	6:H:40:LEU:O	1.97	0.64
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.80	0.64
7:I:83:ASN:C	7:I:83:ASN:HD22	2.06	0.64
9:K:69:ALA:O	9:K:70:ARG:HB3	1.96	0.64
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.33	0.63
3:C:163:ILE:HD13	9:K:10:PHE:CE1	2.33	0.63
1:A:658:LEU:HG	1:A:659:HIS:CD2	2.33	0.63
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.32	0.63
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.63
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.64	0.63
2:B:793:ALA:C	2:B:794:ASN:HD22	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.68	0.63
1:A:1172:LEU:HD23	1:A:1173:HIS:N	2.12	0.63
2:B:60:GLN:O	2:B:63:ILE:HG22	1.99	0.63
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.28	0.63
4:E:88:VAL:HG21	4:E:116:ILE:HD13	1.80	0.63
6:H:114:VAL:CG2	6:H:125:LEU:HB3	2.29	0.63
1:A:198:GLU:CD	1:A:198:GLU:N	2.57	0.63
1:A:317:LYS:N	1:A:317:LYS:HD2	2.14	0.63
6:H:109:LYS:HG2	6:H:111:LEU:HD12	1.80	0.63
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.81	0.63
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.79	0.63
3:C:241:ASP:O	3:C:244:VAL:HG13	1.98	0.63
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.34	0.63
1:A:404:TYR:HA	1:A:413:ILE:O	1.99	0.63
6:H:109:LYS:HD3	6:H:111:LEU:HB2	1.81	0.63
11:R:4:G:H2'	11:R:5:A:C8	2.32	0.63
1:A:630:ILE:HD12	1:A:630:ILE:N	2.14	0.62
2:B:464:GLY:CA	2:B:479:VAL:O	2.47	0.62
1:A:575:LYS:NZ	1:A:615:GLY:O	2.31	0.62
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.80	0.62
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.80	0.62
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.62	0.62
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.81	0.62
1:A:523:ILE:HG23	1:A:527:THR:OG1	2.00	0.62
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.13	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.81	0.62
1:A:158:PRO:HD2	1:A:160:GLN:OE1	1.99	0.62
1:A:699:ALA:HB1	7:I:114:GLN:HG3	1.81	0.62
2:B:803:LEU:H	2:B:822:ASN:HD21	1.45	0.62
7:I:34:TYR:CZ	7:I:36:GLU:HB3	2.35	0.62
1:A:118:HIS:HE1	1:A:155:GLU:HG2	1.63	0.62
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.81	0.62
1:A:845:LEU:O	1:A:848:ILE:HG12	2.00	0.62
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.65	0.62
12:T:6:DG:H2'	12:T:7:DA:C8	2.35	0.62
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.15	0.62
2:B:880:THR:HB	2:B:934:LYS:HB2	1.82	0.62
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.81	0.62
10:L:38:LEU:HD21	10:L:49:LYS:H	1.65	0.62
12:T:14:DG:H2'	12:T:15:DA:C4	2.33	0.62
1:A:55:ASP:O	1:A:58:LEU:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:HIS:HB2	1:A:1086:PHE:HA	1.80	0.61
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.34	0.61
8:J:7:CYS:O	8:J:8:PHE:C	2.43	0.61
2:B:438:GLU:HG2	2:B:440:HIS:CD2	2.34	0.61
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.25	0.61
1:A:118:HIS:CE1	1:A:155:GLU:CG	2.80	0.61
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.82	0.61
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.00	0.61
2:B:340:ALA:O	2:B:342:GLY:N	2.32	0.61
2:B:1072:MET:CE	2:B:1085:ILE:HD12	2.31	0.61
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.82	0.61
1:A:153:PRO:C	1:A:155:GLU:H	2.06	0.61
1:A:158:PRO:HD2	1:A:159:THR:HA	1.82	0.61
1:A:196:GLU:N	1:A:197:PRO:HD3	2.15	0.61
4:E:79:TRP:NE1	4:E:81:GLU:HG3	2.14	0.61
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.82	0.61
1:A:31:SER:HB2	1:A:81:PHE:O	2.01	0.61
1:A:351:THR:OG1	2:B:1103:ILE:HG12	2.01	0.61
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.82	0.61
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.77	0.61
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.15	0.61
2:B:440:HIS:O	2:B:442:PHE:N	2.34	0.61
1:A:107:CYS:SG	1:A:108:MET:N	2.74	0.61
1:A:187:LYS:HD3	1:A:187:LYS:C	2.26	0.61
1:A:332:LYS:H	1:A:337:ARG:HB3	1.65	0.61
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.36	0.61
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.36	0.61
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.00	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.83	0.61
3:C:43:THR:HG23	3:C:74:SER:OG	2.01	0.60
1:A:35:ILE:HG22	1:A:35:ILE:O	2.00	0.60
1:A:185:TRP:HH2	1:A:200:ARG:CD	2.15	0.60
2:B:444:MET:C	2:B:445:LYS:CG	2.68	0.60
3:C:148:ARG:NH2	8:J:64:ASN:HD22	1.99	0.60
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.36	0.60
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.84	0.60
2:B:979:LYS:O	2:B:980:PHE:CD1	2.54	0.60
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.82	0.60
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.37	0.60
2:B:467:GLY:O	2:B:468:GLU:C	2.42	0.60
3:C:259:LEU:HD21	9:K:92:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:75:CYS:SG	7:I:78:CYS:SG	2.99	0.60
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.31	0.60
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.83	0.60
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.30	0.60
1:A:265:LYS:HE2	1:A:303:TYR:HA	1.82	0.60
1:A:302:THR:HG23	1:A:306:ASN:HB3	1.83	0.60
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.14	0.60
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.27	0.60
1:A:907:THR:HG22	1:A:908:LEU:H	1.67	0.60
1:A:814:PHE:O	1:A:817:ALA:HB3	2.02	0.60
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.66	0.60
3:C:180:TYR:O	3:C:181:ASP:HB3	2.02	0.60
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.17	0.60
1:A:1429:ILE:O	1:A:1429:ILE:HG22	2.02	0.60
2:B:459:TYR:C	2:B:459:TYR:HD2	2.10	0.60
2:B:980:PHE:O	2:B:1095:LEU:HG	2.02	0.60
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.01	0.60
2:B:1020:ARG:NH1	2:B:1020:ARG:HB3	2.16	0.60
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.32	0.60
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.41	0.60
2:B:982:SER:OG	2:B:983:ARG:N	2.35	0.60
5:F:97:ARG:HD2	5:F:101:ILE:HG13	1.83	0.60
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.84	0.60
1:A:157:ASP:CG	1:A:157:ASP:O	2.43	0.59
1:A:423:ASP:CG	1:A:424:ILE:H	2.08	0.59
2:B:274:PRO:O	2:B:275:TYR:HB2	2.01	0.59
2:B:428:ILE:O	2:B:432:MET:HG3	2.03	0.59
1:A:765:VAL:HG13	1:A:802:ASN:O	2.03	0.59
2:B:863:GLU:HA	2:B:864:LYS:CG	2.32	0.59
1:A:115:LEU:HD12	1:A:122:MET:HE3	1.83	0.59
2:B:445:LYS:HB3	2:B:447:ALA:HB3	1.84	0.59
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.32	0.59
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.37	0.59
2:B:620:ARG:NE	7:I:89:GLN:HE22	2.00	0.59
2:B:976:ILE:HG23	2:B:977:GLY:N	2.17	0.59
1:A:751:SER:O	1:A:752:LYS:HD3	2.02	0.59
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.32	0.59
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.38	0.59
6:H:109:LYS:CB	6:H:111:LEU:H	2.10	0.59
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.84	0.59
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ASN:OD1	2:B:242:SER:HA	2.02	0.59
1:A:39:GLU:HB3	1:A:41:MET:CB	2.32	0.59
1:A:648:ASN:O	1:A:652:VAL:HG23	2.03	0.59
4:E:179:GLN:O	4:E:182:ASP:HB2	2.03	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.03	0.59
8:J:7:CYS:SG	8:J:7:CYS:O	2.61	0.59
1:A:313:GLN:HG2	1:A:314:ALA:CA	2.32	0.59
1:A:351:THR:CG2	1:A:352:VAL:N	2.65	0.59
1:A:719:VAL:HG12	1:A:723:ASN:HD21	1.66	0.59
1:A:981:LEU:HD12	1:A:1032:LEU:HD21	1.85	0.59
2:B:530:GLY:N	11:R:12:G:H22	2.00	0.59
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.37	0.58
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.28	0.58
2:B:843:GLN:HG2	2:B:993:THR:CB	2.28	0.58
6:H:78:SER:O	6:H:79:TRP:C	2.46	0.58
1:A:752:LYS:NZ	11:R:14:DA:O5'	2.35	0.58
9:K:10:PHE:N	9:K:10:PHE:CD2	2.70	0.58
1:A:302:THR:HG21	1:A:314:ALA:HB3	1.84	0.58
1:A:317:LYS:HD2	1:A:317:LYS:H	1.68	0.58
1:A:1170:ILE:HD11	1:A:1239:ARG:HD2	1.85	0.58
2:B:444:MET:SD	2:B:446:LEU:HD13	2.42	0.58
2:B:806:THR:HG22	2:B:808:ALA:H	1.68	0.58
2:B:1056:SER:CB	2:B:1066:SER:O	2.45	0.58
1:A:249:SER:C	1:A:250:ILE:HG13	2.27	0.58
1:A:858:ASN:C	1:A:858:ASN:ND2	2.62	0.58
6:H:36:CYS:HA	6:H:126:GLU:O	2.04	0.58
1:A:56:PRO:O	1:A:57:ARG:HB2	2.03	0.58
1:A:752:LYS:HG3	2:B:1019:SER:CB	2.33	0.58
1:A:756:ILE:O	1:A:760:GLN:HG2	2.03	0.58
1:A:913:LEU:HD11	1:A:981:LEU:O	2.03	0.58
2:B:901:PRO:HB3	2:B:950:ASP:O	2.03	0.58
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.83	0.58
1:A:464:PRO:HB2	1:A:465:TYR:HD1	1.68	0.58
1:A:1243:VAL:HG13	1:A:1244:ARG:HB2	1.85	0.58
2:B:955:THR:HG22	2:B:956:THR:N	2.09	0.58
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.37	0.58
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.85	0.58
1:A:351:THR:HG21	1:A:466:SER:O	2.03	0.58
1:A:573:SER:O	1:A:576:GLN:HB2	2.03	0.58
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.42	0.58
2:B:716:ASN:N	2:B:716:ASN:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.37	0.58
2:B:338:GLY:HA3	2:B:341:LEU:CG	2.33	0.58
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.33	0.58
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.39	0.58
2:B:445:LYS:HA	2:B:447:ALA:H	1.69	0.58
2:B:485:ARG:HH11	2:B:485:ARG:HG2	1.69	0.58
3:C:101:LEU:HB3	3:C:155:LEU:HB2	1.86	0.58
1:A:298:PHE:CE1	1:A:313:GLN:HG3	2.39	0.58
2:B:308:TRP:O	2:B:311:LEU:N	2.37	0.58
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.39	0.58
5:F:99:LEU:O	5:F:99:LEU:HD13	2.04	0.58
7:I:103:CYS:CB	7:I:108:HIS:HB3	2.33	0.58
12:T:13:DA:H2"	12:T:14:DG:C8	2.39	0.58
2:B:567:GLU:H	2:B:567:GLU:CD	2.12	0.57
1:A:58:LEU:HD21	1:A:244:PRO:CD	2.34	0.57
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.50	0.57
1:A:1006:ILE:HD13	1:A:1006:ILE:H	1.69	0.57
2:B:808:ALA:O	2:B:812:LEU:HG	2.04	0.57
1:A:666:ILE:CD1	1:A:666:ILE:N	2.67	0.57
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.30	0.57
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.04	0.57
3:C:3:GLU:HG2	9:K:100:ALA:HB1	1.86	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.19	0.57
6:H:4:THR:HA	6:H:60:ALA:CB	2.34	0.57
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.69	0.57
1:A:187:LYS:HE3	1:A:188:ASP:HB3	1.85	0.57
1:A:190:ALA:O	1:A:191:THR:CG2	2.52	0.57
2:B:464:GLY:HA3	2:B:479:VAL:O	2.04	0.57
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.85	0.57
1:A:53:LEU:C	1:A:53:LEU:HD23	2.29	0.57
1:A:423:ASP:O	1:A:424:ILE:HB	2.03	0.57
2:B:1168:LEU:HD13	2:B:1208:MET:CE	2.32	0.57
1:A:148:CYS:SG	1:A:167:CYS:HB2	2.45	0.57
1:A:346:ASP:OD1	1:A:346:ASP:N	2.37	0.57
1:A:413:ILE:N	1:A:413:ILE:HD12	2.19	0.57
2:B:87:LYS:HZ1	2:B:436:VAL:HG11	1.69	0.57
3:C:112:ASN:HD21	3:C:146:LYS:HD3	1.70	0.57
6:H:142:LEU:HD12	6:H:143:LEU:N	2.19	0.57
1:A:465:TYR:N	1:A:465:TYR:CD1	2.69	0.57
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.70	0.57
9:K:56:VAL:HG13	9:K:77:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.87	0.57
2:B:1008:PRO:HG3	2:B:1087:PHE:CE1	2.40	0.57
1:A:153:PRO:C	1:A:155:GLU:N	2.62	0.57
4:E:29:PHE:C	4:E:30:ILE:HG13	2.30	0.57
1:A:515:GLN:HG3	1:A:1071:SER:HB3	1.87	0.56
1:A:1187:GLN:HB3	1:A:1188:GLN:HA	1.87	0.56
2:B:417:PHE:CE1	2:B:453:ILE:HD13	2.40	0.56
2:B:603:LEU:HB2	2:B:609:ILE:HG12	1.87	0.56
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.70	0.56
1:A:277:GLU:O	1:A:281:HIS:HD2	1.88	0.56
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.40	0.56
3:C:228:PHE:N	3:C:228:PHE:CD1	2.69	0.56
8:J:10:CYS:SG	8:J:11:GLY:N	2.74	0.56
9:K:11:LEU:N	9:K:11:LEU:HD12	2.20	0.56
1:A:157:ASP:N	1:A:158:PRO:CD	2.66	0.56
1:A:365:GLY:O	1:A:468:PHE:HA	2.04	0.56
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.41	0.56
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.70	0.56
1:A:1172:LEU:CG	1:A:1173:HIS:N	2.68	0.56
2:B:313:MET:HA	2:B:313:MET:HE2	1.87	0.56
2:B:474:SER:O	2:B:475:SER:O	2.23	0.56
2:B:978:ASP:O	2:B:980:PHE:HD1	1.86	0.56
2:B:1020:ARG:NH2	11:R:14:DA:OP2	2.38	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.08	0.56
3:C:71:PRO:O	3:C:133:ILE:HG13	2.04	0.56
6:H:95:TYR:HD2	6:H:95:TYR:C	2.12	0.56
2:B:208:SER:HB2	2:B:482:VAL:HG13	1.88	0.56
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.71	0.56
1:A:242:PRO:HG3	2:B:1209:ALA:HB1	1.87	0.56
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.70	0.56
1:A:789:LYS:HD3	2:B:620:ARG:HH12	1.70	0.56
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.88	0.56
3:C:15:LYS:H	3:C:15:LYS:HD2	1.68	0.56
6:H:107:VAL:O	6:H:109:LYS:HG3	2.06	0.56
1:A:272:ALA:O	1:A:296:LEU:HD13	2.05	0.56
1:A:351:THR:HG22	1:A:352:VAL:O	2.05	0.56
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.20	0.56
2:B:48:LEU:HD23	2:B:173:MET:SD	2.46	0.56
2:B:235:SER:OG	2:B:236:HIS:HD2	1.89	0.56
1:A:858:ASN:ND2	1:A:860:LEU:H	2.02	0.56
1:A:1167:GLU:C	1:A:1170:ILE:CG2	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1120:GLU:HG2	2:B:1121:GLY:H	1.69	0.56
1:A:55:ASP:N	1:A:56:PRO:CD	2.69	0.56
1:A:187:LYS:HZ2	1:A:188:ASP:N	1.86	0.56
1:A:645:LEU:O	1:A:649:ILE:HG13	2.06	0.56
7:I:75:CYS:HB2	7:I:78:CYS:SG	2.46	0.56
8:J:10:CYS:SG	8:J:45:CYS:SG	3.04	0.56
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.05	0.56
1:A:35:ILE:CG2	1:A:270:LEU:HD11	2.33	0.56
2:B:1072:MET:HE2	2:B:1085:ILE:HD12	1.88	0.56
2:B:1095:LEU:C	2:B:1096:ARG:O	2.48	0.56
4:E:45:LYS:HD3	4:E:46:TYR:CE1	2.41	0.56
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.36	0.56
1:A:203:SER:O	1:A:207:ILE:HD11	2.03	0.55
1:A:511:ILE:HG12	1:A:521:MET:CE	2.36	0.55
2:B:955:THR:HG23	10:L:54:ARG:O	2.06	0.55
2:B:1082:MET:HA	3:C:189:THR:HA	1.88	0.55
1:A:443:LEU:HD23	1:A:444:PHE:H	1.70	0.55
2:B:287:ARG:HA	2:B:291:ILE:O	2.05	0.55
2:B:310:MET:O	2:B:313:MET:HB2	2.07	0.55
2:B:662:MET:C	2:B:664:THR:H	2.14	0.55
6:H:95:TYR:C	6:H:95:TYR:CD2	2.84	0.55
8:J:44:TYR:CD1	8:J:44:TYR:C	2.84	0.55
9:K:82:ASP:OD1	9:K:83:PRO:HD2	2.06	0.55
1:A:114:LEU:HD11	1:A:171:GLN:HE22	1.71	0.55
1:A:324:SER:OG	1:A:325:ILE:N	2.39	0.55
1:A:691:LEU:O	1:A:695:LYS:HB2	2.05	0.55
1:A:1167:GLU:O	1:A:1170:ILE:CG2	2.44	0.55
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.72	0.55
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.88	0.55
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.22	0.55
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.42	0.55
1:A:187:LYS:HD3	1:A:188:ASP:CA	2.36	0.55
2:B:122:LEU:HD22	2:B:958:GLN:HG3	1.88	0.55
2:B:523:CYS:SG	2:B:750:GLY:N	2.80	0.55
9:K:70:ARG:O	9:K:70:ARG:HG3	2.05	0.55
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.89	0.55
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.41	0.55
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.71	0.55
2:B:545:ILE:CD1	2:B:633:VAL:HG13	2.36	0.55
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.88	0.55
1:A:470:LEU:CD2	1:A:487:MET:HE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:ARG:HH22	12:T:15:DA:H8	1.54	0.55
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.87	0.55
1:A:55:ASP:O	1:A:57:ARG:N	2.39	0.55
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.55
2:B:98:THR:HG21	2:B:101:MET:HE2	1.88	0.55
2:B:558:LEU:C	2:B:560:GLU:H	2.15	0.55
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.07	0.55
7:I:80:SER:HB3	7:I:105:SER:HB2	1.87	0.55
1:A:628:GLY:O	1:A:632:VAL:HG23	2.07	0.55
1:A:679:ILE:O	1:A:682:THR:HG22	2.07	0.55
2:B:31:TRP:O	2:B:34:ILE:N	2.40	0.55
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.37	0.55
3:C:3:GLU:HG3	3:C:4:GLU:H	1.72	0.55
3:C:147:LEU:HD13	3:C:151:GLN:O	2.06	0.55
9:K:35:PHE:HD1	9:K:35:PHE:H	1.55	0.55
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.42	0.55
12:T:15:DA:H2''	12:T:16:DC:C5'	2.35	0.55
2:B:434:ARG:HA	2:B:437:GLU:HG3	1.89	0.54
1:A:306:ASN:HB2	1:A:313:GLN:OE1	2.07	0.54
2:B:344:LYS:HG2	2:B:347:LYS:HD2	1.89	0.54
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.42	0.54
1:A:46:THR:C	1:A:48:ALA:H	2.14	0.54
1:A:157:ASP:O	1:A:159:THR:HG22	2.06	0.54
1:A:302:THR:O	1:A:324:SER:HB2	2.07	0.54
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.43	0.54
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.88	0.54
3:C:93:ASP:O	3:C:127:ARG:NH2	2.40	0.54
4:E:45:LYS:HD3	4:E:46:TYR:HE1	1.72	0.54
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.88	0.54
2:B:42:GLY:O	2:B:43:LEU:HD23	2.07	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.08	0.54
3:C:262:LEU:HD22	9:K:88:LYS:HE2	1.88	0.54
8:J:7:CYS:SG	8:J:9:SER:OG	2.63	0.54
4:E:157:SER:OG	4:E:160:GLU:HB2	2.07	0.54
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.90	0.54
2:B:71:LEU:H	2:B:88:TYR:HA	1.72	0.54
2:B:516:ASN:H	2:B:516:ASN:ND2	2.04	0.54
2:B:863:GLU:HA	2:B:864:LYS:HG2	1.89	0.54
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.73	0.54
1:A:1223:ASP:O	1:A:1224:LEU:HB3	2.06	0.54
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:GLY:O	2:B:267:ARG:HD3	2.08	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.54
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.89	0.54
8:J:37:SER:OG	8:J:47:ARG:NH2	2.41	0.54
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.08	0.54
1:A:160:GLN:N	1:A:160:GLN:OE1	2.37	0.54
1:A:800:VAL:HG13	1:A:812:GLU:CD	2.33	0.54
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.89	0.54
2:B:831:SER:OG	2:B:832:GLY:N	2.40	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.42	0.54
6:H:30:SER:OG	6:H:33:GLN:HB2	2.08	0.54
6:H:142:LEU:C	6:H:143:LEU:HD12	2.32	0.54
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.43	0.54
1:A:1168:GLU:O	1:A:1168:GLU:HG2	2.08	0.54
2:B:25:ILE:HG22	2:B:26:THR:N	2.23	0.54
2:B:89:GLU:O	2:B:89:GLU:HG2	2.03	0.54
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.54
2:B:1072:MET:HE2	2:B:1085:ILE:CD1	2.38	0.54
4:E:27:GLY:O	4:E:65:THR:HG22	2.08	0.54
5:F:82:THR:HG22	5:F:84:TYR:H	1.72	0.54
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.43	0.54
7:I:80:SER:CB	7:I:105:SER:HB2	2.38	0.54
1:A:189:ARG:CZ	1:A:196:GLU:O	2.56	0.54
1:A:286:HIS:HB3	1:A:287:HIS:CB	2.35	0.54
1:A:295:LEU:HA	1:A:298:PHE:HB3	1.89	0.54
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.54
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.30	0.54
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.73	0.54
2:B:383:ASN:O	2:B:387:LEU:HB2	2.08	0.54
2:B:438:GLU:CG	2:B:440:HIS:NE2	2.71	0.54
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.89	0.54
2:B:957:ASN:HB3	2:B:961:LEU:HG	1.90	0.54
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.89	0.54
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.43	0.54
2:B:301:ILE:HG22	2:B:302:CYS:N	2.22	0.53
2:B:491:THR:O	2:B:495:LEU:HG	2.07	0.53
4:E:94:LYS:HA	4:E:94:LYS:CE	2.21	0.53
9:K:73:LEU:CD2	9:K:75:ILE:HD11	2.38	0.53
1:A:55:ASP:N	1:A:56:PRO:HD2	2.23	0.53
1:A:1085:HIS:CB	1:A:1086:PHE:HA	2.37	0.53
2:B:1084:GLN:H	2:B:1084:GLN:CD	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:NZ	1:A:419:LYS:CB	2.50	0.53
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.90	0.53
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.73	0.53
1:A:1209:MET:O	1:A:1212:VAL:HB	2.07	0.53
2:B:652:LYS:HB3	2:B:689:LEU:CD2	2.39	0.53
1:A:1378:GLN:OE1	1:A:1382:THR:HG21	2.08	0.53
1:A:1449:SER:HA	1:A:1450:LEU:C	2.34	0.53
7:I:17:ARG:HB2	7:I:17:ARG:HH11	1.73	0.53
1:A:390:GLN:O	1:A:394:ASN:HB2	2.08	0.53
2:B:471:LYS:NZ	11:R:4:G:H1'	2.23	0.53
2:B:620:ARG:HE	7:I:89:GLN:HE22	1.57	0.53
2:B:906:SER:HA	2:B:946:ASN:HB3	1.89	0.53
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.24	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.90	0.53
2:B:440:HIS:C	2:B:442:PHE:N	2.61	0.53
2:B:488:TYR:C	2:B:490:SER:H	2.16	0.53
2:B:790:ASP:OD2	2:B:790:ASP:N	2.42	0.53
2:B:1149:GLU:C	2:B:1151:LEU:H	2.17	0.53
2:B:1027:ILE:O	2:B:1030:LEU:N	2.42	0.53
9:K:29:ASN:ND2	9:K:77:THR:O	2.42	0.53
1:A:187:LYS:HZ2	1:A:187:LYS:HB2	1.71	0.53
2:B:827:ILE:HG13	2:B:1086:PHE:O	2.09	0.53
9:K:73:LEU:HD23	9:K:75:ILE:HD11	1.90	0.53
1:A:316:GLN:HB3	1:A:317:LYS:HD2	1.91	0.53
2:B:964:VAL:HG12	2:B:965:LYS:N	2.23	0.53
3:C:228:PHE:N	3:C:228:PHE:HD1	2.06	0.53
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.91	0.53
1:A:741:ASN:ND2	1:A:741:ASN:C	2.67	0.53
6:H:112:ILE:HG22	6:H:128:ASN:HA	1.91	0.53
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.90	0.52
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.92	0.52
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.24	0.52
2:B:71:LEU:HG	2:B:72:GLU:N	2.21	0.52
3:C:163:ILE:H	3:C:163:ILE:HD12	1.73	0.52
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.39	0.52
1:A:353:ILE:HD13	1:A:487:MET:CE	2.37	0.52
1:A:500:GLU:OE1	2:B:1145:SER:N	2.42	0.52
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.90	0.52
2:B:445:LYS:HA	2:B:447:ALA:N	2.25	0.52
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
6:H:105:GLU:HB2	6:H:115:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.91	0.52
2:B:445:LYS:N	2:B:446:LEU:HB3	2.24	0.52
7:I:7:CYS:O	7:I:11:ASN:HA	2.09	0.52
1:A:401:GLY:O	1:A:435:HIS:CD2	2.63	0.52
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.92	0.52
2:B:76:GLN:HA	2:B:82:ASP:HA	1.91	0.52
2:B:132:VAL:HG21	2:B:445:LYS:HZ1	1.74	0.52
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.52
6:H:40:LEU:HD12	6:H:41:ASP:H	1.75	0.52
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.91	0.52
1:A:75:ASN:HA	2:B:1116:ARG:HH22	1.73	0.52
1:A:322:VAL:C	1:A:324:SER:H	2.18	0.52
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.08	0.52
2:B:546:SER:OG	2:B:631:GLY:N	2.32	0.52
2:B:1110:PRO:HB2	2:B:1119:VAL:HG22	1.92	0.52
2:B:1112:GLN:HG3	2:B:1119:VAL:HG12	1.91	0.52
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.90	0.52
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.92	0.52
3:C:143:LEU:C	3:C:143:LEU:HD12	2.34	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.92	0.52
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.09	0.52
2:B:486:TYR:CE2	2:B:777:ALA:O	2.62	0.52
2:B:976:ILE:O	2:B:990:ILE:O	2.26	0.52
3:C:32:SER:O	3:C:36:VAL:CG1	2.44	0.52
3:C:73:GLN:HE21	3:C:75:MET:N	2.07	0.52
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.74	0.52
1:A:867:ILE:HD13	1:A:1014:ALA:HB2	1.92	0.52
1:A:1434:ALA:O	1:A:1436:ILE:N	2.43	0.52
1:A:1082:ASN:HA	1:A:1083:THR:O	2.10	0.52
2:B:344:LYS:O	2:B:347:LYS:N	2.41	0.52
2:B:545:ILE:HD12	2:B:633:VAL:HG13	1.90	0.52
2:B:628:THR:O	2:B:628:THR:HG22	2.10	0.52
2:B:712:PRO:O	2:B:713:ALA:HB2	2.10	0.52
1:A:49:LYS:H	1:A:50:ILE:HA	1.75	0.52
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.52
1:A:1447:GLU:C	1:A:1449:SER:H	2.18	0.52
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.25	0.52
2:B:910:VAL:HG13	2:B:938:SER:OG	2.09	0.52
9:K:6:ARG:C	9:K:8:GLU:H	2.18	0.52
1:A:153:PRO:O	1:A:155:GLU:N	2.43	0.52
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HB2	5:F:133:VAL:CG1	2.40	0.52
2:B:64:CYS:O	2:B:65:GLU:HB3	2.10	0.52
2:B:483:LEU:HD22	2:B:484:ASN:H	1.75	0.52
2:B:1101:ASP:HA	2:B:1122:ARG:HH22	1.75	0.52
4:E:94:LYS:O	4:E:98:ILE:HG12	2.09	0.51
12:T:11:DG:H1	13:N:4:DC:H42	1.58	0.51
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.91	0.51
1:A:91:PHE:H	1:A:297:GLN:NE2	2.05	0.51
1:A:709:THR:HG23	7:I:94:ASP:HA	1.92	0.51
2:B:85:SER:CA	2:B:86:ARG:HB3	2.40	0.51
2:B:878:GLN:O	2:B:879:ARG:NH2	2.42	0.51
2:B:1051:THR:HB	2:B:1054:GLY:H	1.74	0.51
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.92	0.51
9:K:56:VAL:HA	9:K:77:THR:HG22	1.92	0.51
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.91	0.51
2:B:604:ARG:HD2	2:B:615:MET:HE2	1.92	0.51
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.91	0.51
2:B:715:ALA:H	2:B:716:ASN:HA	1.74	0.51
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.92	0.51
1:A:834:THR:CG2	1:A:1077:THR:HA	2.41	0.51
1:A:942:PHE:C	1:A:942:PHE:CD2	2.87	0.51
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.42	0.51
6:H:12:VAL:CG1	6:H:51:ALA:HA	2.40	0.51
1:A:37:PHE:HB3	1:A:39:GLU:OE1	2.09	0.51
1:A:190:ALA:O	1:A:191:THR:CB	2.58	0.51
4:E:199:ILE:O	4:E:199:ILE:HG22	2.10	0.51
1:A:1082:ASN:HD22	1:A:1082:ASN:N	2.08	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.91	0.51
2:B:339:THR:O	2:B:340:ALA:CB	2.58	0.51
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.75	0.51
7:I:32:CYS:O	7:I:33:SER:OG	2.18	0.51
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.76	0.51
1:A:48:ALA:O	1:A:49:LYS:HD2	2.11	0.51
1:A:172:PRO:CD	1:A:185:TRP:NE1	2.74	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.51
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.93	0.51
1:A:1131:ALA:HA	1:A:1134:ILE:HD12	1.93	0.51
1:A:1177:LEU:O	1:A:1177:LEU:HD13	2.10	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.68	0.51
2:B:905:VAL:CG1	2:B:941:LEU:HG	2.40	0.51
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.92	0.51
12:T:19:DT:H2'	12:T:20:DC:C6	2.46	0.51
1:A:219:PHE:O	1:A:222:LEU:HD12	2.11	0.51
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.10	0.51
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.92	0.51
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.10	0.51
7:I:73:ARG:HG3	7:I:101:PHE:CE2	2.46	0.51
9:K:51:LEU:HD11	9:K:59:ALA:HB3	1.92	0.51
10:L:31:CYS:SG	10:L:34:CYS:HB2	2.51	0.51
1:A:665:GLY:O	1:A:668:ASP:HB2	2.11	0.51
1:A:943:LEU:C	1:A:945:GLU:H	2.19	0.51
2:B:69:LEU:H	2:B:90:ILE:HG22	1.75	0.51
2:B:785:TYR:CD1	2:B:785:TYR:C	2.88	0.51
6:H:118:PHE:O	6:H:120:GLY:N	2.44	0.51
7:I:105:SER:O	7:I:106:CYS:CB	2.58	0.51
8:J:35:ALA:O	8:J:39:LEU:HD13	2.10	0.51
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.46	0.51
1:A:33:ALA:HB3	1:A:82:GLY:CA	2.40	0.51
2:B:715:ALA:HB3	2:B:716:ASN:O	2.10	0.51
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.40	0.51
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.76	0.50
2:B:71:LEU:HG	2:B:72:GLU:HB2	1.93	0.50
2:B:542:MET:SD	2:B:747:MET:HE2	2.51	0.50
2:B:628:THR:O	2:B:628:THR:CG2	2.59	0.50
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.93	0.50
5:F:84:TYR:CE1	5:F:152:ILE:HD12	2.47	0.50
1:A:152:VAL:C	1:A:161:LEU:HD23	2.36	0.50
1:A:235:ILE:O	1:A:235:ILE:HD12	2.10	0.50
3:C:43:THR:HG22	3:C:44:LEU:N	2.25	0.50
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.92	0.50
1:A:158:PRO:N	1:A:159:THR:HG22	2.25	0.50
1:A:351:THR:HG23	1:A:352:VAL:N	2.25	0.50
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.77	0.50
2:B:365:THR:HG21	2:B:370:PHE:CG	2.47	0.50
2:B:599:THR:O	2:B:603:LEU:HG	2.12	0.50
2:B:955:THR:CG2	2:B:956:THR:H	2.07	0.50
6:H:109:LYS:CD	6:H:111:LEU:HB2	2.41	0.50
7:I:10:CYS:SG	7:I:29:CYS:SG	3.10	0.50
1:A:50:ILE:HG12	1:A:51:GLY:N	2.27	0.50
1:A:741:ASN:HD22	1:A:741:ASN:C	2.19	0.50
2:B:386:LEU:C	2:B:388:CYS:N	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:MET:HE3	2:B:1010:LEU:CD1	2.40	0.50
4:E:62:ALA:N	4:E:78:LEU:O	2.42	0.50
7:I:106:CYS:O	7:I:107:SER:HB2	2.12	0.50
1:A:239:LEU:HD21	1:A:304:MET:HE1	1.93	0.50
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.93	0.50
1:A:310:GLY:H	1:A:311:GLN:HB2	1.73	0.50
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.12	0.50
3:C:148:ARG:N	3:C:151:GLN:OE1	2.43	0.50
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.94	0.50
1:A:852:TYR:O	5:F:81:THR:HG22	2.12	0.50
1:A:1178:ASP:HB2	1:A:1179:GLU:C	2.37	0.50
2:B:232:SER:C	2:B:261:ARG:HH21	2.18	0.50
3:C:75:MET:C	3:C:77:ILE:H	2.19	0.50
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.47	0.50
1:A:815:PHE:O	1:A:818:MET:N	2.45	0.50
2:B:291:ILE:N	2:B:291:ILE:CD1	2.75	0.50
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.77	0.50
2:B:1008:PRO:HG3	2:B:1087:PHE:HE1	1.77	0.50
3:C:165:LYS:O	9:K:6:ARG:NH1	2.44	0.50
1:A:125:ALA:O	1:A:128:ILE:HG22	2.12	0.50
1:A:591:PHE:HA	1:A:595:THR:HG21	1.94	0.50
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.94	0.50
1:A:1166:ASP:C	1:A:1170:ILE:HG21	2.37	0.50
1:A:1172:LEU:HG	1:A:1173:HIS:N	2.26	0.50
4:E:201:LYS:HE2	4:E:207:ARG:NH1	2.27	0.50
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.77	0.50
8:J:32:GLU:O	8:J:36:LEU:HG	2.11	0.50
1:A:187:LYS:CE	1:A:188:ASP:HB3	2.42	0.49
1:A:273:ASN:HD22	1:A:296:LEU:HD21	1.77	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
2:B:830:TYR:O	2:B:831:SER:CB	2.59	0.49
3:C:43:THR:HG23	3:C:44:LEU:H	1.75	0.49
3:C:172:PRO:C	3:C:235:VAL:HG23	2.37	0.49
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.77	0.49
5:F:118:LEU:O	5:F:122:MET:HG3	2.12	0.49
7:I:111:THR:HG22	7:I:113:ASP:H	1.77	0.49
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.36	0.49
2:B:728:ARG:HH21	2:B:1048:THR:H	1.58	0.49
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.94	0.49
1:A:67:CYS:O	1:A:70:CYS:HB2	2.12	0.49
1:A:158:PRO:N	1:A:159:THR:CG2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:PRO:HG3	1:A:1188:GLN:HE21	1.76	0.49
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.93	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.93	0.49
1:A:255:SER:HA	1:A:256:GLN:O	2.13	0.49
1:A:531:ILE:O	1:A:531:ILE:HG12	2.13	0.49
1:A:577:ILE:O	1:A:580:VAL:HB	2.12	0.49
1:A:908:LEU:H	1:A:908:LEU:CD2	2.25	0.49
2:B:213:ILE:HG23	2:B:497:ARG:O	2.12	0.49
2:B:386:LEU:C	2:B:388:CYS:H	2.19	0.49
2:B:467:GLY:O	2:B:468:GLU:O	2.30	0.49
2:B:549:THR:HG22	2:B:550:ASP:H	1.77	0.49
2:B:591:ARG:O	2:B:592:ASN:HB3	2.12	0.49
2:B:637:LEU:O	2:B:690:VAL:HA	2.11	0.49
9:K:44:ASN:HA	9:K:61:TYR:HE2	1.77	0.49
1:A:286:HIS:CB	1:A:287:HIS:HB2	2.37	0.49
1:A:679:ILE:HA	1:A:682:THR:HG22	1.95	0.49
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.12	0.49
1:A:1030:ARG:C	1:A:1032:LEU:H	2.21	0.49
1:A:1039:LYS:HE2	1:A:1043:ASP:OD2	2.12	0.49
2:B:87:LYS:HZ3	2:B:436:VAL:HG11	1.78	0.49
2:B:363:HIS:O	2:B:364:ILE:HB	2.11	0.49
3:C:92:CYS:O	3:C:96:SER:OG	2.25	0.49
1:A:84:ILE:HG22	1:A:239:LEU:O	2.11	0.49
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.48	0.49
1:A:556:TRP:O	1:A:558:GLY:N	2.46	0.49
1:A:907:THR:HG22	1:A:908:LEU:N	2.27	0.49
1:A:1436:ILE:O	1:A:1437:GLY:C	2.55	0.49
2:B:112:LEU:HD11	2:B:117:ALA:HB2	1.94	0.49
2:B:760:ASP:OD2	2:B:1046:PRO:O	2.31	0.49
2:B:998:ASP:OD2	3:C:35:ARG:NH2	2.45	0.49
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.94	0.49
1:A:19:PHE:O	1:A:1416:ALA:HA	2.13	0.49
1:A:381:THR:C	1:A:383:TYR:N	2.70	0.49
1:A:815:PHE:O	1:A:816:HIS:C	2.56	0.49
1:A:1167:GLU:O	1:A:1170:ILE:O	2.30	0.49
1:A:1251:GLU:HG2	1:A:1252:THR:H	1.78	0.49
2:B:794:ASN:HD22	2:B:794:ASN:N	2.10	0.49
2:B:817:LEU:N	2:B:818:PRO:HD3	2.27	0.49
3:C:112:ASN:ND2	3:C:146:LYS:HD3	2.26	0.49
3:C:124:LEU:C	3:C:126:GLY:N	2.66	0.49
3:C:183:TRP:CD1	3:C:183:TRP:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:82:THR:O	5:F:136:ARG:NH1	2.44	0.49
12:T:27:DA:H2	12:T:28:DT:H1'	1.77	0.49
1:A:391:LEU:HD23	1:A:400:PRO:C	2.37	0.49
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.95	0.49
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.95	0.49
2:B:620:ARG:HH11	7:I:68:LEU:HD21	1.78	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.95	0.49
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.94	0.49
8:J:17:LYS:HB3	8:J:39:LEU:HD23	1.94	0.49
1:A:368:LYS:O	1:A:369:SER:C	2.55	0.49
2:B:363:HIS:C	2:B:365:THR:H	2.19	0.49
3:C:92:CYS:SG	3:C:93:ASP:N	2.85	0.49
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.93	0.49
2:B:344:LYS:CB	2:B:347:LYS:HB2	2.43	0.49
2:B:1020:ARG:HB3	2:B:1020:ARG:CZ	2.43	0.49
2:B:1098:MET:O	2:B:1099:VAL:C	2.53	0.49
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.41	0.49
3:C:167:HIS:CD2	3:C:167:HIS:C	2.90	0.49
1:A:635:ARG:HE	1:A:877:HIS:HA	1.77	0.48
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.95	0.48
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.48	0.48
2:B:202:TYR:C	2:B:203:PHE:CD1	2.91	0.48
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.95	0.48
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.27	0.48
1:A:360:GLU:HB2	1:A:363:GLN:OE1	2.13	0.48
2:B:345:LYS:HG2	2:B:348:ARG:HH21	1.78	0.48
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.48	0.48
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.43	0.48
7:I:62:ILE:C	7:I:64:SER:H	2.21	0.48
1:A:254:GLU:HG3	2:B:918:ILE:HG21	1.95	0.48
1:A:465:TYR:HD1	1:A:465:TYR:N	2.09	0.48
1:A:488:ASN:ND2	2:B:1128:LEU:HD12	2.27	0.48
1:A:901:LEU:N	1:A:926:GLN:HE21	2.11	0.48
1:A:1170:ILE:HG22	1:A:1170:ILE:O	2.12	0.48
2:B:441:ASP:C	2:B:443:ASN:H	2.21	0.48
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.13	0.48
2:B:560:GLU:O	2:B:561:TRP:CD1	2.66	0.48
1:A:55:ASP:HA	1:A:58:LEU:O	2.13	0.48
1:A:185:TRP:CH2	1:A:200:ARG:HD2	2.39	0.48
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.43	0.48
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:PRO:O	3:C:183:TRP:C	2.57	0.48
3:C:258:ILE:HG22	3:C:259:LEU:N	2.27	0.48
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.48	0.48
1:A:24:PRO:HG3	1:A:237:THR:HB	1.95	0.48
1:A:147:VAL:HG12	1:A:170:THR:HG22	1.95	0.48
1:A:374:LEU:O	1:A:436:ILE:HD13	2.13	0.48
1:A:419:LYS:HZ2	1:A:419:LYS:CB	2.13	0.48
2:B:865:LYS:HA	2:B:870:ILE:O	2.13	0.48
2:B:1163:CYS:HB3	2:B:1167:GLY:H	1.78	0.48
4:E:205:SER:O	4:E:206:GLY:C	2.55	0.48
1:A:40:THR:HB	1:A:41:MET:HA	1.94	0.48
1:A:193:ASP:O	1:A:193:ASP:OD2	2.30	0.48
1:A:557:ASP:OD1	1:A:559:VAL:HB	2.13	0.48
1:A:666:ILE:CG1	2:B:1026:LEU:HB3	2.43	0.48
1:A:1063:MET:HE3	1:A:1063:MET:HB3	1.66	0.48
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.95	0.48
2:B:515:HIS:O	2:B:516:ASN:C	2.57	0.48
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.95	0.48
3:C:44:LEU:HD12	3:C:160:LYS:O	2.14	0.48
9:K:35:PHE:N	9:K:35:PHE:CD1	2.80	0.48
1:A:53:LEU:HD23	1:A:54:ASN:N	2.28	0.48
1:A:261:ASP:HB3	1:A:322:VAL:HG12	1.96	0.48
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.95	0.48
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.95	0.48
2:B:445:LYS:HB3	2:B:447:ALA:CB	2.43	0.48
2:B:1023:VAL:O	2:B:1024:ALA:C	2.57	0.48
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.44	0.48
1:A:298:PHE:HE1	1:A:313:GLN:HG3	1.78	0.48
1:A:423:ASP:O	1:A:424:ILE:CB	2.62	0.48
1:A:731:ARG:CG	1:A:755:PHE:CE1	2.95	0.48
1:A:814:PHE:CZ	2:B:514:LEU:HD21	2.49	0.48
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.96	0.48
7:I:11:ASN:CG	7:I:11:ASN:O	2.56	0.48
1:A:256:GLN:HA	12:T:29:DA:C2	2.49	0.48
1:A:313:GLN:CD	1:A:313:GLN:C	2.82	0.48
1:A:662:PHE:O	2:B:828:ALA:HA	2.14	0.48
2:B:465:ASN:O	2:B:466:TRP:C	2.57	0.48
4:E:171:LYS:HB2	4:E:174:GLN:HG3	1.96	0.48
7:I:33:SER:O	7:I:35:VAL:HG23	2.14	0.48
1:A:549:MET:O	1:A:552:TRP:HB2	2.14	0.48
1:A:1171:GLN:O	1:A:1171:GLN:CD	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:ASN:C	2:B:795:ILE:HD12	2.39	0.48
2:B:864:LYS:HD2	2:B:872:GLU:CD	2.39	0.48
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.79	0.48
1:A:381:THR:O	1:A:383:TYR:N	2.47	0.47
1:A:812:GLU:O	1:A:813:PHE:C	2.57	0.47
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.39	0.47
2:B:31:TRP:HA	2:B:34:ILE:HG13	1.96	0.47
2:B:1131:GLY:O	2:B:1132:GLU:C	2.56	0.47
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.48	0.47
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.29	0.47
1:A:464:PRO:HB3	9:K:4:PRO:HG3	1.95	0.47
1:A:738:LYS:HZ3	3:C:194:GLU:HA	1.78	0.47
1:A:869:GLY:O	4:E:204:THR:HG21	2.15	0.47
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.79	0.47
9:K:56:VAL:HG13	9:K:77:THR:CG2	2.44	0.47
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.74	0.47
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.44	0.47
2:B:26:THR:HB	2:B:27:ALA:H	1.49	0.47
2:B:441:ASP:O	2:B:443:ASN:N	2.42	0.47
1:A:546:VAL:O	1:A:550:LEU:HD22	2.15	0.47
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.49	0.47
1:A:1082:ASN:HD22	1:A:1082:ASN:H	1.61	0.47
2:B:842:ASN:ND2	2:B:845:SER:H	2.11	0.47
2:B:1006:ILE:HD12	8:J:45:CYS:HB3	1.96	0.47
2:B:1116:ARG:HD2	2:B:1198:TYR:CE2	2.50	0.47
3:C:57:VAL:HG21	8:J:57:ILE:CD1	2.40	0.47
6:H:24:CYS:O	6:H:41:ASP:HA	2.14	0.47
9:K:63:VAL:O	9:K:63:VAL:CG2	2.62	0.47
1:A:190:ALA:C	1:A:191:THR:OG1	2.57	0.47
1:A:296:LEU:O	1:A:300:VAL:HG23	2.15	0.47
1:A:1060:PRO:HD2	5:F:86:THR:CG2	2.44	0.47
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.14	0.47
2:B:703:ILE:HG22	2:B:704:ALA:O	2.14	0.47
3:C:76:ASP:O	3:C:79:GLN:HG2	2.15	0.47
3:C:101:LEU:HD23	3:C:155:LEU:HD12	1.95	0.47
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.50	0.47
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.95	0.47
1:A:1329:THR:HG23	1:A:1331:SER:H	1.79	0.47
1:A:1428:VAL:C	1:A:1430:LEU:H	2.22	0.47
2:B:121:ASN:N	2:B:121:ASN:HD22	2.12	0.47
2:B:363:HIS:C	2:B:365:THR:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:CZ	1:A:207:ILE:HD12	2.50	0.47
1:A:323:LYS:O	1:A:324:SER:HB3	2.14	0.47
1:A:548:ASN:OD1	9:K:60:ALA:HB1	2.15	0.47
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.96	0.47
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.61	0.47
1:A:1172:LEU:CD2	1:A:1173:HIS:N	2.76	0.47
1:A:1209:MET:HE3	1:A:1228:TRP:HB2	1.97	0.47
1:A:1341:ILE:HG22	4:E:182:ASP:OD2	2.15	0.47
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.80	0.47
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.96	0.47
2:B:791:THR:O	2:B:792:MET:CB	2.63	0.47
2:B:1072:MET:HE3	2:B:1085:ILE:HD12	1.96	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.14	0.47
6:H:109:LYS:CG	6:H:111:LEU:HB2	2.44	0.47
6:H:118:PHE:CZ	6:H:142:LEU:HD23	2.50	0.47
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
2:B:358:LYS:O	2:B:362:PRO:HG3	2.15	0.47
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.22	0.47
1:A:58:LEU:HD23	1:A:80:HIS:HB2	1.97	0.47
1:A:119:ASN:O	1:A:120:GLU:O	2.33	0.47
1:A:964:ILE:HG21	1:A:1035:TYR:CD2	2.50	0.47
2:B:41:LYS:HB3	2:B:45:SER:HB3	1.97	0.47
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.97	0.47
2:B:711:GLU:N	2:B:712:PRO:HD3	2.30	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:CB	2.77	0.47
9:K:7:PHE:CD1	9:K:7:PHE:C	2.92	0.47
10:L:50:ASP:CG	10:L:50:ASP:O	2.57	0.47
1:A:158:PRO:CD	1:A:159:THR:HB	2.45	0.47
1:A:161:LEU:HD22	1:A:162:VAL:O	2.14	0.47
1:A:278:THR:O	1:A:282:ASN:HB2	2.15	0.47
1:A:469:ARG:NH2	2:B:991:GLY:O	2.48	0.47
1:A:575:LYS:HB3	1:A:612:ILE:CD1	2.36	0.47
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.97	0.47
2:B:210:LYS:HZ2	2:B:482:VAL:HG22	1.80	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.47
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.15	0.47
5:F:101:ILE:CD1	5:F:120:ILE:HG22	2.41	0.47
7:I:50:THR:HG22	7:I:52:ILE:H	1.80	0.47
8:J:6:ARG:HG2	8:J:11:GLY:O	2.15	0.47
11:R:8:G:O2'	11:R:9:G:H5'	2.15	0.47
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.80	0.46
1:A:892:ALA:HA	1:A:895:LYS:NZ	2.31	0.46
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.95	0.46
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.97	0.46
1:A:913:LEU:HG	1:A:915:SER:H	1.80	0.46
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.40	0.46
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.97	0.46
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.97	0.46
7:I:74:GLU:HG3	7:I:79:HIS:HA	1.98	0.46
7:I:106:CYS:SG	7:I:107:SER:N	2.88	0.46
1:A:190:ALA:O	1:A:191:THR:OG1	2.30	0.46
1:A:1172:LEU:O	1:A:1174:PHE:CA	2.56	0.46
1:A:1336:MET:HE3	1:A:1381:LEU:H	1.80	0.46
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.24	0.46
2:B:301:ILE:HA	2:B:379:GLY:O	2.14	0.46
2:B:715:ALA:H	2:B:716:ASN:CA	2.27	0.46
4:E:28:TYR:HA	4:E:64:PRO:HA	1.97	0.46
9:K:61:TYR:HA	9:K:72:LYS:O	2.15	0.46
1:A:527:THR:O	1:A:653:VAL:HG11	2.16	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.97	0.46
2:B:102:VAL:HG12	2:B:112:LEU:HB2	1.96	0.46
1:A:446:ARG:NH1	1:A:478:TYR:O	2.48	0.46
1:A:897:TYR:HE2	1:A:1024:SER:O	1.99	0.46
1:A:917:SER:C	1:A:919:ILE:H	2.21	0.46
1:A:1039:LYS:HD3	1:A:1039:LYS:C	2.40	0.46
1:A:1151:GLU:HG3	1:A:1153:TYR:HE1	1.81	0.46
2:B:616:ILE:HG12	2:B:696:GLU:HG3	1.96	0.46
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.97	0.46
10:L:28:LYS:HG3	10:L:39:SER:OG	2.16	0.46
1:A:78:PRO:HB3	2:B:1160:VAL:HG13	1.98	0.46
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.97	0.46
1:A:445:ASN:HB2	1:A:454:SER:O	2.16	0.46
1:A:1344:GLY:O	1:A:1345:ARG:C	2.57	0.46
2:B:1106:ARG:HH12	2:B:1110:PRO:HD2	1.79	0.46
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.16	0.46
12:T:12:DC:H42	13:N:3:DG:H1	1.62	0.46
1:A:160:GLN:O	1:A:161:LEU:HB2	2.16	0.46
1:A:341:MET:HE1	1:A:1425:SER:OG	2.15	0.46
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.46	0.46
2:B:128:LEU:HB2	2:B:167:ILE:O	2.15	0.46
2:B:745:PRO:C	2:B:747:MET:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:THR:HG22	2:B:809:MET:SD	2.55	0.46
3:C:5:GLY:O	3:C:6:PRO:C	2.58	0.46
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.51	0.46
3:C:262:LEU:CD1	9:K:87:LEU:HD23	2.46	0.46
1:A:179:LEU:HB3	1:A:297:GLN:HG2	1.98	0.46
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.98	0.46
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.46	0.46
2:B:340:ALA:C	2:B:342:GLY:N	2.74	0.46
2:B:638:PHE:CE1	2:B:743:ILE:HD13	2.51	0.46
2:B:1019:SER:HG	11:R:14:DA:P	2.39	0.46
7:I:5:ARG:HG3	7:I:6:PHE:H	1.81	0.46
12:T:26:DG:N3	12:T:27:DA:C8	2.83	0.46
1:A:203:SER:O	1:A:207:ILE:CG1	2.63	0.46
1:A:687:LYS:HD2	1:A:794:PRO:CG	2.46	0.46
1:A:913:LEU:HD12	1:A:914:GLU:H	1.81	0.46
2:B:475:SER:O	2:B:477:ALA:N	2.48	0.46
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.41	0.46
8:J:38:ARG:HB2	8:J:38:ARG:HH11	1.80	0.46
1:A:55:ASP:O	1:A:56:PRO:C	2.58	0.46
1:A:61:ILE:O	1:A:63:ARG:NH2	2.49	0.46
1:A:239:LEU:HD13	1:A:240:PRO:HD2	1.97	0.46
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.46	0.46
2:B:25:ILE:HG22	2:B:26:THR:H	1.80	0.46
2:B:1084:GLN:HE22	3:C:192:TRP:HB2	1.80	0.46
3:C:173:ALA:O	3:C:174:ALA:HB3	2.16	0.46
1:A:168:GLY:O	1:A:169:ASN:O	2.34	0.46
1:A:387:ARG:HH11	1:A:437:MET:HE1	1.81	0.46
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.56	0.46
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.97	0.46
2:B:473:MET:HA	2:B:474:SER:HA	1.47	0.46
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.98	0.46
2:B:905:VAL:HG11	2:B:941:LEU:HG	1.98	0.46
2:B:1131:GLY:O	2:B:1134:GLU:N	2.39	0.46
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.46
3:C:163:ILE:HD12	3:C:163:ILE:N	2.31	0.46
6:H:98:TYR:C	6:H:118:PHE:HD2	2.24	0.46
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.97	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.98	0.45
1:A:1044:TRP:O	1:A:1045:VAL:C	2.60	0.45
2:B:636:PRO:O	2:B:691:GLU:O	2.33	0.45
3:C:44:LEU:HD12	3:C:160:LYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:CG	1:A:185:TRP:HE1	2.23	0.45
1:A:172:PRO:CD	1:A:185:TRP:HE1	2.29	0.45
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.98	0.45
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.31	0.45
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.98	0.45
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.98	0.45
2:B:1215:ARG:HB3	2:B:1217:TYR:HE1	1.81	0.45
7:I:71:SER:OG	7:I:73:ARG:HG2	2.16	0.45
10:L:60:ARG:HG3	10:L:61:THR:H	1.81	0.45
11:R:3:C:N4	11:R:4:G:C6	2.84	0.45
11:R:5:A:C2	11:R:6:G:C5	3.04	0.45
1:A:188:ASP:C	1:A:189:ARG:CG	2.89	0.45
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.98	0.45
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.51	0.45
1:A:690:VAL:O	1:A:694:THR:OG1	2.35	0.45
2:B:20:ASP:O	2:B:21:GLU:HG2	2.16	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.34	0.45
2:B:487:THR:HG22	2:B:488:TYR:N	2.31	0.45
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.81	0.45
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.81	0.45
1:A:109:HIS:C	1:A:167:CYS:SG	3.00	0.45
3:C:44:LEU:HD22	3:C:129:ILE:HD11	1.99	0.45
7:I:17:ARG:HB2	7:I:17:ARG:NH1	2.31	0.45
12:T:1:DC:H4'	12:T:2:DT:OP1	2.17	0.45
1:A:55:ASP:H	1:A:56:PRO:CD	2.26	0.45
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.45
1:A:413:ILE:N	1:A:413:ILE:CD1	2.80	0.45
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.31	0.45
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.97	0.45
2:B:721:LEU:HA	2:B:722:ASP:HA	1.71	0.45
2:B:757:PRO:HB3	2:B:1044:ALA:CB	2.47	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.97	0.45
7:I:83:ASN:C	7:I:83:ASN:ND2	2.73	0.45
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.52	0.45
1:A:658:LEU:HD12	1:A:658:LEU:O	2.17	0.45
1:A:737:LEU:HA	1:A:737:LEU:HD23	1.57	0.45
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.99	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.31	0.45
2:B:978:ASP:O	2:B:980:PHE:CD1	2.67	0.45
2:B:1019:SER:OG	11:R:14:DA:O5'	2.32	0.45
2:B:1120:GLU:O	2:B:1124:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HA	1:A:312:PRO:HA	1.83	0.45
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.80	0.45
1:A:1364:ASN:O	1:A:1365:TYR:C	2.60	0.45
2:B:20:ASP:O	2:B:20:ASP:CG	2.60	0.45
3:C:58:LEU:HB3	3:C:62:PHE:HD2	1.81	0.45
3:C:142:VAL:HG21	8:J:5:VAL:CG1	2.45	0.45
1:A:194:ALA:O	1:A:195:ASP:O	2.34	0.45
1:A:848:ILE:CD1	1:A:858:ASN:HB3	2.47	0.45
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.98	0.45
3:C:34:ARG:HG2	3:C:35:ARG:N	2.31	0.45
3:C:130:GLY:O	3:C:132:PRO:HD3	2.17	0.45
3:C:167:HIS:CE1	10:L:70:ARG:HA	2.51	0.45
4:E:64:PRO:HD3	4:E:76:GLY:O	2.16	0.45
5:F:120:ILE:O	5:F:123:LYS:N	2.45	0.45
6:H:102:TYR:O	6:H:103:LYS:HB2	2.17	0.45
8:J:48:ARG:NH1	8:J:49:MET:HE1	2.32	0.45
1:A:473:SER:OG	1:A:522:GLY:O	2.30	0.45
1:A:811:GLN:O	1:A:812:GLU:C	2.60	0.45
1:A:1189:SER:CB	1:A:1241:ARG:HB3	2.47	0.45
2:B:441:ASP:C	2:B:443:ASN:N	2.75	0.45
2:B:483:LEU:CD2	2:B:484:ASN:H	2.29	0.45
2:B:616:ILE:HD12	2:B:616:ILE:N	2.32	0.45
2:B:766:ARG:HH22	2:B:1020:ARG:HH12	1.63	0.45
2:B:821:GLN:HE22	2:B:851:PHE:H	1.65	0.45
8:J:63:TYR:N	8:J:63:TYR:CD1	2.84	0.45
1:A:203:SER:O	1:A:207:ILE:HG13	2.17	0.45
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.82	0.45
1:A:464:PRO:HD2	9:K:67:PHE:CD1	2.52	0.45
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.62	0.45
1:A:507:VAL:HG12	1:A:521:MET:HE1	1.98	0.45
2:B:273:LEU:HA	2:B:274:PRO:HD3	1.86	0.45
2:B:635:ARG:O	2:B:636:PRO:C	2.59	0.45
2:B:715:ALA:CB	2:B:716:ASN:CA	2.90	0.45
2:B:716:ASN:C	2:B:717:GLU:HG3	2.41	0.45
2:B:899:ILE:CD1	2:B:911:ILE:HG23	2.43	0.45
2:B:1072:MET:CE	2:B:1085:ILE:CD1	2.95	0.45
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.95	0.44
1:A:545:GLN:O	1:A:549:MET:HG3	2.17	0.44
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.99	0.44
2:B:31:TRP:O	2:B:32:ALA:C	2.60	0.44
3:C:33:LEU:O	3:C:37:MET:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:LEU:HD12	3:C:144:ILE:N	2.33	0.44
12:T:2:DT:H3	13:N:13:DA:H61	1.65	0.44
1:A:172:PRO:N	1:A:185:TRP:CD1	2.85	0.44
1:A:353:ILE:O	1:A:353:ILE:HG13	2.18	0.44
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	1.99	0.44
3:C:39:ALA:CB	3:C:164:ALA:HB3	2.47	0.44
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.52	0.44
7:I:32:CYS:O	7:I:33:SER:CB	2.65	0.44
10:L:32:ALA:CB	10:L:55:ILE:HD11	2.47	0.44
1:A:75:ASN:HA	2:B:1116:ARG:NH2	2.32	0.44
1:A:185:TRP:HE3	1:A:198:GLU:HG2	1.81	0.44
1:A:379:VAL:HG22	1:A:431:LYS:HG2	2.00	0.44
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.51	0.44
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.98	0.44
2:B:944:THR:CG2	2:B:1122:ARG:NH2	2.75	0.44
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.52	0.44
3:C:142:VAL:HA	8:J:16:ASP:HB3	1.98	0.44
7:I:111:THR:HG22	7:I:112:SER:N	2.33	0.44
1:A:41:MET:CG	1:A:42:ASP:H	2.21	0.44
1:A:530:GLY:HA2	1:A:533:LYS:HG3	2.00	0.44
1:A:553:VAL:HA	1:A:554:PRO:HD3	1.91	0.44
1:A:590:ARG:O	1:A:591:PHE:HB2	2.17	0.44
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.98	0.44
2:B:874:PHE:CE1	2:B:964:VAL:HG23	2.52	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.40	0.44
1:A:11:LEU:HA	2:B:1193:GLN:O	2.18	0.44
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.33	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.44
1:A:1398:MET:C	1:A:1400:CYS:N	2.72	0.44
2:B:38:PHE:HD2	2:B:42:GLY:O	2.00	0.44
2:B:315:LYS:N	2:B:316:PRO:CD	2.80	0.44
6:H:12:VAL:HG13	6:H:26:ILE:CD1	2.46	0.44
1:A:13:THR:HG22	1:A:14:VAL:N	2.31	0.44
1:A:402:ALA:N	1:A:435:HIS:CD2	2.84	0.44
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.86	0.44
2:B:203:PHE:CD1	2:B:203:PHE:N	2.85	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.00	0.44
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.44
4:E:78:LEU:HD23	4:E:79:TRP:N	2.33	0.44
7:I:73:ARG:HG3	7:I:101:PHE:CD2	2.53	0.44
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:HIS:CD2	1:A:877:HIS:H	2.34	0.44
1:A:982:THR:HB	1:A:985:ASP:H	1.83	0.44
2:B:498:THR:HB	2:B:537:LYS:HB2	2.00	0.44
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.99	0.44
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.41	0.44
3:C:27:LEU:HD12	3:C:228:PHE:CZ	2.52	0.44
6:H:12:VAL:HG11	6:H:51:ALA:HA	2.00	0.44
1:A:4:GLN:O	1:A:5:GLN:HG3	2.17	0.44
1:A:91:PHE:HZ	1:A:207:ILE:CD1	2.30	0.44
1:A:153:PRO:CA	1:A:161:LEU:HD23	2.48	0.44
1:A:337:ARG:NH2	1:A:839:ARG:NH2	2.66	0.44
1:A:456:MET:HE3	1:A:507:VAL:HG22	1.99	0.44
1:A:650:GLN:O	1:A:651:LYS:C	2.61	0.44
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.18	0.44
1:A:709:THR:CG2	7:I:94:ASP:HA	2.48	0.44
1:A:715:GLU:O	1:A:716:ASP:C	2.59	0.44
1:A:921:GLY:O	1:A:922:ASP:HB3	2.18	0.44
2:B:770:GLN:O	2:B:770:GLN:NE2	2.51	0.44
3:C:167:HIS:CD2	3:C:168:ALA:N	2.86	0.44
9:K:31:VAL:HG12	9:K:32:VAL:N	2.32	0.44
12:T:23:DC:C2'	12:T:24:DT:H5'	2.48	0.44
1:A:188:ASP:O	1:A:189:ARG:HG2	2.17	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.89	0.44
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.00	0.44
2:B:188:ASP:HA	2:B:191:LYS:HE3	2.00	0.44
2:B:487:THR:O	2:B:490:SER:HB3	2.18	0.44
2:B:604:ARG:HD2	2:B:615:MET:CE	2.48	0.44
2:B:613:VAL:HG22	2:B:628:THR:HA	2.00	0.44
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.18	0.44
2:B:879:ARG:HA	2:B:879:ARG:NE	2.33	0.44
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.77	0.44
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.53	0.44
5:F:111:LEU:H	5:F:111:LEU:CD2	2.28	0.44
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.18	0.44
1:A:153:PRO:HA	1:A:161:LEU:HD23	2.00	0.43
1:A:160:GLN:CD	1:A:160:GLN:H	2.10	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
1:A:871:ASP:HB3	4:E:205:SER:HB3	2.00	0.43
1:A:889:SER:C	1:A:891:ALA:N	2.75	0.43
2:B:119:LEU:HD22	2:B:789:MET:HB2	1.99	0.43
2:B:600:LEU:HB3	2:B:615:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:CA	2:B:946:ASN:HB2	2.42	0.43
3:C:215:GLU:CD	3:C:216:GLY:N	2.76	0.43
4:E:15:ALA:HA	4:E:140:LEU:O	2.18	0.43
9:K:6:ARG:O	9:K:8:GLU:N	2.51	0.43
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.99	0.43
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.53	0.43
1:A:516:SER:HB3	1:A:1362:TYR:O	2.18	0.43
1:A:809:THR:CB	1:A:810:PRO:CD	2.94	0.43
1:A:917:SER:C	1:A:919:ILE:N	2.76	0.43
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.53	0.43
1:A:1443:VAL:C	1:A:1444:MET:HG2	2.42	0.43
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.53	0.43
2:B:290:GLY:C	2:B:291:ILE:HD12	2.43	0.43
2:B:463:THR:HG21	2:B:465:ASN:HD21	1.81	0.43
3:C:115:SER:C	3:C:117:ASP:N	2.74	0.43
3:C:142:VAL:CG2	3:C:143:LEU:N	2.75	0.43
4:E:88:VAL:HG23	4:E:116:ILE:HA	2.00	0.43
7:I:5:ARG:HG3	7:I:6:PHE:N	2.33	0.43
7:I:78:CYS:SG	7:I:106:CYS:SG	3.08	0.43
8:J:31:ASP:OD1	8:J:34:THR:OG1	2.36	0.43
1:A:782:ARG:HB3	1:A:788:SER:O	2.19	0.43
1:A:851:HIS:CD2	1:A:857:ARG:HG3	2.53	0.43
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.49	0.43
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.93	0.43
2:B:598:GLU:HA	2:B:598:GLU:OE2	2.18	0.43
2:B:642:ASP:C	2:B:644:GLU:H	2.26	0.43
3:C:173:ALA:O	3:C:233:GLU:O	2.35	0.43
1:A:208:LEU:HB2	1:A:235:ILE:HD11	2.01	0.43
1:A:323:LYS:HG3	1:A:327:ALA:HB3	2.01	0.43
1:A:391:LEU:O	1:A:392:VAL:C	2.60	0.43
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.82	0.43
1:A:492:PRO:HB3	1:A:497:THR:CG2	2.48	0.43
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.91	0.43
1:A:592:ASP:O	1:A:593:GLU:OE1	2.36	0.43
1:A:645:LEU:O	1:A:646:PHE:C	2.59	0.43
1:A:1189:SER:HB3	1:A:1241:ARG:HD3	2.00	0.43
2:B:463:THR:HG22	2:B:465:ASN:ND2	2.29	0.43
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.53	0.43
2:B:1200:ALA:O	2:B:1203:LEU:N	2.51	0.43
3:C:43:THR:CG2	3:C:44:LEU:H	2.26	0.43
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:93:TYR:CG	6:H:143:LEU:HB3	2.54	0.43
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.53	0.43
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.00	0.43
1:A:738:LYS:HZ1	3:C:194:GLU:HA	1.83	0.43
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.84	0.43
2:B:34:ILE:HG23	2:B:542:MET:CE	2.48	0.43
2:B:471:LYS:HA	2:B:472:ALA:HA	1.63	0.43
2:B:730:ARG:O	2:B:731:VAL:C	2.62	0.43
2:B:1117:GLN:CG	2:B:1156:ASP:OD2	2.65	0.43
12:T:18:DA:C2	12:T:19:DT:N3	2.87	0.43
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.84	0.43
1:A:513:SER:HA	1:A:514:PRO:HD3	1.86	0.43
1:A:870:GLU:OE1	4:E:202:SER:HB2	2.19	0.43
1:A:1080:THR:CG2	1:A:1081:LEU:N	2.80	0.43
3:C:37:MET:O	3:C:38:ILE:C	2.61	0.43
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.53	0.43
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.52	0.43
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.83	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.83	0.43
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.85	0.43
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.81	0.43
1:A:1193:LEU:HD21	1:A:1267:MET:CE	2.42	0.43
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.83	0.43
2:B:698:GLU:HA	2:B:701:ILE:CD1	2.49	0.43
2:B:982:SER:O	2:B:1093:GLN:HG3	2.18	0.43
2:B:1095:LEU:O	2:B:1096:ARG:O	2.37	0.43
8:J:16:ASP:OD1	8:J:16:ASP:N	2.40	0.43
1:A:815:PHE:C	1:A:817:ALA:N	2.77	0.43
1:A:867:ILE:O	1:A:868:TYR:C	2.61	0.43
2:B:202:TYR:C	2:B:203:PHE:HD1	2.26	0.43
2:B:464:GLY:CA	2:B:480:SER:HB3	2.46	0.43
3:C:46:ILE:HA	3:C:159:ALA:HA	2.01	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.01	0.43
1:A:789:LYS:HE2	7:I:67:THR:HB	2.00	0.43
1:A:943:LEU:C	1:A:945:GLU:N	2.77	0.43
2:B:292:ILE:H	2:B:293:PRO:HD3	1.83	0.43
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.34	0.43
2:B:797:TYR:OH	2:B:971:THR:OG1	2.30	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.89	0.43
3:C:137:LYS:C	3:C:139:GLY:H	2.26	0.43
5:F:93:ILE:O	5:F:94:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:60:ARG:HG3	10:L:61:THR:N	2.34	0.43
1:A:33:ALA:HB3	1:A:82:GLY:HA2	2.00	0.43
1:A:302:THR:HG23	1:A:306:ASN:CB	2.49	0.43
1:A:402:ALA:CB	1:A:434:ARG:HA	2.47	0.43
1:A:534:LEU:HA	1:A:539:THR:HG21	2.01	0.43
1:A:775:ILE:O	1:A:797:LYS:HE2	2.19	0.43
1:A:1133:LEU:HD23	1:A:1133:LEU:HA	1.89	0.43
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.53	0.43
2:B:579:ARG:HG3	2:B:623:GLU:HG2	1.99	0.43
7:I:27:PHE:O	7:I:28:GLU:HB3	2.19	0.43
8:J:8:PHE:O	8:J:9:SER:O	2.37	0.43
8:J:23:ASN:O	8:J:27:GLU:HB3	2.19	0.43
1:A:187:LYS:HB2	1:A:187:LYS:HZ3	1.81	0.42
1:A:464:PRO:HD2	9:K:67:PHE:HD1	1.84	0.42
1:A:1080:THR:CG2	1:A:1081:LEU:H	2.32	0.42
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.53	0.42
2:B:464:GLY:HA2	2:B:480:SER:CB	2.45	0.42
2:B:770:GLN:O	2:B:770:GLN:CD	2.62	0.42
2:B:856:PHE:HB3	2:B:967:ARG:HD2	2.00	0.42
3:C:167:HIS:CE1	10:L:70:ARG:HB3	2.54	0.42
12:T:26:DG:C4	12:T:27:DA:C8	3.07	0.42
1:A:305:ASP:OD1	1:A:306:ASN:N	2.52	0.42
1:A:649:ILE:HG13	1:A:649:ILE:H	1.62	0.42
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.87	0.42
1:A:1033:GLN:HE21	1:A:1033:GLN:HB3	1.61	0.42
1:A:1092:LYS:H	1:A:1093:LYS:HA	1.83	0.42
1:A:1144:LYS:HD2	1:A:1269:GLU:HG2	2.00	0.42
2:B:204:ILE:O	2:B:205:ILE:HD13	2.18	0.42
2:B:215:GLN:O	2:B:406:LEU:HA	2.19	0.42
2:B:550:ASP:O	2:B:553:PRO:HD2	2.20	0.42
2:B:803:LEU:HD13	2:B:1032:SER:O	2.20	0.42
3:C:258:ILE:C	3:C:260:LEU:N	2.77	0.42
5:F:133:VAL:O	5:F:133:VAL:HG13	2.19	0.42
7:I:104:LEU:HD22	7:I:104:LEU:HA	1.84	0.42
9:K:10:PHE:N	9:K:10:PHE:HD2	2.16	0.42
1:A:267:ALA:O	1:A:271:LYS:HB2	2.20	0.42
1:A:315:LEU:HD22	1:A:315:LEU:H	1.83	0.42
1:A:391:LEU:HD23	1:A:400:PRO:O	2.19	0.42
1:A:402:ALA:HA	1:A:435:HIS:HD2	1.85	0.42
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.32	0.42
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.19	0.42
1:A:784:LEU:C	1:A:786:HIS:H	2.27	0.42
1:A:979:SER:OG	1:A:980:ASP:N	2.51	0.42
2:B:711:GLU:H	2:B:712:PRO:HD3	1.84	0.42
5:F:79:ARG:O	5:F:81:THR:N	2.52	0.42
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.31	0.42
1:A:648:ASN:O	1:A:649:ILE:C	2.60	0.42
1:A:726:ARG:HD3	1:A:766:GLY:HA3	2.02	0.42
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.33	0.42
1:A:1168:GLU:C	1:A:1169:ILE:HD12	2.31	0.42
1:A:1319:VAL:O	1:A:1322:ILE:HD12	2.19	0.42
2:B:89:GLU:O	2:B:89:GLU:CG	2.62	0.42
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.01	0.42
3:C:46:ILE:HD12	3:C:157:CYS:CB	2.48	0.42
4:E:88:VAL:CG2	4:E:116:ILE:HD13	2.48	0.42
1:A:140:THR:O	1:A:140:THR:HG22	2.20	0.42
1:A:179:LEU:HD13	1:A:297:GLN:HG3	2.02	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.19	0.42
1:A:356:ASP:HA	1:A:357:PRO:HD3	1.78	0.42
2:B:64:CYS:O	2:B:67:SER:OG	2.30	0.42
2:B:816:GLU:C	2:B:817:LEU:HD12	2.44	0.42
4:E:52:ARG:HA	4:E:53:PRO:HD3	1.72	0.42
12:T:6:DG:H2''	12:T:7:DA:O5'	2.20	0.42
12:T:28:DT:H2'	12:T:29:DA:O4'	2.20	0.42
1:A:41:MET:HG3	1:A:42:ASP:N	2.26	0.42
1:A:158:PRO:C	1:A:159:THR:HG22	2.44	0.42
1:A:381:THR:C	1:A:383:TYR:H	2.28	0.42
1:A:494:SER:O	1:A:498:ARG:HG3	2.20	0.42
1:A:919:ILE:HD13	1:A:919:ILE:HA	1.82	0.42
1:A:1169:ILE:HG21	1:A:1170:ILE:HD11	1.96	0.42
2:B:294:ASP:C	2:B:296:GLU:H	2.27	0.42
2:B:445:LYS:CA	2:B:447:ALA:N	2.79	0.42
2:B:457:LEU:HD23	2:B:457:LEU:HA	1.86	0.42
2:B:488:TYR:C	2:B:490:SER:N	2.77	0.42
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.20	0.42
4:E:161:LYS:HD2	4:E:195:VAL:HG23	2.02	0.42
9:K:6:ARG:C	9:K:8:GLU:N	2.77	0.42
1:A:363:GLN:HG3	1:A:459:ARG:NH1	2.34	0.42
1:A:818:MET:HG2	2:B:514:LEU:O	2.19	0.42
2:B:218:SER:HB3	2:B:241:ARG:NH1	2.35	0.42
2:B:324:ILE:HG21	2:B:330:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LEU:O	2:B:382:ILE:HG12	2.19	0.42
2:B:680:THR:O	2:B:683:SER:OG	2.37	0.42
2:B:839:MET:CE	2:B:1010:LEU:HD12	2.43	0.42
3:C:245:VAL:HG13	9:K:102:LYS:HD2	2.02	0.42
9:K:82:ASP:HA	9:K:83:PRO:HD3	1.93	0.42
1:A:306:ASN:N	1:A:306:ASN:HD22	2.18	0.42
1:A:523:ILE:HG22	1:A:528:LEU:HB2	2.01	0.42
2:B:282:ILE:H	2:B:282:ILE:HG13	1.72	0.42
2:B:469:GLN:O	2:B:470:LYS:HB2	2.19	0.42
2:B:757:PRO:HB3	2:B:1044:ALA:HB1	2.01	0.42
2:B:771:SER:O	2:B:775:LYS:HG3	2.20	0.42
2:B:1041:GLU:HG2	2:B:1042:GLY:N	2.35	0.42
3:C:127:ARG:HG3	3:C:129:ILE:CG2	2.49	0.42
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.55	0.42
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.83	0.42
1:A:1158:PRO:HG3	1:A:1188:GLN:NE2	2.35	0.42
2:B:213:ILE:CD1	2:B:481:GLN:OE1	2.65	0.42
2:B:414:ALA:C	2:B:416:LEU:H	2.27	0.42
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.20	0.42
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.50	0.42
2:B:789:MET:HE3	2:B:965:LYS:HB3	2.02	0.42
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.55	0.42
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.42
3:C:120:ILE:H	3:C:120:ILE:HG12	1.39	0.42
4:E:153:HIS:O	4:E:154:ILE:HD13	2.19	0.42
7:I:7:CYS:SG	7:I:8:ARG:O	2.78	0.42
7:I:17:ARG:HH11	7:I:17:ARG:CB	2.32	0.42
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.59	0.42
1:A:74:MET:HE3	1:A:74:MET:HB2	1.98	0.42
1:A:156:ASP:OD2	1:A:160:GLN:OE1	2.36	0.42
1:A:261:ASP:O	1:A:264:PHE:HB2	2.20	0.42
1:A:343:LYS:NZ	2:B:1156:ASP:CG	2.78	0.42
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.75	0.42
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.45	0.42
1:A:1172:LEU:CD2	1:A:1173:HIS:H	2.20	0.42
2:B:488:TYR:O	2:B:490:SER:N	2.53	0.42
2:B:945:GLU:O	2:B:946:ASN:HB3	2.20	0.42
2:B:1149:GLU:C	2:B:1151:LEU:N	2.78	0.42
5:F:93:ILE:HG23	5:F:132:LEU:HD12	2.02	0.42
8:J:18:TRP:O	8:J:21:TYR:HB3	2.20	0.42
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:O	1:A:569:LYS:N	2.53	0.41
1:A:902:LEU:CD2	1:A:923:LEU:HD23	2.50	0.41
1:A:1021:LEU:CD1	1:A:1025:ARG:HE	2.30	0.41
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.19	0.41
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.20	0.41
1:A:1193:LEU:O	1:A:1193:LEU:HG	2.19	0.41
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.41
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.53	0.41
2:B:658:ILE:O	2:B:661:LEU:HB2	2.20	0.41
3:C:77:ILE:HD11	3:C:161:LYS:HG3	2.02	0.41
1:A:148:CYS:SG	1:A:167:CYS:CB	3.08	0.41
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.55	0.41
1:A:857:ARG:HD2	5:F:139:PRO:HG3	2.02	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.19	0.41
2:B:273:LEU:CD1	2:B:285:ILE:HD12	2.50	0.41
2:B:567:GLU:OE1	2:B:567:GLU:N	2.39	0.41
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.20	0.41
6:H:109:LYS:HB3	6:H:111:LEU:CA	2.50	0.41
7:I:75:CYS:CB	7:I:78:CYS:SG	3.07	0.41
7:I:87:GLN:NE2	7:I:97:MET:HG2	2.34	0.41
1:A:79:GLY:HA3	2:B:1205:GLN:HE21	1.86	0.41
1:A:265:LYS:HZ3	1:A:265:LYS:HB2	1.84	0.41
1:A:991:LYS:HD2	1:A:991:LYS:HA	1.88	0.41
1:A:1193:LEU:CD2	1:A:1267:MET:HE2	2.44	0.41
1:A:1343:ALA:HA	4:E:149:LEU:O	2.21	0.41
2:B:582:VAL:HA	2:B:626:ILE:O	2.19	0.41
3:C:46:ILE:H	3:C:46:ILE:HG12	1.63	0.41
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.76	0.41
1:A:164:ARG:HB3	1:A:165:GLY:H	1.78	0.41
1:A:1081:LEU:HG	11:R:13:C:H41	1.86	0.41
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	2.03	0.41
2:B:47:GLN:O	2:B:173:MET:HE1	2.20	0.41
2:B:85:SER:N	2:B:86:ARG:CB	2.79	0.41
2:B:463:THR:HG21	2:B:465:ASN:ND2	2.33	0.41
3:C:178:PHE:CD2	3:C:178:PHE:C	2.99	0.41
3:C:266:ASP:C	3:C:268:ASP:H	2.28	0.41
1:A:80:HIS:C	1:A:243:PRO:HG3	2.46	0.41
1:A:241:VAL:HA	1:A:242:PRO:HD3	1.92	0.41
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.71	0.41
1:A:453:MET:HE2	1:A:453:MET:HB2	1.83	0.41
1:A:1192:LEU:HD11	1:A:1239:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:VAL:O	1:A:1322:ILE:CD1	2.69	0.41
2:B:777:ALA:HB2	2:B:1093:GLN:NE2	2.35	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.41
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.34	0.41
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.56	0.41
1:A:631:HIS:HE1	1:A:879:GLU:HB3	1.86	0.41
1:A:935:GLN:NE2	1:A:939:ASP:OD1	2.53	0.41
1:A:1037:LEU:HD12	1:A:1042:PHE:HD1	1.86	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD3	1.82	0.41
1:A:1198:ASP:C	1:A:1200:ALA:N	2.78	0.41
1:A:1394:THR:HG22	1:A:1398:MET:HE3	2.02	0.41
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.56	0.41
2:B:815:ARG:O	8:J:54:VAL:HG21	2.20	0.41
2:B:825:VAL:HG11	2:B:1090:THR:HB	2.02	0.41
2:B:874:PHE:CE2	2:B:914:LYS:HD3	2.55	0.41
3:C:180:TYR:O	3:C:180:TYR:CD1	2.74	0.41
6:H:12:VAL:HG12	6:H:51:ALA:HA	2.02	0.41
7:I:80:SER:C	7:I:82:GLU:H	2.28	0.41
1:A:91:PHE:CZ	1:A:207:ILE:CD1	3.04	0.41
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.03	0.41
7:I:59:VAL:HG12	7:I:60:GLN:H	1.86	0.41
1:A:174:ILE:HA	1:A:182:VAL:O	2.21	0.41
1:A:306:ASN:O	1:A:307:ASP:HB2	2.21	0.41
1:A:387:ARG:NH1	1:A:437:MET:HE1	2.36	0.41
1:A:605:MET:HE3	1:A:614:PHE:O	2.21	0.41
1:A:1052:GLN:O	1:A:1055:ARG:HB2	2.21	0.41
2:B:791:THR:O	2:B:792:MET:HB2	2.21	0.41
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	2.03	0.41
2:B:880:THR:O	2:B:882:THR:N	2.51	0.41
2:B:915:THR:HB	2:B:934:LYS:HB3	2.02	0.41
2:B:969:ARG:HG2	2:B:970:THR:N	2.35	0.41
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.51	0.41
1:A:55:ASP:HB3	1:A:56:PRO:HD3	2.02	0.41
1:A:80:HIS:O	1:A:243:PRO:HG3	2.21	0.41
1:A:230:ARG:HD3	1:A:232:GLU:OE2	2.21	0.41
1:A:230:ARG:HA	1:A:231:PRO:HD3	1.84	0.41
1:A:239:LEU:HA	1:A:240:PRO:HD3	1.91	0.41
1:A:262:LEU:HD11	1:A:325:ILE:HG12	2.02	0.41
1:A:273:ASN:ND2	1:A:296:LEU:HD21	2.36	0.41
1:A:320:ARG:HA	1:A:320:ARG:NE	2.30	0.41
1:A:343:LYS:HZ1	2:B:1156:ASP:CG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:O	1:A:526:ASP:C	2.64	0.41
1:A:543:LEU:O	1:A:547:LEU:HG	2.21	0.41
1:A:578:LEU:C	1:A:580:VAL:H	2.29	0.41
1:A:662:PHE:HD2	2:B:829:CYS:SG	2.44	0.41
1:A:831:THR:C	1:A:833:GLU:N	2.79	0.41
1:A:880:LYS:HG3	1:A:880:LYS:O	2.21	0.41
2:B:66:ASP:O	2:B:66:ASP:OD1	2.39	0.41
2:B:173:MET:HG3	2:B:201:GLY:HA2	2.02	0.41
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.35	0.41
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.85	0.41
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.56	0.41
2:B:593:PRO:HA	2:B:596:LEU:HB3	2.03	0.41
2:B:843:GLN:O	2:B:844:SER:C	2.64	0.41
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.20	0.41
2:B:976:ILE:HD11	2:B:991:GLY:O	2.21	0.41
2:B:1002:THR:C	2:B:1004:GLU:N	2.78	0.41
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	2.02	0.41
2:B:1146:PHE:CD2	2:B:1146:PHE:C	2.97	0.41
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.36	0.41
3:C:33:LEU:O	3:C:37:MET:HB2	2.20	0.41
3:C:45:ALA:O	3:C:46:ILE:C	2.61	0.41
3:C:57:VAL:HG21	8:J:61:LEU:HD23	2.03	0.41
6:H:31:THR:C	6:H:33:GLN:H	2.29	0.41
8:J:3:VAL:CG2	8:J:18:TRP:CG	3.04	0.41
1:A:343:LYS:HZ1	2:B:1156:ASP:CB	2.34	0.41
1:A:360:GLU:HA	1:A:360:GLU:OE2	2.21	0.41
1:A:449:SER:OG	2:B:1134:GLU:OE2	2.36	0.41
1:A:752:LYS:HD2	1:A:752:LYS:HA	1.81	0.41
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.61	0.41
1:A:1170:ILE:CG2	1:A:1170:ILE:O	2.69	0.41
2:B:769:TYR:OH	11:R:12:G:H2'	2.21	0.41
2:B:826:ALA:O	2:B:1011:ILE:HA	2.21	0.41
2:B:833:TYR:OH	9:K:65:HIS:CE1	2.74	0.41
1:A:250:ILE:HD12	1:A:251:SER:H	1.85	0.40
1:A:343:LYS:HE2	2:B:1151:LEU:HD23	2.04	0.40
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.90	0.40
2:B:57:TYR:O	2:B:58:THR:C	2.64	0.40
2:B:100:PRO:HD3	2:B:178:ASN:O	2.21	0.40
2:B:344:LYS:HB3	2:B:347:LYS:HB2	2.03	0.40
2:B:756:ILE:HA	2:B:757:PRO:HD3	1.88	0.40
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.01	0.40
3:C:63:ILE:O	3:C:66:ARG:HB2	2.21	0.40
3:C:142:VAL:HG23	8:J:15:GLY:HA3	2.02	0.40
3:C:167:HIS:HD2	3:C:169:LYS:N	1.93	0.40
7:I:46:HIS:O	7:I:47:GLU:O	2.40	0.40
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.56	0.40
1:A:33:ALA:HB3	1:A:82:GLY:HA3	2.02	0.40
1:A:384:ASN:O	1:A:385:ILE:C	2.64	0.40
1:A:508:PRO:HB3	1:A:643:ALA:HB2	2.02	0.40
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.22	0.40
2:B:292:ILE:H	2:B:293:PRO:CD	2.34	0.40
2:B:706:GLN:O	2:B:707:PRO:C	2.64	0.40
2:B:801:LYS:HA	2:B:802:PRO:HD2	1.91	0.40
2:B:834:ASN:HB2	2:B:839:MET:HA	2.02	0.40
7:I:85:PHE:CD1	7:I:99:LEU:HD22	2.56	0.40
1:A:46:THR:C	1:A:48:ALA:N	2.79	0.40
1:A:287:HIS:HA	1:A:288:ALA:HA	1.47	0.40
1:A:622:VAL:O	1:A:630:ILE:HD11	2.22	0.40
1:A:655:PHE:O	1:A:658:LEU:HB3	2.21	0.40
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	2.04	0.40
2:B:34:ILE:O	2:B:37:PHE:N	2.53	0.40
2:B:210:LYS:NZ	2:B:482:VAL:HG22	2.36	0.40
2:B:797:TYR:HH	2:B:971:THR:HG1	1.62	0.40
2:B:825:VAL:CG1	2:B:1090:THR:HB	2.52	0.40
2:B:899:ILE:HD11	2:B:911:ILE:CG2	2.46	0.40
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.36	0.40
7:I:85:PHE:C	7:I:86:PHE:CD2	2.99	0.40
1:A:567:LYS:O	1:A:568:PRO:C	2.64	0.40
1:A:1134:ILE:H	1:A:1134:ILE:HG13	1.66	0.40
1:A:1192:LEU:HG	1:A:1193:LEU:H	1.87	0.40
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.99	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.84	0.40
2:B:662:MET:C	2:B:664:THR:N	2.79	0.40
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.55	0.40
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.76	0.40
6:H:118:PHE:C	6:H:120:GLY:N	2.80	0.40
1:A:535:THR:HG22	1:A:575:LYS:HG2	2.03	0.40
1:A:667:GLY:C	3:C:192:TRP:HZ2	2.28	0.40
1:A:1198:ASP:C	1:A:1200:ALA:H	2.30	0.40
1:A:1317:MET:HB3	1:A:1327:ILE:HD13	2.03	0.40
2:B:242:SER:HB2	2:B:362:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.98	0.40
10:L:32:ALA:HB3	10:L:55:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1438/1733 (83%)	1083 (75%)	289 (20%)	66 (5%)	2	18
2	B	1145/1224 (94%)	877 (77%)	219 (19%)	49 (4%)	2	19
3	C	269/318 (85%)	205 (76%)	57 (21%)	7 (3%)	4	27
4	E	213/215 (99%)	180 (84%)	28 (13%)	5 (2%)	5	30
5	F	83/155 (54%)	66 (80%)	13 (16%)	4 (5%)	2	17
6	H	132/146 (90%)	100 (76%)	26 (20%)	6 (4%)	2	18
7	I	117/122 (96%)	82 (70%)	26 (22%)	9 (8%)	1	11
8	J	63/70 (90%)	53 (84%)	6 (10%)	4 (6%)	1	14
9	K	112/120 (93%)	97 (87%)	13 (12%)	2 (2%)	6	33
10	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	18
All	All	3616/4173 (87%)	2772 (77%)	690 (19%)	154 (4%)	2	19

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	117	GLU
1	A	120	GLU
1	A	169	ASN
1	A	186	LYS

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Mol	Chain	Res	Type
1	A	191	THR
1	A	193	ASP
1	A	194	ALA
1	A	195	ASP
1	A	320	ARG
1	A	567	LYS
1	A	1170	ILE
1	A	1173	HIS
1	A	1270	ASN
2	B	439	ALA
2	B	468	GLU
2	B	475	SER
2	B	483	LEU
2	B	636	PRO
2	B	713	ALA
2	B	717	GLU
2	B	718	GLU
2	B	864	LYS
2	B	1021	MET
2	B	1096	ARG
3	C	142	VAL
3	C	182	PRO
4	E	206	GLY
7	I	33	SER
7	I	47	GLU
7	I	79	HIS
7	I	106	CYS
7	I	116	ASN
8	J	9	SER
8	J	10	CYS
1	A	56	PRO
1	A	155	GLU
1	A	250	ILE
1	A	258	GLY
1	A	307	ASP
1	A	424	ILE
1	A	846	GLU
1	A	958	VAL
1	A	1169	ILE
1	A	1221	LYS
1	A	1390	ASN
1	A	1437	GLY

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Mol	Chain	Res	Type
2	B	91	SER
2	B	176	SER
2	B	340	ALA
2	B	441	ASP
2	B	478	GLY
2	B	531	GLN
2	B	575	PRO
2	B	831	SER
2	B	881	ASN
5	F	72	LYS
6	H	78	SER
6	H	119	GLY
7	I	107	SER
9	K	70	ARG
1	A	154	SER
1	A	185	TRP
1	A	255	SER
1	A	311	GLN
1	A	418	SER
1	A	557	ASP
1	A	1031	VAL
1	A	1081	LEU
1	A	1156	PRO
1	A	1218	GLN
1	A	1407	GLU
2	B	21	GLU
2	B	489	SER
2	B	712	PRO
2	B	732	SER
2	B	943	SER
4	E	76	GLY
5	F	77	ASP
5	F	78	GLN
5	F	80	ALA
6	H	82	PRO
6	H	109	LYS
7	I	3	THR
7	I	9	ASP
8	J	6	ARG
9	K	7	PHE
1	A	48	ALA
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	149	GLU
1	A	323	LYS
1	A	1190	PRO
1	A	1224	LEU
1	A	1388	GLY
1	A	1435	PRO
2	B	74	LEU
2	B	76	GLN
2	B	79	THR
2	B	290	GLY
2	B	559	SER
2	B	946	ASN
2	B	1017	ILE
2	B	1150	ARG
3	C	28	ALA
3	C	214	ASN
4	E	86	PRO
6	H	60	ALA
6	H	75	ALA
8	J	8	PHE
10	L	59	ALA
1	A	248	PRO
1	A	287	HIS
1	A	332	LYS
1	A	599	SER
1	A	1171	GLN
2	B	277	LYS
2	B	647	GLY
2	B	676	VAL
2	B	711	GLU
2	B	792	MET
2	B	974	PRO
3	C	125	MET
3	C	227	THR
4	E	124	VAL
7	I	11	ASN
10	L	46	VAL
1	A	78	PRO
1	A	119	ASN
1	A	157	ASP
1	A	308	ILE
1	A	364	VAL

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Mol	Chain	Res	Type
1	A	392	VAL
1	A	568	PRO
2	B	555	ILE
2	B	1214	PRO
3	C	129	ILE
1	A	158	PRO
1	A	338	GLY
1	A	639	PRO
1	A	756	ILE
1	A	1424	VAL
1	A	1429	ILE
2	B	292	ILE
2	B	731	VAL
1	A	197	PRO
2	B	70	ILE
2	B	93	GLY
2	B	901	PRO
4	E	38	PRO
1	A	570	PRO
1	A	1379	GLY
2	B	410	GLY
2	B	976	ILE
2	B	1046	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1258/1520 (83%)	1079 (86%)	179 (14%)	3	17
2	B	1000/1061 (94%)	861 (86%)	139 (14%)	3	18
3	C	238/274 (87%)	208 (87%)	30 (13%)	4	21
4	E	196/197 (100%)	182 (93%)	14 (7%)	13	39
5	F	74/137 (54%)	71 (96%)	3 (4%)	27	51
6	H	119/128 (93%)	110 (92%)	9 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	113/116 (97%)	101 (89%)	12 (11%)	6	26
8	J	60/65 (92%)	52 (87%)	8 (13%)	4	19
9	K	99/102 (97%)	88 (89%)	11 (11%)	6	24
10	L	40/57 (70%)	36 (90%)	4 (10%)	7	28
All	All	3197/3657 (87%)	2788 (87%)	409 (13%)	4	21

All (409) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	23	SER
1	A	30	ILE
1	A	32	VAL
1	A	49	LYS
1	A	58	LEU
1	A	63	ARG
1	A	65	LEU
1	A	69	THR
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	108	MET
1	A	113	LEU
1	A	121	LEU
1	A	154	SER
1	A	155	GLU
1	A	159	THR
1	A	160	GLN
1	A	161	LEU
1	A	164	ARG
1	A	167	CYS
1	A	180	LYS
1	A	187	LYS
1	A	191	THR
1	A	193	ASP
1	A	195	ASP
1	A	198	GLU
1	A	208	LEU
1	A	216	VAL
1	A	222	LEU
1	A	226	GLU

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Mol	Chain	Res	Type
1	A	227	VAL
1	A	239	LEU
1	A	250	ILE
1	A	263	THR
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	295	LEU
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN
1	A	317	LYS
1	A	322	VAL
1	A	323	LYS
1	A	332	LYS
1	A	333	GLU
1	A	346	ASP
1	A	351	THR
1	A	373	THR
1	A	403	LYS
1	A	405	VAL
1	A	411	ASP
1	A	413	ILE
1	A	419	LYS
1	A	424	ILE
1	A	440	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	454	SER
1	A	463	ILE
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	474	VAL
1	A	475	THR
1	A	516	SER
1	A	517	ASN
1	A	518	LYS
1	A	527	THR

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Mol	Chain	Res	Type
1	A	535	THR
1	A	545	GLN
1	A	550	LEU
1	A	565	ILE
1	A	576	GLN
1	A	618	GLU
1	A	652	VAL
1	A	658	LEU
1	A	663	SER
1	A	666	ILE
1	A	687	LYS
1	A	694	THR
1	A	732	LEU
1	A	740	LEU
1	A	741	ASN
1	A	747	VAL
1	A	752	LYS
1	A	756	ILE
1	A	758	ILE
1	A	762	SER
1	A	764	CYS
1	A	765	VAL
1	A	770	VAL
1	A	771	GLU
1	A	783	THR
1	A	788	SER
1	A	803	SER
1	A	824	LEU
1	A	837	ILE
1	A	838	GLN
1	A	858	ASN
1	A	867	ILE
1	A	884	ASP
1	A	885	THR
1	A	895	LYS
1	A	902	LEU
1	A	904	THR
1	A	908	LEU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	929	LEU

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Mol	Chain	Res	Type
1	A	961	ARG
1	A	969	GLN
1	A	970	THR
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1031	VAL
1	A	1033	GLN
1	A	1035	TYR
1	A	1037	LEU
1	A	1039	LYS
1	A	1046	LEU
1	A	1049	ILE
1	A	1058	VAL
1	A	1067	LEU
1	A	1079	MET
1	A	1081	LEU
1	A	1082	ASN
1	A	1089	VAL
1	A	1095	THR
1	A	1113	THR
1	A	1116	LEU
1	A	1118	VAL
1	A	1142	THR
1	A	1146	VAL
1	A	1152	ILE
1	A	1168	GLU
1	A	1169	ILE
1	A	1172	LEU
1	A	1174	PHE
1	A	1175	SER
1	A	1176	LEU
1	A	1177	LEU
1	A	1178	ASP
1	A	1179	GLU
1	A	1222	ASN
1	A	1224	LEU
1	A	1227	ILE

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Mol	Chain	Res	Type
1	A	1237	ILE
1	A	1243	VAL
1	A	1264	GLU
1	A	1271	ILE
1	A	1283	VAL
1	A	1322	ILE
1	A	1327	ILE
1	A	1329	THR
1	A	1333	ILE
1	A	1341	ILE
1	A	1354	ASN
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1407	GLU
1	A	1408	ILE
1	A	1428	VAL
2	B	26	THR
2	B	34	ILE
2	B	35	SER
2	B	39	ARG
2	B	44	VAL
2	B	63	ILE
2	B	66	ASP
2	B	67	SER
2	B	68	THR
2	B	69	LEU
2	B	71	LEU
2	B	72	GLU
2	B	74	LEU
2	B	80	GLU
2	B	84	ILE
2	B	89	GLU
2	B	90	ILE
2	B	98	THR
2	B	120	ARG
2	B	130	VAL
2	B	178	ASN

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Mol	Chain	Res	Type
2	B	203	PHE
2	B	204	ILE
2	B	213	ILE
2	B	222	ILE
2	B	223	VAL
2	B	225	VAL
2	B	246	LYS
2	B	268	THR
2	B	282	ILE
2	B	283	VAL
2	B	291	ILE
2	B	298	LEU
2	B	305	VAL
2	B	310	MET
2	B	315	LYS
2	B	327	ARG
2	B	336	ARG
2	B	353	LYS
2	B	355	ILE
2	B	371	GLU
2	B	396	ASP
2	B	404	LYS
2	B	412	LEU
2	B	416	LEU
2	B	419	THR
2	B	420	LEU
2	B	424	LEU
2	B	425	THR
2	B	438	GLU
2	B	440	HIS
2	B	441	ASP
2	B	444	MET
2	B	445	LYS
2	B	453	ILE
2	B	459	TYR
2	B	463	THR
2	B	466	TRP
2	B	469	GLN
2	B	470	LYS
2	B	471	LYS
2	B	474	SER
2	B	479	VAL

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Mol	Chain	Res	Type
2	B	483	LEU
2	B	516	ASN
2	B	527	THR
2	B	537	LYS
2	B	542	MET
2	B	545	ILE
2	B	549	THR
2	B	570	VAL
2	B	582	VAL
2	B	626	ILE
2	B	633	VAL
2	B	637	LEU
2	B	644	GLU
2	B	645	SER
2	B	651	LEU
2	B	658	ILE
2	B	661	LEU
2	B	678	GLU
2	B	694	ASP
2	B	701	ILE
2	B	711	GLU
2	B	723	VAL
2	B	748	ILE
2	B	762	ASN
2	B	790	ASP
2	B	827	ILE
2	B	844	SER
2	B	864	LYS
2	B	871	THR
2	B	878	GLN
2	B	891	ASP
2	B	899	ILE
2	B	916	THR
2	B	941	LEU
2	B	943	SER
2	B	963	PHE
2	B	968	VAL
2	B	970	THR
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS

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Mol	Chain	Res	Type
2	B	989	THR
2	B	992	ILE
2	B	995	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1012	ILE
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1048	THR
2	B	1050	ILE
2	B	1051	THR
2	B	1052	VAL
2	B	1071	VAL
2	B	1082	MET
2	B	1087	PHE
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1128	LEU
2	B	1132	GLU
2	B	1145	SER
2	B	1147	LEU
2	B	1156	ASP
2	B	1165	ILE
2	B	1175	LEU
2	B	1190	ASP
2	B	1194	ILE
2	B	1196	ILE
3	C	4	GLU
3	C	10	ILE
3	C	18	VAL
3	C	21	ILE
3	C	22	LEU
3	C	25	VAL
3	C	27	LEU
3	C	36	VAL

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Mol	Chain	Res	Type
3	C	43	THR
3	C	50	GLU
3	C	57	VAL
3	C	58	LEU
3	C	69	LEU
3	C	77	ILE
3	C	109	SER
3	C	120	ILE
3	C	129	ILE
3	C	134	ILE
3	C	143	LEU
3	C	158	VAL
3	C	163	ILE
3	C	195	GLN
3	C	197	SER
3	C	199	LYS
3	C	203	GLN
3	C	215	GLU
3	C	228	PHE
3	C	240	VAL
3	C	244	VAL
3	C	258	ILE
4	E	14	ARG
4	E	30	ILE
4	E	31	THR
4	E	33	GLU
4	E	43	LYS
4	E	88	VAL
4	E	92	THR
4	E	95	THR
4	E	131	THR
4	E	134	THR
4	E	150	VAL
4	E	156	LEU
4	E	159	ASP
4	E	169	ARG
5	F	97	ARG
5	F	111	LEU
5	F	148	VAL
6	H	11	GLN
6	H	15	VAL
6	H	23	VAL

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Mol	Chain	Res	Type
6	H	55	LEU
6	H	56	THR
6	H	62	SER
6	H	94	ASP
6	H	121	LEU
6	H	142	LEU
7	I	8	ARG
7	I	9	ASP
7	I	17	ARG
7	I	29	CYS
7	I	31	THR
7	I	59	VAL
7	I	75	CYS
7	I	78	CYS
7	I	83	ASN
7	I	95	THR
7	I	96	SER
7	I	104	LEU
8	J	5	VAL
8	J	7	CYS
8	J	13	VAL
8	J	29	GLU
8	J	31	ASP
8	J	34	THR
8	J	43	ARG
8	J	50	ILE
9	K	6	ARG
9	K	10	PHE
9	K	33	ILE
9	K	41	THR
9	K	42	LEU
9	K	50	LEU
9	K	101	LEU
9	K	102	LYS
9	K	106	GLU
9	K	107	THR
9	K	113	THR
10	L	49	LYS
10	L	55	ILE
10	L	61	THR
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	83	HIS
1	A	119	ASN
1	A	171	GLN
1	A	253	ASN
1	A	273	ASN
1	A	281	HIS
1	A	299	HIS
1	A	306	ASN
1	A	311	GLN
1	A	316	GLN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	471	ASN
1	A	493	GLN
1	A	503	GLN
1	A	660	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	760	GLN
1	A	838	GLN
1	A	854	ASN
1	A	858	ASN
1	A	877	HIS
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1082	ASN
1	A	1173	HIS
1	A	1188	GLN
1	A	1218	GLN
1	A	1222	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1387	HIS
1	A	1427	ASN
1	A	1432	GLN
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	110	HIS
2	B	121	ASN
2	B	178	ASN
2	B	206	ASN
2	B	215	GLN
2	B	236	HIS
2	B	278	GLN
2	B	300	HIS
2	B	366	GLN
2	B	395	GLN
2	B	440	HIS
2	B	465	ASN
2	B	494	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	761	HIS
2	B	762	ASN
2	B	767	ASN
2	B	794	ASN
2	B	821	GLN
2	B	822	ASN
2	B	842	ASN
2	B	878	GLN
2	B	975	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1084	GLN
2	B	1141	HIS
2	B	1178	ASN
2	B	1195	HIS
3	C	31	ASN
3	C	73	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN

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Mol	Chain	Res	Type
3	C	167	HIS
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
3	C	206	ASN
3	C	271	ASN
4	E	3	GLN
4	E	8	ASN
4	E	104	ASN
4	E	147	HIS
4	E	174	GLN
4	E	179	GLN
6	H	11	GLN
6	H	35	GLN
6	H	131	ASN
7	I	60	GLN
7	I	83	ASN
7	I	87	GLN
7	I	89	GLN
8	J	64	ASN
9	K	65	HIS
9	K	76	GLN
10	L	66	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	1442/1733 (83%)	-0.21	11 (0%) 82 62	77, 132, 243, 401	0
2	B	1153/1224 (94%)	-0.16	9 (0%) 82 62	77, 116, 250, 399	0
3	C	271/318 (85%)	-0.37	1 (0%) 88 74	86, 111, 177, 330	0
4	E	215/215 (100%)	-0.20	1 (0%) 87 71	107, 153, 272, 354	0
5	F	85/155 (54%)	-0.40	0 100 100	107, 129, 169, 217	0
6	H	136/146 (93%)	0.02	2 (1%) 72 50	120, 167, 307, 372	0
7	I	119/122 (97%)	-0.04	2 (1%) 69 47	106, 148, 191, 275	0
8	J	65/70 (92%)	-0.39	0 100 100	83, 101, 151, 176	0
9	K	114/120 (95%)	-0.42	0 100 100	83, 115, 150, 171	0
10	L	46/70 (65%)	0.18	2 (4%) 40 28	102, 161, 254, 269	0
11	R	14/18 (77%)	-0.01	1 (7%) 22 19	106, 130, 215, 216	0
12	T	29/29 (100%)	0.43	1 (3%) 48 33	105, 216, 417, 435	0
13	N	14/14 (100%)	0.53	0 100 100	263, 310, 353, 397	0
All	All	3703/4234 (87%)	-0.19	30 (0%) 82 62	77, 128, 255, 435	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	3.6
1	A	157	ASP	3.4
7	I	57	GLY	3.3
2	B	441	ASP	3.2
11	R	14	DA	3.2
1	A	158	PRO	2.9
10	L	32	ALA	2.8
10	L	27	LEU	2.7
6	H	139	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
7	I	105	SER	2.6
6	H	120	GLY	2.5
2	B	1211	ASN	2.5
1	A	195	ASP	2.5
1	A	186	LYS	2.5
1	A	193	ASP	2.5
4	E	88	VAL	2.4
1	A	190	ALA	2.4
1	A	188	ASP	2.4
2	B	477	ALA	2.4
12	T	3	DA	2.3
2	B	643	ASP	2.3
1	A	197	PRO	2.1
1	A	155	GLU	2.1
3	C	157	CYS	2.1
2	B	471	LYS	2.1
2	B	440	HIS	2.1
1	A	159	THR	2.0
2	B	439	ALA	2.0
1	A	192	GLY	2.0
2	B	1019	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	I	204	1/1	0.95	0.08	310,310,310,310	0
14	ZN	A	1734	1/1	0.98	0.03	228,228,228,228	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	A	1735	1/1	0.99	0.07	149,149,149,149	0
14	ZN	J	101	1/1	0.99	0.03	193,193,193,193	0
14	ZN	L	105	1/1	0.99	0.03	131,131,131,131	0
14	ZN	B	1307	1/1	1.00	0.02	157,157,157,157	0
14	ZN	C	319	1/1	1.00	0.02	136,136,136,136	0
14	ZN	I	203	1/1	1.00	0.02	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.