



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:40 AM EDT

PDB ID : 2R7Z / pdb_00002r7z
Title : Cisplatin lesion containing RNA polymerase II elongation complex
Authors : Damsma, G.E.; Alt, A.; Brueckner, F.; Carell, T.; Cramer, P.
Deposited on : 2007-09-10
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

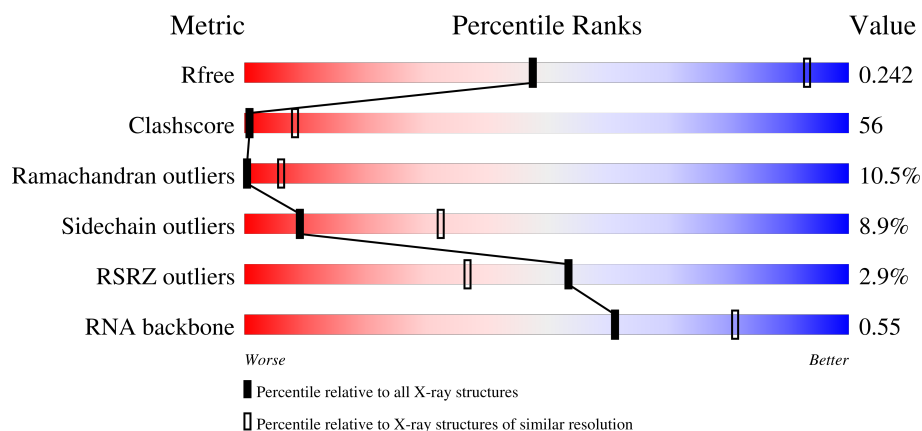
1 Overall quality at a glance

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)
RNA backbone	3983	1007 (4.50-3.10)

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	T	17	6% 76% 18% 6%
2	N	7	14% 43% 57%
3	P	10	10% 20% 60% 10% 10%
4	A	1733	2% 22% 46% 12% 18%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31804 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 DNA chain called 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	17	Total	C	N	O	P	0	0	0
			336	163	53	104	16			

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	0	0	0
			143	69	30	38	6			

- Molecule 3 is a RNA chain called 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			216	97	41	69	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

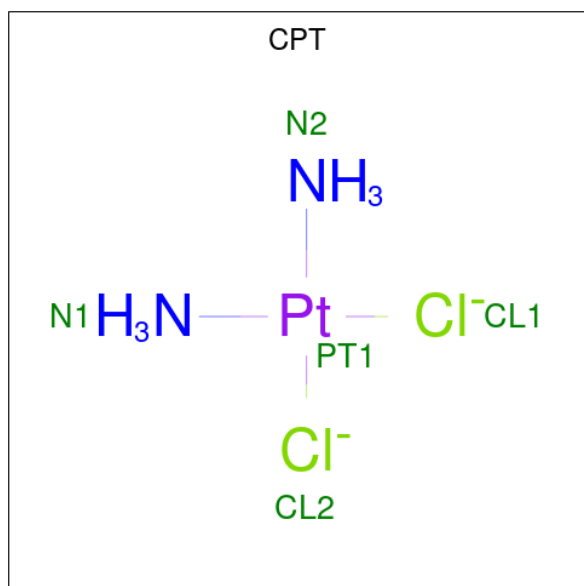
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 16 is Cisplatin (CCD ID: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	T	1	Total	N	Pt	0	0
			3	2	1		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		

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

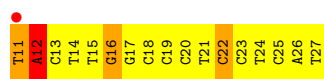
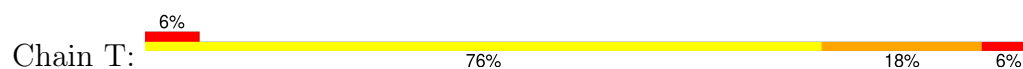
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 1	Mg 1	0	0

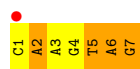
3 Residue-property plots

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: 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3',



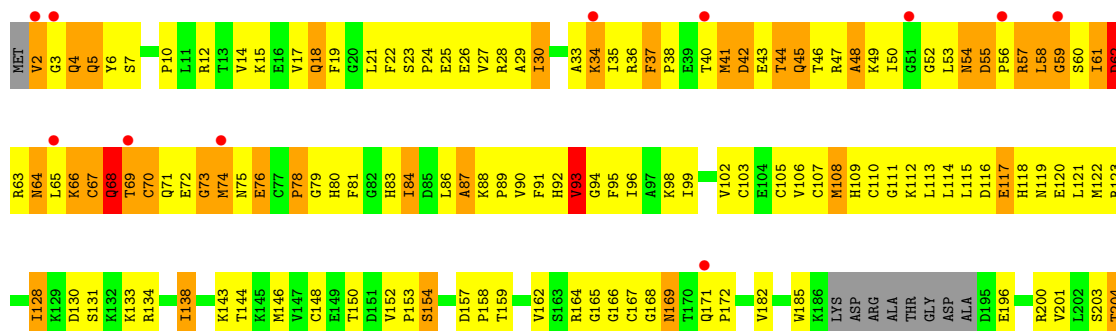
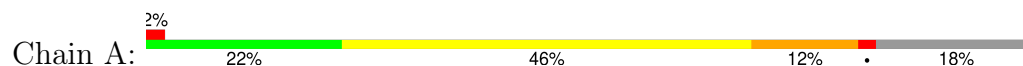
- Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'



- Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

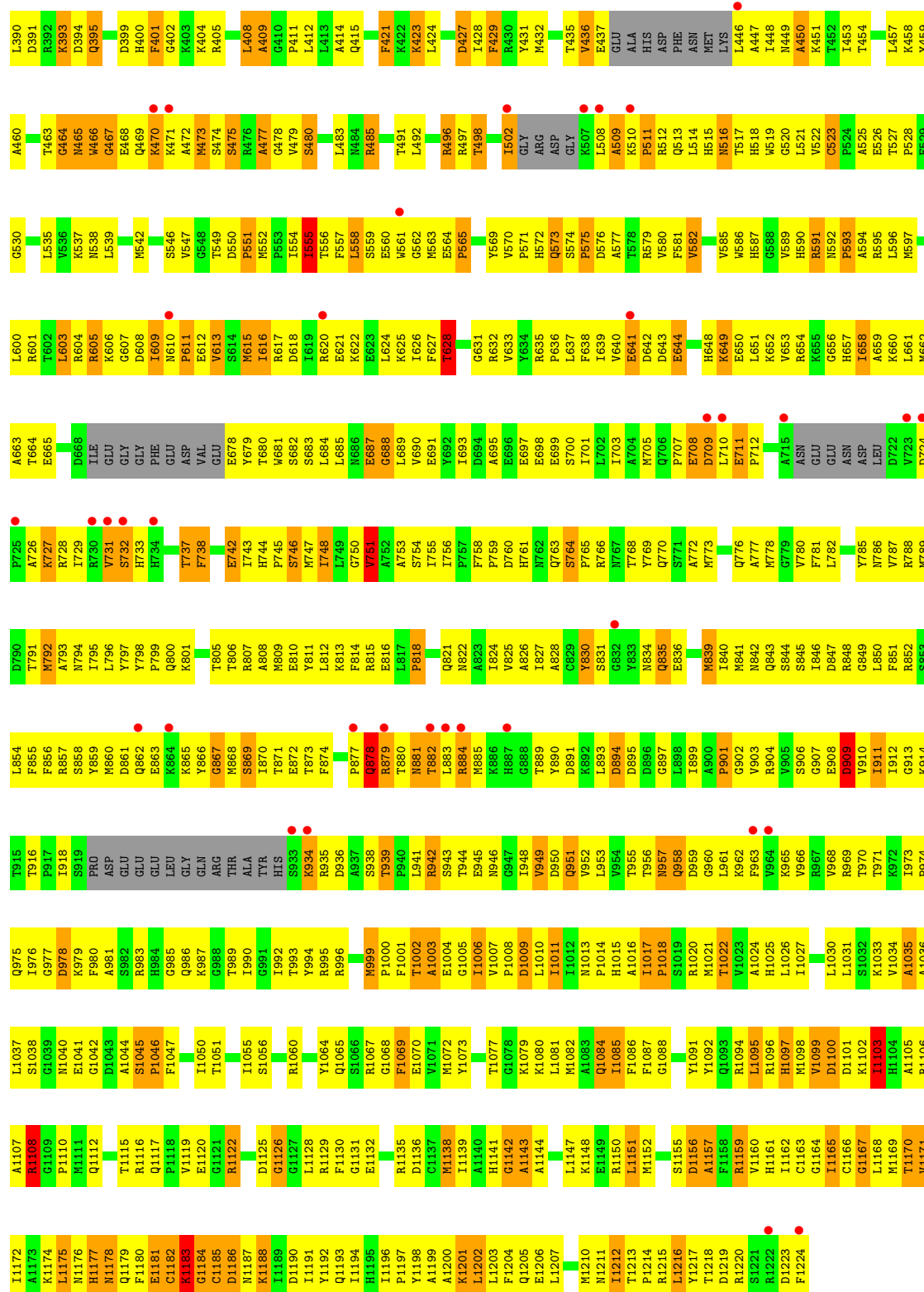


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



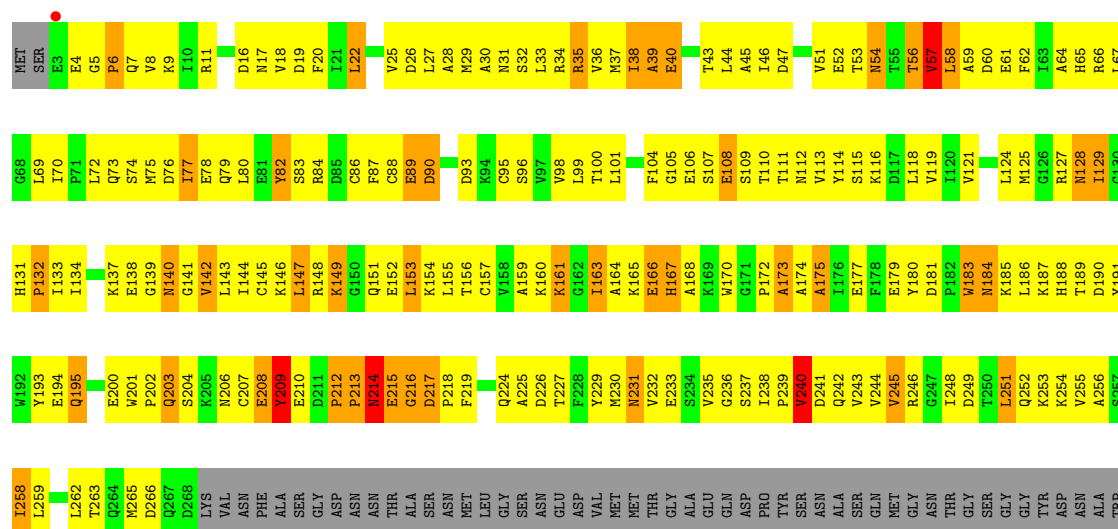
Q1130	A1069	G1002	K938	E870	G807	L737	I670	S599	L528	I463	G401	G334	D268	E205
A1131	Q1070	A1003	D939	D871	L808	K738	A671	P600	I531	P464	Y404	R335	I269	E206
K1132	S1072	E1004	R940	M872	T809	D739	D672	D602	Y405	Y465	Y406	R336	I270	I207
L1133	I1072	E1005	R941	M873	P810	L740	A673	G601	G406	S466	L406	R337	L267	L208
I1134	G1073	I1006	F942	D874	Q811	N741	G673	M605	L534	T467	R407	G338	L276	N209
E1074	E1074	I1007	L943	A875	R812	N742	P674	L606	T535	F468	D408	N339	L277	I210
A1075	A1075	Q1008	R944	D876	F813	V743	T675	L606	L536	R469	L340	N340	T278	F211
A1076	A1076	Q1009	E945	I878	F814	K744	M676	I607	R537	L470	S409	K341	L279	
T1077	T1077	A1010	V946		F815	Q745		L608	P538	N471	G410	G342	E280	I214
Q1078	Q1078	Q1011	F947	S882	H816	K746	T680	D609	T539	L472	R412	K343	H281	S215
T1141	T1141	R1012		L883	A817	V747	I683		F540	S473	R413	K344	N282	
K1143	K1080	D1013	G950	T884	M818	N748	E681	L612	I541	V474	I413	V345	O283	D218
L1144	L1081	A1014		T885		K749	T682	L613	I542	T475	D414	D346	O284	F219
S1145	ASN	V1015	N953	I886	R821	G750	I683	F614	L543	S476	L415	F347	O285	T220
V1146	THR	T1016	N954	G887		S751	A684	G615	D544	P477	R416	S348	H286	S221
T1147	PHE	L1017	P955	G888	I825	K752	A685	G616	I545	Y478	R417	A349	L222	T222
L1148	HIS	F1018	L956	G889	D826	G753	E686	Q545	V546	N479	S418	R350	G223	G223
A1149	PHE	C1019	P957	D890	T927	S754	K687	E618	L547	A480	K419	T351	F224	F224
S1150	ALA	C1020	V958	A891	A828		K688	K619	N548	O481	R420	V352	N290	N295
E1151	GLY	L1021	N959		V829	N757	K689	K620	N549	F482		I353	E291	E226
I1152	VAL	L1022	R896	R896	R830		G690	T621	L550	D485	D423	S354	E292	V227
Y1153	ALA		Y897	Y897	T831	M761	L691	G622	Y551	I424	Q425	G355	E293	F228
Y1154	SER	R1025	R898	R898	A832	G762	D692	G623	M552	E486	Q426	D356		S229
D1155	K1092		T963	V899	E833	A763	V693	S624		K487	L426	P357		R230
P1156	K1093	R1029	T964	D900	T834	G764	T694	S625	N556	N488	Q427		Q297	P231
D1157	V1094	R1030	Q965	L901	G835	V765	K685	N626	D557	L489	Y428	E360	H299	E232
P1158	T1095	V1031	N966	L902	Y836	G766	E696	G627	G558	H490	Q429	L361	V300	M233
S1159	S1096	L1032	A967	N903	I837	Q767	A697	G628	V559	V491	W430		A301	M234
T1160	G1097	Q1033	Q968	T904	Q838	Q768	Q698	L629	I560	P492	K431	G365	T302	L235
L1161	E1034	E1034	Q969	D905	R839	Q768	A699	L630	P561	Q493	V432	V366	Y303	L236
V1162	V1035	R1035	T970	H906	R840	R774	N700	H631	T562	S494	R433	V367	T237	T237
L1163	R1036	L1036	F971	T907	L841	I775	L701	V632	P563	E495	R434	K368	D305	C238
P1164	L1037	L1037	H972	L908	V842		L702	V633	A564	E496	H435	S369	N306	L239
E1165	T1038	R1038	1973	D909	K843	G778		T634	I565	T497	L436		D307	P240
D1166	K1039	P910	K977	P910	A844	F779	T709	R635	I566	R498	N437	K372	I308	V241
E1167	Q1040	S911	K978	S911	L845	V780	L710	P639	P568	A499	D438	T373	A309	P242
E1168	L1104	L912	P878	L912	E846	D781	R711	Q640	K569	E500	N439	L374	G310	P243
T1169	F1042	L913	S979	L913	D847	R782	E712	V641	S573		D440	T375	N311	P244
I1170	D1043	S914	D980	S914	I848	T783	S713	C642	L571	Q503	P441	T376	Q313	P245
Q1171	W1044	S915	L981	S915	M849	L784	F714		N572	L504	V442	P377	A314	V246
L1172	V1045	G916	T982	G916	V850	P785	E715	F646	S574	Q507	F444		L315	R247
H1173	L1046	S917	L983	S917	H851	H786	D716	F646	Q575	V507	R445	P382	P248	P248
F1174	S1047	E918	D985	E918	Y852	F787	N717	G647	K575		R446	Y383	S249	S249
S1175	L1048	I919	D986	I919	D853	S788	N718	N648	G576	T611	Q447	N384	I250	I250
L1176	I1049	L920	T987	L920	N854	K789	V719	I649	Q676	V512		P382	S251	S251
LEU	E1050	D921	V987	D921	T855		R720	Q650	L577	P514	S449	D386	G319	F252
ASP	A1051	N922	G989	N922	R857	P794	F721	K651	L578	Q515	L450	R387	R320	N253
GLU	Q1052	L925	G989	L925	N858	S796	N723	N654	V580	S516	H451	L388	P321	E254
GLU	V1058	Q926	V990	Q926	S859	S796	E724	F655		N517	K452		V322	S255
ALA	H1058	V927	K991	V927	L860	K797	A725		L588	K518	M453	L391	K323	Q256
GLN	P1060	L992	D992	L992	G861	G798	R726	L658	Q689	P519	S454	V392	S324	E259
SER	G1061	L993	L993	L993	N862	F799	D727		R590	C520	M455	R393	I325	D260
PHE	E1062	E995	E995	E995	V863	V800	K728	G661	F591	M521	M456	N394	A327	D261
ASP	M1063	N996	N996	N996	I864	E801	A729	F662	D592	G522	A457	G395	F328	L262
Q1187	V1064	Y933	L997	Y933	Q865	N802	G730	S663	T523	P396	L329	P396	L329	T263
Q1188	G1065	K934	L993	K934	F866	S803	R731	T664	T595	V524	R459	N397	K330	F264
S1189	V1066	Q935	V999	Q935	I867	Y804	L732	G665	T596	Q525	V460	E398	G331	K265
P1190	L1067	L1067	L1000	L1067	Y868	L805	L732	R666	L597	D526	K461	N399	K332	L266
W1191	E1129		R1001	V937	G969	R806	N736	G667	L598	T527	V462	P400	E333	A267



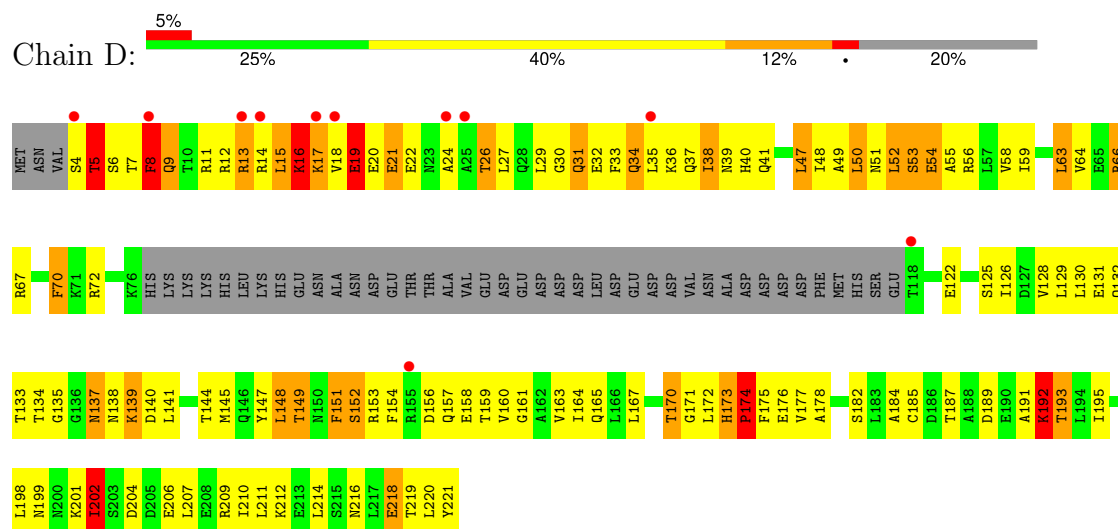


• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

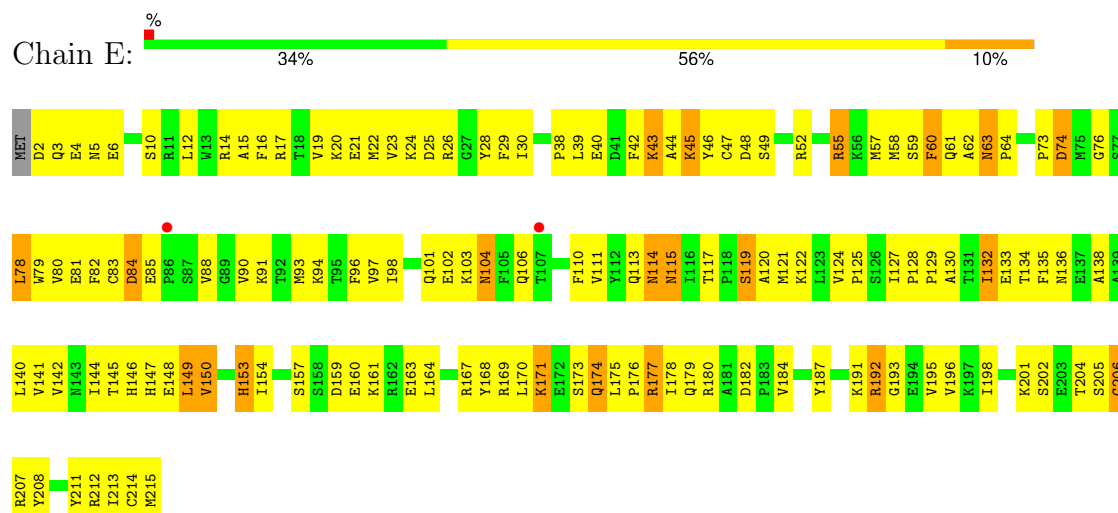
Chain C: 20% 49% 13% 16%



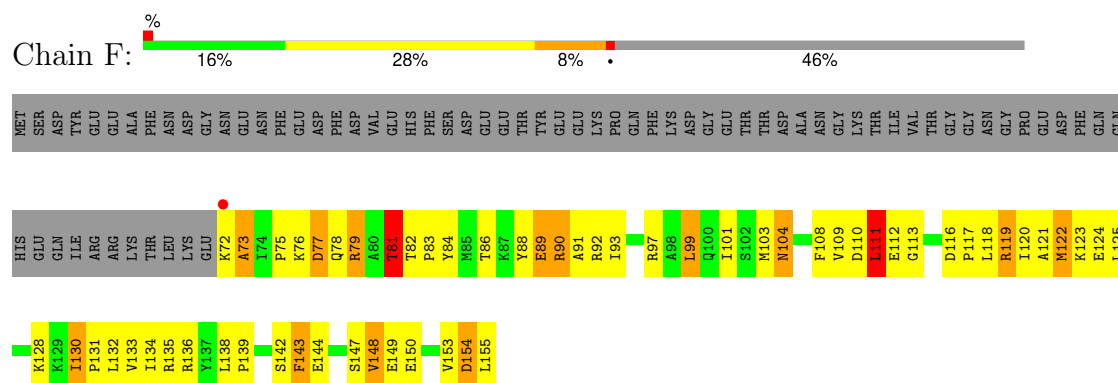
- Molecule 7: DNA-directed RNA polymerase II subunit RPB4



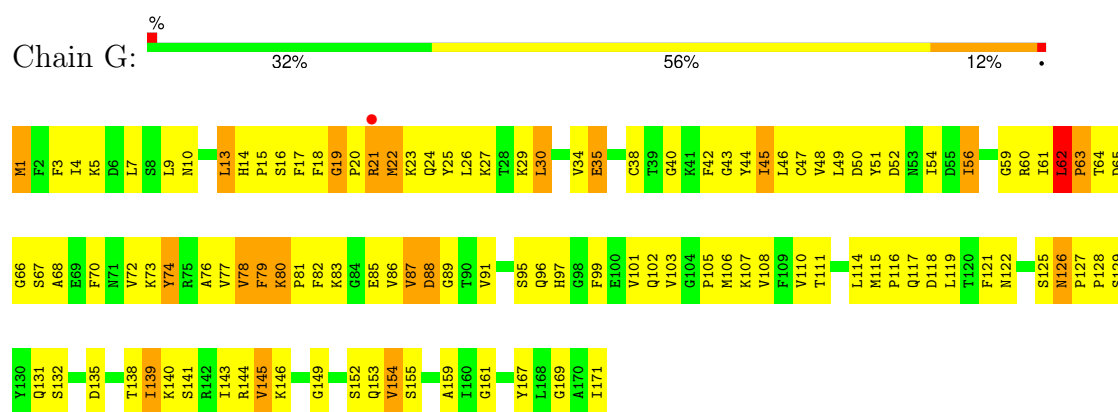
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



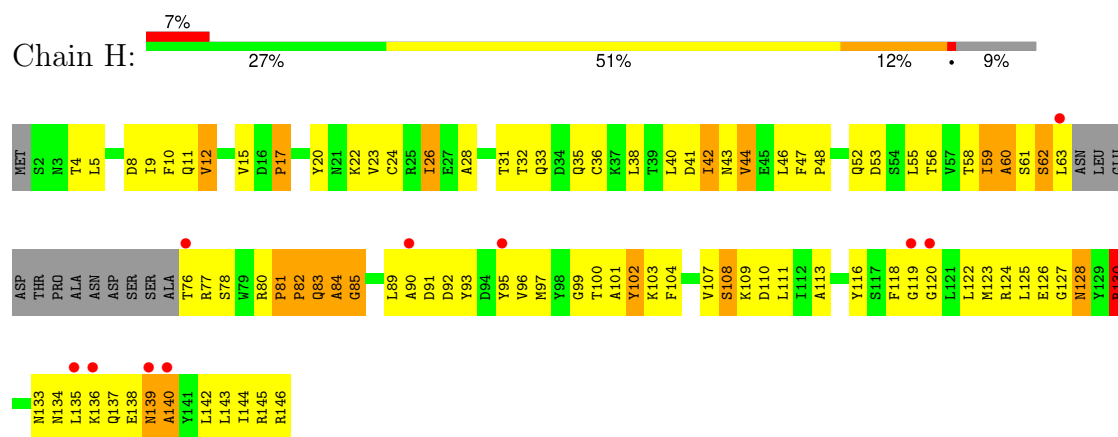
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



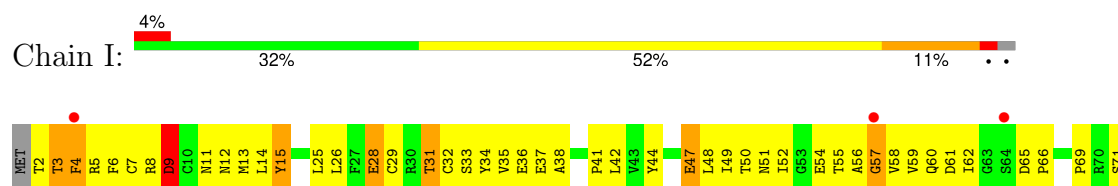
• Molecule 10: DNA-directed RNA polymerase II subunit RPB7

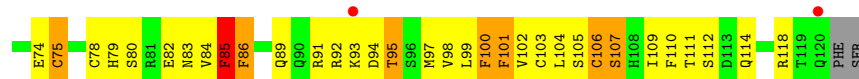


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

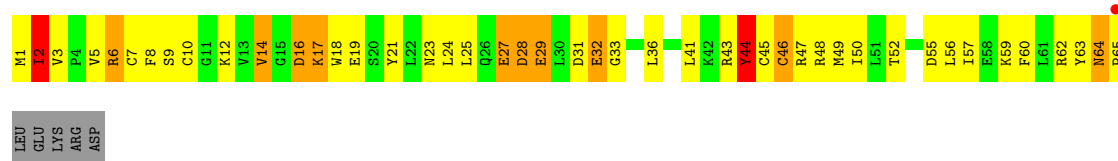


• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

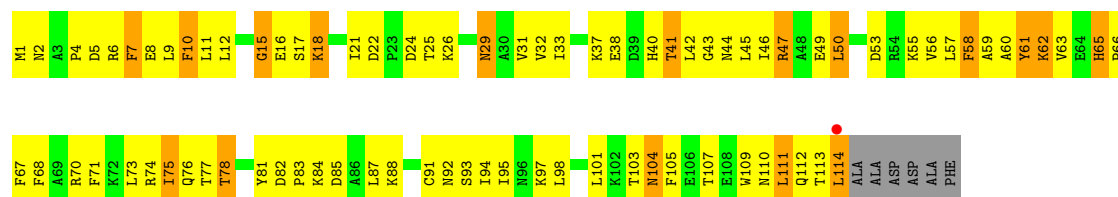




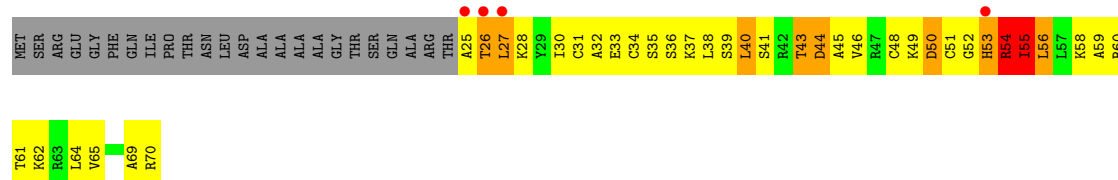
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 14: DNA-directed RNA polymerase II subunit RPB11



- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.06Å 393.12Å 283.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.7 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.240 0.216 , 0.242	Depositor DCC
R_{free} test set	2410 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	106.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31804	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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, MG, CPT

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	T	0.77	0/373	1.53	4/572 (0.7%)
2	N	0.71	0/161	1.19	2/247 (0.8%)
3	P	0.55	0/242	0.89	2/377 (0.5%)
4	A	0.54	0/11339	1.09	84/15334 (0.5%)
5	B	0.50	1/8981 (0.0%)	1.04	48/12108 (0.4%)
6	C	0.53	0/2133	1.07	11/2891 (0.4%)
7	D	0.49	0/1437	1.12	10/1925 (0.5%)
8	E	0.48	0/1788	1.06	13/2406 (0.5%)
9	F	0.60	0/691	1.15	6/933 (0.6%)
10	G	0.51	0/1368	1.12	13/1844 (0.7%)
11	H	0.47	0/1086	0.99	5/1470 (0.3%)
12	I	0.43	0/989	0.99	5/1331 (0.4%)
13	J	0.53	0/541	0.99	1/727 (0.1%)
14	K	0.51	0/937	1.06	8/1265 (0.6%)
15	L	0.55	0/366	0.90	0/485
All	All	0.52	1/32432 (0.0%)	1.07	212/43915 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	2
2	N	0	2
6	C	0	1
13	J	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	292	ILE	CA-CB	5.17	1.57	1.53

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	452	LYS	N-CA-C	-12.53	97.62	111.28
5	B	1185	CYS	N-CA-C	-12.31	98.93	114.56
7	D	26	THR	N-CA-C	-12.05	97.33	112.88
5	B	1177	HIS	N-CA-C	-10.70	101.63	112.97
10	G	62	LEU	CA-C-N	-10.21	107.08	119.84
10	G	62	LEU	C-N-CA	-10.21	107.08	119.84
7	D	171	GLY	N-CA-C	-9.71	101.03	115.00
4	A	1261	LYS	N-CA-C	-9.35	103.97	114.62
4	A	567	LYS	CA-C-N	-9.05	108.53	119.84
4	A	567	LYS	C-N-CA	-9.05	108.53	119.84
7	D	54	GLU	N-CA-C	-8.90	101.24	112.90
10	G	52	ASP	N-CA-C	8.64	120.31	111.07
5	B	427	ASP	N-CA-C	-8.58	103.33	113.88
4	A	983	ILE	N-CA-C	-8.56	102.08	110.72
4	A	143	LYS	N-CA-C	-8.44	102.03	111.82
4	A	344	ARG	N-CA-C	-8.40	98.08	110.52
5	B	1009	ASP	N-CA-C	-8.40	102.81	113.23
4	A	1275	GLY	N-CA-C	8.33	120.50	112.08
5	B	882	THR	N-CA-C	8.33	121.18	111.02
4	A	425	GLN	N-CA-C	-8.16	96.38	109.76
5	B	473	MET	N-CA-C	-8.10	103.11	113.16
7	D	72	ARG	N-CA-C	-8.09	103.41	113.28
4	A	266	LEU	N-CA-C	-8.04	102.20	110.97
8	E	171	LYS	N-CA-C	-8.00	98.68	110.52
5	B	395	GLN	N-CA-C	-7.99	99.01	110.59
4	A	864	ILE	N-CA-C	-7.96	105.73	113.53
7	D	38	ILE	N-CA-C	7.87	119.19	108.17
4	A	138	ILE	N-CA-C	-7.70	103.19	110.42
4	A	320	ARG	CA-C-N	7.56	129.29	119.84
4	A	320	ARG	C-N-CA	7.56	129.29	119.84
6	C	39	ALA	N-CA-C	7.55	123.16	113.88
4	A	598	LEU	N-CA-C	-7.53	102.66	113.21
8	E	55	ARG	N-CA-C	7.51	119.10	111.07
5	B	606	LYS	N-CA-C	-7.46	104.15	113.55
4	A	1277	GLU	N-CA-C	7.44	120.18	110.43
5	B	464	GLY	N-CA-C	-7.38	105.70	114.48
5	B	628	THR	N-CA-C	-7.32	103.94	114.12
5	B	296	GLU	N-CA-C	-7.13	103.54	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	982	THR	N-CA-C	-7.13	101.12	110.53
10	G	64	THR	N-CA-C	-7.11	105.80	114.75
4	A	710	LEU	N-CA-C	-6.98	103.69	111.71
9	F	77	ASP	N-CA-C	-6.91	99.65	110.36
4	A	1291	VAL	CA-C-N	6.90	128.46	119.84
4	A	1291	VAL	C-N-CA	6.90	128.46	119.84
4	A	244	PRO	N-CA-C	6.89	119.10	110.70
7	D	157	GLN	N-CA-C	-6.89	105.00	113.19
11	H	85	GLY	N-CA-C	-6.88	105.19	113.99
4	A	30	ILE	N-CA-C	6.86	117.01	110.42
4	A	466	SER	N-CA-C	6.82	125.33	110.80
5	B	555	ILE	N-CA-C	-6.81	104.02	110.42
4	A	1262	LYS	N-CA-C	-6.79	104.25	112.54
4	A	288	ALA	N-CA-C	-6.75	103.43	112.94
5	B	573	GLN	N-CA-C	-6.74	104.53	112.89
4	A	860	LEU	N-CA-C	-6.73	105.22	113.50
13	J	44	TYR	N-CA-C	6.72	119.46	111.33
4	A	311	GLN	N-CA-C	6.66	124.53	109.81
5	B	475	SER	N-CA-C	6.65	118.75	109.31
4	A	158	PRO	N-CA-C	-6.60	106.28	114.20
1	T	16	DG	C4'-C3'-O3'	6.59	119.89	110.00
7	D	66	ARG	N-CA-C	-6.59	103.36	111.40
6	C	38	ILE	N-CA-C	6.57	116.67	110.30
14	K	18	LYS	N-CA-C	-6.50	103.46	111.33
5	B	648	HIS	N-CA-C	6.49	114.10	108.78
8	E	6	GLU	N-CA-C	-6.44	105.28	113.01
6	C	40	GLU	N-CA-C	6.38	120.77	112.92
5	B	1142	GLY	N-CA-C	-6.32	106.52	115.43
5	B	1184	GLY	N-CA-C	-6.30	105.79	114.67
4	A	478	TYR	N-CA-C	-6.29	105.09	112.89
4	A	778	GLY	N-CA-C	-6.27	106.57	114.16
8	E	84	ASP	N-CA-C	-6.27	105.91	112.93
8	E	63	ASN	CA-C-N	6.23	127.63	119.84
8	E	63	ASN	C-N-CA	6.23	127.63	119.84
4	A	229	SER	N-CA-C	6.17	117.51	107.32
4	A	81	PHE	N-CA-C	6.16	118.25	110.24
5	B	934	LYS	N-CA-C	6.15	119.37	108.24
5	B	291	ILE	CA-C-N	6.10	124.08	120.24
5	B	291	ILE	C-N-CA	6.10	124.08	120.24
4	A	467	THR	N-CA-C	6.09	119.47	109.85
8	E	119	SER	N-CA-C	-6.08	104.22	111.69
10	G	30	LEU	N-CA-C	-6.07	103.61	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	348	ARG	N-CA-C	6.07	117.90	111.28
1	T	22	DC	C5'-C4'-C3'	-6.07	105.80	114.90
8	E	150	VAL	CA-C-N	6.04	126.23	120.31
8	E	150	VAL	C-N-CA	6.04	126.23	120.31
5	B	112	LEU	N-CA-C	6.03	119.40	110.48
5	B	648	HIS	CA-C-O	6.01	121.43	117.94
4	A	491	VAL	N-CA-C	5.96	113.45	107.55
10	G	56	ILE	CB-CA-C	-5.96	105.81	111.06
12	I	28	GLU	N-CA-C	5.96	115.96	108.45
5	B	911	ILE	N-CA-C	-5.95	107.70	113.53
1	T	12	DA	C5'-C4'-C3'	-5.93	106.01	114.90
10	G	129	SER	N-CA-C	5.93	116.38	108.38
14	K	62	LYS	N-CA-C	5.92	117.41	108.46
10	G	19	GLY	CA-C-N	5.92	127.23	119.84
10	G	19	GLY	C-N-CA	5.92	127.23	119.84
3	P	2	U	C4'-C3'-O3'	-5.90	104.16	113.00
9	F	130	ILE	CA-C-N	5.89	127.20	119.84
9	F	130	ILE	C-N-CA	5.89	127.20	119.84
5	B	523	CYS	CA-C-N	5.88	127.19	119.84
5	B	523	CYS	C-N-CA	5.88	127.19	119.84
4	A	436	ILE	N-CA-C	-5.87	101.22	109.21
5	B	535	LEU	N-CA-C	-5.87	105.95	113.23
4	A	827	THR	N-CA-C	-5.87	105.38	112.54
11	H	130	ARG	N-CA-C	-5.86	106.76	112.97
5	B	292	ILE	N-CA-C	5.85	121.10	112.61
4	A	830	LYS	N-CA-C	-5.82	106.52	113.21
4	A	539	THR	N-CA-C	5.80	118.12	109.25
4	A	1264	GLU	N-CA-C	-5.80	104.96	111.28
4	A	472	LEU	N-CA-C	5.79	117.28	110.97
4	A	1422	ARG	N-CA-C	-5.79	104.92	113.61
10	G	40	GLY	N-CA-C	-5.78	105.19	113.86
4	A	564	ALA	N-CA-C	-5.78	104.95	112.23
4	A	950	GLY	N-CA-C	-5.75	107.45	114.92
5	B	949	VAL	N-CA-C	-5.70	101.54	110.09
4	A	424	ILE	N-CA-C	5.70	121.19	109.34
7	D	173	HIS	CA-C-N	5.69	126.95	119.84
7	D	173	HIS	C-N-CA	5.69	126.95	119.84
14	K	65	HIS	CA-C-N	5.67	126.93	119.84
14	K	65	HIS	C-N-CA	5.67	126.93	119.84
6	C	96	SER	N-CA-C	5.66	117.69	108.76
5	B	805	THR	N-CA-C	5.64	117.54	109.14
10	G	22	MET	N-CA-C	-5.63	105.19	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	75	ILE	N-CA-C	5.63	116.23	108.12
4	A	78	PRO	N-CA-C	-5.62	102.98	111.41
5	B	609	ILE	N-CA-C	-5.61	99.81	107.99
5	B	732	SER	N-CA-C	5.59	116.46	108.74
4	A	507	VAL	CB-CA-C	-5.59	108.39	113.70
4	A	1299	VAL	N-CA-C	5.59	118.18	108.90
4	A	204	THR	N-CA-C	-5.59	104.20	111.02
4	A	468	PHE	N-CA-C	-5.58	99.44	108.41
4	A	999	VAL	N-CA-C	-5.57	106.38	111.67
5	B	1201	LYS	N-CA-C	-5.56	104.23	111.02
4	A	68	GLN	N-CA-C	-5.56	103.78	111.28
4	A	1104	ILE	N-CA-C	5.55	115.75	110.53
5	B	574	SER	CA-C-N	5.53	126.76	119.84
5	B	574	SER	C-N-CA	5.53	126.76	119.84
4	A	227	VAL	N-CA-C	5.53	116.92	111.67
12	I	31	THR	N-CA-C	-5.52	105.65	112.72
4	A	243	PRO	CA-C-N	5.48	126.02	120.38
4	A	243	PRO	C-N-CA	5.48	126.02	120.38
4	A	1404	GLU	N-CA-C	5.48	119.67	113.15
7	D	34	GLN	N-CA-C	-5.47	102.18	110.28
4	A	1268	LEU	N-CA-C	5.46	117.31	111.36
6	C	258	ILE	N-CA-C	-5.46	105.21	110.72
6	C	203	GLN	N-CA-C	-5.45	103.19	110.55
4	A	293	GLU	N-CA-C	-5.44	105.77	112.90
14	K	58	PHE	N-CA-C	5.43	116.66	108.46
6	C	245	VAL	N-CA-C	-5.43	105.55	110.82
5	B	472	ALA	N-CA-C	5.43	117.34	108.55
8	E	149	LEU	N-CA-C	5.43	119.07	112.23
5	B	292	ILE	CB-CA-C	-5.41	108.61	114.35
4	A	682	THR	N-CA-C	-5.41	105.94	112.54
4	A	453	MET	N-CA-C	5.41	118.97	112.38
6	C	183	TRP	N-CA-C	-5.41	97.82	107.98
3	P	3	U	C4'-C3'-O3'	-5.39	104.91	113.00
5	B	1025	HIS	N-CA-C	-5.39	105.30	111.07
9	F	111	LEU	N-CA-C	-5.39	101.39	109.15
6	C	225	ALA	N-CA-C	5.38	116.22	107.23
4	A	1038	THR	N-CA-C	-5.38	102.23	110.14
6	C	57	VAL	N-CA-C	-5.37	105.76	113.07
2	N	7	DG	C2'-C3'-O3'	-5.36	103.45	111.50
4	A	497	THR	N-CA-C	-5.36	105.13	110.97
4	A	729	ALA	N-CA-C	-5.34	105.36	111.07
5	B	66	ASP	N-CA-C	-5.33	104.20	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	808	LEU	N-CA-C	5.30	117.17	110.33
11	H	80	ARG	CA-C-N	5.30	125.84	120.38
11	H	80	ARG	C-N-CA	5.30	125.84	120.38
4	A	750	GLY	N-CA-C	-5.29	107.81	115.27
4	A	64	ASN	N-CA-C	5.29	117.01	108.34
6	C	4	GLU	N-CA-C	5.29	119.65	112.04
4	A	1421	CYS	N-CA-C	-5.28	104.00	111.56
9	F	121	ALA	N-CA-C	-5.28	105.53	111.28
5	B	1151	LEU	N-CA-C	5.27	117.94	111.82
4	A	1010	ALA	N-CA-C	-5.26	105.66	111.71
1	T	17	DG	O4'-C1'-N9	5.26	116.29	108.40
8	E	177	ARG	N-CA-C	5.25	118.55	110.42
14	K	22	ASP	CA-C-N	5.24	125.40	119.90
14	K	22	ASP	C-N-CA	5.24	125.40	119.90
4	A	351	THR	CB-CA-C	-5.23	106.97	114.87
5	B	423	LYS	N-CA-C	-5.23	106.16	112.54
2	N	2	DA	C2'-C3'-O3'	5.22	119.33	111.50
5	B	213	ILE	N-CA-C	5.22	116.09	108.53
4	A	1096	SER	N-CA-C	5.20	116.97	108.76
10	G	145	VAL	N-CA-C	5.20	117.26	109.20
4	A	977	LYS	CA-C-N	5.20	125.65	120.14
4	A	977	LYS	C-N-CA	5.20	125.65	120.14
5	B	363	HIS	N-CA-C	-5.18	103.76	110.19
4	A	87	ALA	N-CA-C	-5.18	105.79	112.68
5	B	277	LYS	N-CA-C	5.17	117.58	111.33
8	E	111	VAL	N-CA-C	5.16	114.72	106.88
11	H	42	ILE	N-CA-C	5.15	115.78	108.42
4	A	1444	MET	N-CA-C	5.14	117.20	109.23
4	A	511	ILE	N-CA-C	5.13	116.47	110.62
4	A	398	GLU	N-CA-C	-5.12	104.11	110.41
4	A	323	LYS	N-CA-C	5.11	117.02	108.23
12	I	65	ASP	CA-C-N	5.10	124.60	119.19
12	I	65	ASP	C-N-CA	5.10	124.60	119.19
4	A	1440	ALA	N-CA-C	-5.10	106.91	112.72
4	A	440	ASP	N-CA-C	-5.09	101.30	109.04
4	A	219	PHE	N-CA-C	-5.08	99.97	110.80
5	B	687	GLU	N-CA-C	-5.06	105.58	112.26
9	F	89	GLU	N-CA-C	-5.05	105.42	111.03
10	G	140	LYS	N-CA-C	5.05	118.54	112.38
8	E	5	ASN	N-CA-C	-5.05	107.07	114.39
5	B	558	LEU	N-CA-C	5.04	116.47	110.97
12	I	85	PHE	N-CA-C	5.04	117.92	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	487	MET	N-CA-C	5.04	116.73	109.07
4	A	445	ASN	N-CA-C	5.03	116.17	108.42
4	A	1155	ASP	CA-C-N	5.03	125.85	120.47
4	A	1155	ASP	C-N-CA	5.03	125.85	120.47
5	B	650	GLU	N-CA-C	5.01	116.68	108.76
5	B	660	LYS	N-CA-C	-5.01	107.17	113.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	82	TYR	Sidechain
13	J	44	TYR	Sidechain
2	N	5	DT	Sidechain
2	N	6	DA	Sidechain
1	T	11	DT	Sidechain
1	T	12	DA	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	336	0	195	46	0
2	N	143	0	80	20	0
3	P	216	0	108	13	0
4	A	11140	0	11217	1389	0
5	B	8810	0	8847	1093	0
6	C	2095	0	2052	269	0
7	D	1427	0	1451	145	0
8	E	1752	0	1776	166	0
9	F	679	0	701	82	0
10	G	1340	0	1357	167	0
11	H	1068	0	1040	136	0
12	I	971	0	930	106	0
13	J	532	0	543	111	0
14	K	919	0	929	121	0
15	L	364	0	388	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	T	3	0	0	1	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31804	0	31614	3579	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 56.

All (3579) 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)
11:H:100:THR:HG23	11:H:138:GLU:HA	1.26	1.16
10:G:138:THR:HG22	10:G:139:ILE:H	1.09	1.12
4:A:53:LEU:HD23	4:A:54:ASN:H	0.99	1.12
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.32	1.11
5:B:510:LYS:HG3	5:B:511:PRO:HD3	1.12	1.11
5:B:273:LEU:HB2	5:B:276:ILE:HD12	1.30	1.09
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.31	1.09
1:T:22:DC:H2"	1:T:23:DC:H5"	1.16	1.08
5:B:792:MET:HE2	5:B:857:ARG:HH12	1.16	1.08
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.37	1.06
4:A:1017:LEU:HB2	8:E:206:GLY:H	1.17	1.05
5:B:806:THR:HG22	5:B:808:ALA:H	1.22	1.03
4:A:855:THR:HG21	4:A:857:ARG:HE	1.17	1.02
12:I:111:THR:HG22	12:I:112:SER:H	1.25	1.02
5:B:882:THR:HG22	5:B:884:ARG:H	1.26	1.01
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.26	1.01
5:B:589:VAL:HG12	5:B:590:HIS:H	1.22	1.01
5:B:172:ILE:HD13	5:B:178:ASN:HB3	1.42	1.01
6:C:116:LYS:HD3	6:C:140:ASN:HB3	1.40	1.00
14:K:47:ARG:HB3	14:K:47:ARG:HH11	1.24	1.00
4:A:828:ALA:CB	5:B:530:GLY:HA2	1.92	1.00
6:C:43:THR:HG22	6:C:44:LEU:H	1.24	1.00
4:A:40:THR:HG22	4:A:41:MET:HG3	1.44	1.00
5:B:918:ILE:HB	5:B:935:ARG:HD2	1.43	0.99
4:A:475:THR:HG23	4:A:476:SER:H	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:22:DC:H2''	1:T:23:DC:C5'	1.92	0.99
4:A:535:THR:HG21	4:A:616:VAL:HA	1.46	0.98
4:A:53:LEU:HD23	4:A:54:ASN:N	1.76	0.98
8:E:19:VAL:O	8:E:23:VAL:HG23	1.63	0.98
5:B:510:LYS:CG	5:B:511:PRO:HD3	1.92	0.98
4:A:1445:ILE:H	4:A:1445:ILE:HD12	1.23	0.98
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.80	0.96
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.45	0.96
6:C:44:LEU:HB2	6:C:77:ILE:HD11	1.48	0.95
5:B:879:ARG:HH11	5:B:883:LEU:HD22	1.29	0.95
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.46	0.95
10:G:7:LEU:HB2	10:G:74:TYR:CE2	2.02	0.95
6:C:166:GLU:HG3	14:K:10:PHE:HZ	1.32	0.95
5:B:365:THR:HG23	5:B:367:LEU:H	1.30	0.94
5:B:233:PRO:HG2	5:B:234:ILE:HD12	1.48	0.94
8:E:94:LYS:HE2	8:E:98:ILE:HD11	1.50	0.94
11:H:4:THR:HA	11:H:60:ALA:HB2	1.49	0.94
13:J:1:MET:H2	13:J:57:ILE:H	1.03	0.94
4:A:779:PHE:HE1	4:A:785:PRO:HD3	1.32	0.93
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.47	0.93
4:A:1189:SER:O	4:A:1241:ARG:HD3	1.67	0.93
6:C:47:ASP:HA	15:L:69:ALA:HB3	1.51	0.93
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.48	0.93
5:B:98:THR:O	5:B:126:SER:HB2	1.69	0.92
4:A:903:ASN:HD22	4:A:904:THR:N	1.68	0.92
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.51	0.91
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.51	0.91
4:A:1004:ASN:ND2	8:E:167:ARG:HD2	1.86	0.91
5:B:579:ARG:HB2	5:B:586:TRP:NE1	1.85	0.91
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.51	0.91
5:B:217:ARG:HE	5:B:405:ARG:HB2	1.33	0.91
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.35	0.91
4:A:829:VAL:HG21	5:B:508:LEU:HD13	1.50	0.90
10:G:1:MET:SD	10:G:79:PHE:HD1	1.93	0.90
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.52	0.90
13:J:64:ASN:HB3	13:J:65:PRO:CD	2.00	0.90
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.52	0.90
5:B:579:ARG:HB2	5:B:586:TRP:HE1	1.35	0.90
6:C:98:VAL:O	6:C:99:LEU:HD23	1.72	0.90
9:F:86:THR:OG1	9:F:89:GLU:HG3	1.72	0.90
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:510:LYS:HG3	5:B:511:PRO:CD	2.02	0.89
1:T:11:DT:H2''	1:T:12:DA:O5'	1.71	0.89
5:B:25:ILE:HD11	5:B:653:VAL:O	1.72	0.89
5:B:594:ALA:HA	5:B:617:ARG:HH12	1.38	0.89
13:J:44:TYR:HA	13:J:47:ARG:HB2	1.53	0.89
4:A:763:ALA:O	4:A:803:SER:HB3	1.72	0.89
3:P:3:U:H4'	4:A:323:LYS:HZ1	1.34	0.89
8:E:22:MET:HE3	8:E:26:ARG:HE	1.35	0.89
13:J:5:VAL:HG12	13:J:6:ARG:HG3	1.53	0.89
14:K:53:ASP:HB3	14:K:56:VAL:HG23	1.53	0.89
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.02	0.89
4:A:709:THR:HG22	4:A:711:ARG:H	1.36	0.89
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.55	0.89
4:A:1116:LEU:N	4:A:1308:THR:HG22	1.88	0.88
6:C:7:GLN:HG2	14:K:104:ASN:HD22	1.38	0.88
4:A:646:PHE:O	4:A:650:GLN:HG3	1.73	0.88
8:E:153:HIS:HB3	8:E:196:VAL:HG11	1.56	0.88
9:F:93:ILE:HD11	9:F:134:ILE:HD11	1.56	0.88
15:L:32:ALA:HB3	15:L:55:ILE:HD12	1.54	0.88
5:B:879:ARG:NH1	5:B:883:LEU:HD22	1.87	0.88
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.74	0.88
10:G:13:LEU:HD21	10:G:17:PHE:HB2	1.55	0.88
4:A:356:ASP:HB2	4:A:469:ARG:NH1	1.89	0.88
4:A:366:VAL:HG21	4:A:460:VAL:HG22	1.56	0.88
4:A:55:ASP:C	4:A:57:ARG:H	1.81	0.88
4:A:901:LEU:H	4:A:926:GLN:NE2	1.72	0.88
6:C:133:ILE:HD11	6:C:237:SER:HA	1.54	0.88
5:B:211:VAL:O	5:B:480:SER:HA	1.73	0.87
5:B:1166:CYS:HB2	5:B:1215:ARG:NH1	1.90	0.87
1:T:24:DT:H2''	1:T:25:DC:O5'	1.74	0.87
8:E:14:ARG:HH21	8:E:141:VAL:HG12	1.37	0.87
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	1.57	0.87
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.55	0.87
4:A:49:LYS:NZ	4:A:61:ILE:HG13	1.89	0.87
5:B:1159:ARG:HB3	5:B:1159:ARG:NH1	1.89	0.87
4:A:321:PRO:O	4:A:322:VAL:HB	1.73	0.87
4:A:225:ASN:HD22	4:A:228:PHE:H	1.23	0.86
6:C:57:VAL:HG11	13:J:60:PHE:HB3	1.54	0.86
4:A:115:LEU:HB2	4:A:122:MET:HE2	1.57	0.86
10:G:127:PRO:HG2	10:G:138:THR:HG21	1.58	0.86
5:B:1165:ILE:HG22	5:B:1166:CYS:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:441:PRO:HD2	4:A:498:ARG:NH2	1.90	0.86
9:F:82:THR:HG22	9:F:84:TYR:H	1.36	0.86
4:A:754:SER:H	4:A:757:ASN:HD22	1.23	0.86
5:B:594:ALA:HA	5:B:617:ARG:NH1	1.89	0.86
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.39	0.86
8:E:177:ARG:HD3	8:E:215:MET:HG3	1.57	0.86
4:A:427:GLN:HG3	4:A:430:TRP:CZ2	2.11	0.85
4:A:537:ARG:HD2	11:H:20:TYR:HE1	1.39	0.85
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.56	0.85
9:F:111:LEU:HD12	9:F:111:LEU:H	1.41	0.85
5:B:467:GLY:H	5:B:475:SER:HB3	1.40	0.85
5:B:516:ASN:HD22	5:B:516:ASN:N	1.74	0.85
5:B:199:MET:HE2	5:B:492:LEU:HD23	1.58	0.85
5:B:563:MET:HE3	5:B:580:VAL:HB	1.59	0.84
10:G:18:PHE:HA	10:G:22:MET:CE	2.07	0.84
5:B:798:TYR:HE2	6:C:62:PHE:CE2	1.95	0.84
1:T:22:DC:C2'	1:T:23:DC:H5''	2.06	0.84
2:N:6:DA:H2''	2:N:7:DG:OP2	1.76	0.84
4:A:249:SER:O	4:A:250:ILE:HG13	1.76	0.84
6:C:32:SER:O	6:C:36:VAL:HG23	1.78	0.84
4:A:567:LYS:HB3	11:H:96:VAL:H	1.43	0.84
4:A:1283:VAL:HG12	4:A:1284:MET:H	1.42	0.83
11:H:4:THR:HA	11:H:60:ALA:CB	2.08	0.83
5:B:1224:PHE:HE2	8:E:171:LYS:HG3	1.43	0.83
5:B:1065:GLN:HE21	5:B:1067:ARG:N	1.75	0.83
10:G:23:LYS:HG3	10:G:56:ILE:HD11	1.61	0.83
10:G:34:VAL:HG12	10:G:45:ILE:HG21	1.60	0.83
11:H:42:ILE:HG23	11:H:95:TYR:HE1	1.40	0.83
5:B:1180:PHE:HB3	5:B:1191:ILE:HD12	1.61	0.83
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.60	0.83
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.61	0.83
7:D:48:ILE:HG21	10:G:4:ILE:HB	1.60	0.83
1:T:18:DC:H2''	1:T:19:DC:O5'	1.79	0.83
8:E:117:THR:HG22	8:E:119:SER:H	1.44	0.83
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.61	0.83
11:H:130:ARG:H	11:H:130:ARG:HD2	1.44	0.83
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.61	0.83
9:F:111:LEU:C	9:F:113:GLY:H	1.86	0.82
11:H:100:THR:OG1	11:H:138:GLU:HG3	1.78	0.82
4:A:809:THR:HG23	4:A:812:GLU:OE1	1.78	0.82
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:860:LEU:HD11	4:A:1393:ASN:HB2	1.59	0.82
4:A:56:PRO:O	4:A:57:ARG:HG3	1.80	0.82
10:G:14:HIS:ND1	10:G:15:PRO:HD2	1.94	0.82
8:E:16:PHE:CZ	8:E:20:LYS:HE2	2.14	0.82
1:T:20:DC:H2''	1:T:21:DT:O5'	1.80	0.82
4:A:1017:LEU:HB2	8:E:206:GLY:N	1.95	0.82
5:B:613:VAL:HG13	5:B:627:PHE:O	1.79	0.82
7:D:144:THR:O	7:D:148:LEU:HB2	1.79	0.82
13:J:12:LYS:O	13:J:14:VAL:HG23	1.79	0.82
4:A:70:CYS:O	4:A:72:GLU:HG2	1.79	0.82
4:A:743:VAL:O	4:A:747:VAL:HG23	1.79	0.82
5:B:801:LYS:O	13:J:52:THR:HG23	1.78	0.82
11:H:93:TYR:HB3	11:H:144:ILE:O	1.80	0.82
4:A:23:SER:HA	4:A:233:TRP:NE1	1.94	0.82
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.15	0.82
5:B:23:ALA:HB1	5:B:24:PRO:HD2	1.62	0.82
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.62	0.82
1:T:25:DC:H2''	1:T:26:DA:O5'	1.79	0.81
4:A:1127:ASP:HB3	4:A:1130:GLN:CB	2.09	0.81
13:J:57:ILE:HA	13:J:60:PHE:HD2	1.43	0.81
4:A:567:LYS:CD	4:A:568:PRO:HD2	2.11	0.81
10:G:18:PHE:HA	10:G:22:MET:HE3	1.61	0.81
5:B:821:GLN:HE22	5:B:851:PHE:HA	1.45	0.81
4:A:1076:ALA:HA	4:A:1079:MET:HE2	1.64	0.80
10:G:79:PHE:HZ	10:G:106:MET:HE2	1.44	0.80
4:A:886:ILE:HG22	4:A:887:GLY:N	1.95	0.80
5:B:53:GLN:HG2	5:B:547:VAL:HG22	1.61	0.80
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.60	0.80
6:C:6:PRO:HB3	6:C:25:VAL:HG12	1.64	0.80
5:B:563:MET:CE	5:B:580:VAL:HB	2.11	0.80
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.63	0.80
8:E:202:SER:OG	8:E:204:THR:HG22	1.81	0.80
4:A:858:ASN:ND2	4:A:860:LEU:H	1.80	0.80
5:B:710:LEU:HA	5:B:733:HIS:HB3	1.64	0.80
11:H:102:TYR:OH	11:H:122:LEU:HD22	1.81	0.80
6:C:172:PRO:O	6:C:235:VAL:HG23	1.81	0.80
5:B:244:LEU:HD21	5:B:366:GLN:NE2	1.97	0.80
11:H:59:ILE:HG22	11:H:60:ALA:N	1.97	0.80
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.46	0.80
4:A:598:LEU:HA	11:H:122:LEU:HD13	1.64	0.79
6:C:43:THR:HG22	6:C:44:LEU:N	1.93	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:35:LEU:HD23	7:D:174:PRO:HD2	1.65	0.79
4:A:524:VAL:HG12	4:A:525:GLN:H	1.47	0.79
5:B:782:LEU:HD12	5:B:788:ARG:HH11	1.46	0.79
3:P:3:U:H2'	3:P:4:G:C8	2.17	0.79
5:B:792:MET:HE2	5:B:857:ARG:NH1	1.96	0.79
4:A:534:LEU:O	4:A:574:GLY:HA3	1.82	0.79
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.63	0.79
10:G:81:PRO:HG3	10:G:106:MET:SD	2.23	0.79
4:A:475:THR:HG23	4:A:476:SER:N	1.96	0.79
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.64	0.79
12:I:55:THR:HG21	12:I:109:ILE:HD13	1.65	0.79
4:A:265:LYS:HD2	4:A:265:LYS:H	1.47	0.79
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.48	0.79
5:B:847:ASP:HB3	6:C:167:HIS:NE2	1.98	0.79
5:B:859:TYR:OH	5:B:941:LEU:HD12	1.83	0.78
4:A:741:ASN:HD22	4:A:744:LYS:H	1.31	0.78
5:B:882:THR:CG2	5:B:884:ARG:HB2	2.12	0.78
4:A:866:PHE:C	4:A:867:ILE:HD12	2.07	0.78
5:B:125:SER:HA	5:B:171:PRO:HA	1.63	0.78
5:B:549:THR:HG22	5:B:550:ASP:H	1.46	0.78
1:T:11:DT:H2''	1:T:12:DA:C5'	2.12	0.78
10:G:122:ASN:ND2	10:G:125:SER:HB3	1.98	0.78
12:I:85:PHE:H	12:I:85:PHE:HD2	1.27	0.78
4:A:341:MET:HE1	5:B:1135:ARG:NH1	1.99	0.78
7:D:40:HIS:CB	10:G:73:LYS:HZ2	1.96	0.78
7:D:49:ALA:HB2	7:D:174:PRO:HB3	1.66	0.78
8:E:213:ILE:HG12	8:E:214:CYS:H	1.47	0.78
14:K:45:LEU:HG	14:K:94:ILE:HD13	1.63	0.78
5:B:953:LEU:HD21	5:B:965:LYS:HB2	1.65	0.78
4:A:55:ASP:CG	4:A:55:ASP:O	2.22	0.78
5:B:35:SER:HA	5:B:811:TYR:HE2	1.46	0.78
8:E:135:PHE:HB3	8:E:140:LEU:HD11	1.64	0.78
4:A:670:ILE:HG23	4:A:805:LEU:HD21	1.64	0.78
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.64	0.78
7:D:40:HIS:CB	10:G:73:LYS:NZ	2.47	0.78
14:K:65:HIS:CD2	14:K:67:PHE:H	2.01	0.78
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.64	0.78
5:B:217:ARG:NE	5:B:405:ARG:HB2	1.99	0.78
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.66	0.78
7:D:189:ASP:O	7:D:193:THR:HB	1.84	0.78
4:A:446:ARG:CD	4:A:480:ALA:HB2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.66	0.77
13:J:1:MET:N	13:J:57:ILE:H	1.81	0.77
4:A:53:LEU:CD2	4:A:54:ASN:H	1.91	0.77
5:B:520:GLY:H	5:B:748:ILE:HG22	1.49	0.77
5:B:603:LEU:HD13	5:B:608:ASP:HB2	1.65	0.77
7:D:17:LYS:HE2	7:D:17:LYS:N	1.99	0.77
10:G:138:THR:HG22	10:G:139:ILE:N	1.91	0.77
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.19	0.77
14:K:47:ARG:HB3	14:K:47:ARG:NH1	1.99	0.77
5:B:789:MET:HE2	5:B:953:LEU:HD22	1.65	0.77
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.18	0.77
4:A:885:THR:O	4:A:940:ARG:HD2	1.84	0.77
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.65	0.77
8:E:179:GLN:HB2	8:E:182:ASP:HB2	1.67	0.77
12:I:75:CYS:HG	12:I:78:CYS:HG	1.32	0.77
4:A:1420:ASP:HB3	4:A:1422:ARG:HG3	1.65	0.77
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.66	0.77
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.67	0.77
10:G:15:PRO:HA	10:G:18:PHE:CD1	2.19	0.77
10:G:80:LYS:HD3	10:G:80:LYS:N	1.98	0.77
5:B:1085:ILE:N	5:B:1085:ILE:HD12	1.99	0.77
13:J:1:MET:N	13:J:56:LEU:N	2.33	0.77
4:A:49:LYS:HZ1	4:A:61:ILE:HG13	1.48	0.77
8:E:22:MET:HE3	8:E:26:ARG:NE	1.98	0.77
13:J:3:VAL:HG21	13:J:18:TRP:HB2	1.65	0.77
4:A:718:VAL:O	4:A:722:LEU:HD12	1.85	0.77
5:B:978:ASP:OD2	5:B:1098:MET:HG2	1.84	0.77
4:A:746:MET:HE3	5:B:1018:PRO:HG2	1.65	0.76
4:A:853:ASP:O	4:A:854:ASN:HB2	1.85	0.76
5:B:1065:GLN:HE21	5:B:1067:ARG:H	1.30	0.76
10:G:80:LYS:HD3	10:G:80:LYS:H	1.50	0.76
13:J:16:ASP:OD1	13:J:17:LYS:HD2	1.84	0.76
4:A:709:THR:HG23	12:I:94:ASP:HA	1.68	0.76
14:K:113:THR:O	14:K:114:LEU:HB2	1.83	0.76
5:B:996:ARG:NH2	6:C:175:ALA:H	1.84	0.76
6:C:66:ARG:NH1	13:J:2:ILE:HG21	2.00	0.76
9:F:103:MET:O	9:F:104:ASN:HB2	1.84	0.76
4:A:496:GLU:HG2	9:F:99:LEU:HD23	1.67	0.76
4:A:1208:THR:HG22	4:A:1210:GLY:H	1.51	0.76
5:B:1162:ILE:HD11	5:B:1194:ILE:HD13	1.66	0.76
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:705:MET:H	5:B:710:LEU:HD12	1.51	0.76
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.15	0.76
4:A:414:ASP:OD1	4:A:416:ARG:HG2	1.86	0.76
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.51	0.76
5:B:467:GLY:N	5:B:475:SER:HB3	2.01	0.76
5:B:957:ASN:HD22	5:B:961:LEU:HD12	1.49	0.76
8:E:2:ASP:O	8:E:3:GLN:HG2	1.84	0.76
8:E:180:ARG:HH21	8:E:192:ARG:HB2	1.51	0.76
11:H:38:LEU:HD12	11:H:124:ARG:O	1.85	0.76
11:H:89:LEU:HB3	11:H:91:ASP:OD1	1.86	0.76
4:A:849:MET:HE3	4:A:1061:GLY:HA2	1.66	0.76
5:B:309:GLN:OE1	12:I:52:ILE:HD11	1.86	0.76
4:A:1341:ILE:HD12	4:A:1379:GLY:O	1.86	0.75
4:A:1424:VAL:HG13	4:A:1436:ILE:CD1	2.17	0.75
9:F:90:ARG:HD3	9:F:155:LEU:HD12	1.67	0.75
5:B:278:GLN:HG2	5:B:279:ASP:H	1.49	0.75
5:B:800:GLN:HB3	13:J:52:THR:HG21	1.66	0.75
5:B:882:THR:HG22	5:B:884:ARG:N	1.98	0.75
4:A:590:ARG:HH21	4:A:620:LYS:CB	1.99	0.75
6:C:239:PRO:HB2	6:C:241:ASP:OD1	1.87	0.75
10:G:43:GLY:HA3	10:G:80:LYS:HB3	1.69	0.75
12:I:8:ARG:HG3	12:I:34:TYR:HE1	1.52	0.75
5:B:806:THR:HG22	5:B:808:ALA:N	2.01	0.75
8:E:14:ARG:HH21	8:E:141:VAL:CG1	1.99	0.75
13:J:44:TYR:H	13:J:44:TYR:HD2	1.34	0.75
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.67	0.75
5:B:363:HIS:O	5:B:364:ILE:HB	1.84	0.75
6:C:33:LEU:HG	6:C:37:MET:HE2	1.69	0.75
14:K:7:PHE:HA	14:K:10:PHE:CE2	2.22	0.75
4:A:466:SER:O	5:B:1103:ILE:HD11	1.86	0.74
4:A:537:ARG:HD2	11:H:20:TYR:CE1	2.21	0.74
5:B:758:PHE:HB3	5:B:761:HIS:HD2	1.52	0.74
11:H:83:GLN:C	11:H:85:GLY:H	1.92	0.74
12:I:111:THR:HG22	12:I:112:SER:N	2.02	0.74
3:P:3:U:H2'	3:P:4:G:H8	1.50	0.74
6:C:7:GLN:HG2	14:K:104:ASN:ND2	2.03	0.74
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	1.86	0.74
5:B:1072:MET:CE	5:B:1085:ILE:HB	2.18	0.74
6:C:147:LEU:HB2	6:C:151:GLN:HB2	1.69	0.74
14:K:65:HIS:HD2	14:K:67:PHE:H	1.36	0.74
4:A:341:MET:HE2	4:A:843:LYS:HZ1	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.17	0.74
4:A:1341:ILE:HG23	4:A:1342:GLU:N	2.01	0.74
5:B:1152:MET:CE	5:B:1157:ALA:HA	2.18	0.74
4:A:1279:ILE:HD11	4:A:1316:VAL:CG2	2.17	0.74
5:B:214:ALA:HB3	5:B:498:THR:HA	1.69	0.74
5:B:1182:CYS:O	5:B:1182:CYS:SG	2.45	0.74
6:C:5:GLY:O	6:C:7:GLN:HG3	1.88	0.74
7:D:12:ARG:NH2	7:D:12:ARG:HB3	2.03	0.74
5:B:637:LEU:HD12	5:B:693:ILE:HD12	1.68	0.74
4:A:185:TRP:CZ3	4:A:200:ARG:HG2	2.22	0.74
5:B:542:MET:HE2	5:B:743:ILE:HG13	1.69	0.74
5:B:971:THR:OG1	6:C:61:GLU:HG3	1.88	0.74
7:D:52:LEU:HD21	7:D:147:TYR:HE2	1.52	0.74
11:H:23:VAL:HG22	11:H:43:ASN:HA	1.70	0.74
11:H:89:LEU:C	11:H:91:ASP:H	1.96	0.74
13:J:8:PHE:H	13:J:49:MET:HE3	1.52	0.74
4:A:19:PHE:O	4:A:1416:ALA:HA	1.86	0.74
4:A:311:GLN:O	4:A:312:PRO:C	2.31	0.74
4:A:528:LEU:O	4:A:531:ILE:HG22	1.88	0.74
4:A:1004:ASN:O	4:A:1008:GLN:HB2	1.87	0.74
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.87	0.74
4:A:808:LEU:HD23	4:A:813:PHE:HA	1.70	0.73
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.22	0.73
4:A:855:THR:HG21	4:A:857:ARG:NE	2.00	0.73
4:A:982:THR:HB	4:A:985:ASP:H	1.53	0.73
4:A:1444:MET:HG2	10:G:60:ARG:HA	1.70	0.73
5:B:770:GLN:CD	5:B:983:ARG:HA	2.13	0.73
7:D:9:GLN:HE21	7:D:38:ILE:HD12	1.53	0.73
4:A:288:ALA:HA	4:A:291:GLU:OE2	1.89	0.73
4:A:567:LYS:HB3	11:H:95:TYR:HA	1.70	0.73
5:B:273:LEU:CB	5:B:276:ILE:HD12	2.16	0.73
4:A:164:ARG:HG3	4:A:165:GLY:N	2.03	0.73
4:A:518:LYS:HE2	4:A:624:SER:O	1.88	0.73
4:A:682:THR:HG23	4:A:728:LYS:HE3	1.70	0.73
5:B:1077:THR:HG22	14:K:44:ASN:ND2	2.03	0.73
5:B:1077:THR:HG22	14:K:44:ASN:HD21	1.52	0.73
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.70	0.73
5:B:1065:GLN:NE2	5:B:1067:ARG:HG2	2.03	0.73
5:B:642:ASP:HA	5:B:649:LYS:HA	1.68	0.73
4:A:283:GLY:O	4:A:285:PRO:HD3	1.88	0.73
4:A:351:THR:HB	5:B:1103:ILE:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.69	0.73
4:A:960:ILE:HA	4:A:963:ILE:HG22	1.69	0.73
4:A:628:GLY:O	4:A:632:VAL:HG23	1.88	0.73
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.70	0.73
7:D:12:ARG:HB3	7:D:12:ARG:HH21	1.53	0.73
13:J:43:ARG:HG3	13:J:45:CYS:SG	2.28	0.73
8:E:153:HIS:HB3	8:E:196:VAL:CG1	2.18	0.73
6:C:194:GLU:O	6:C:195:GLN:HG3	1.87	0.73
7:D:56:ARG:HB2	7:D:148:LEU:HD22	1.69	0.73
4:A:963:ILE:HD11	4:A:1048:ASN:CB	2.19	0.72
5:B:603:LEU:HB3	5:B:609:ILE:HD11	1.70	0.72
5:B:175:ARG:HG2	5:B:175:ARG:HH11	1.53	0.72
5:B:435:THR:C	5:B:437:GLU:H	1.97	0.72
6:C:262:LEU:HD11	14:K:87:LEU:HD23	1.71	0.72
3:P:10:G:H4'	4:A:485:ASP:OD1	1.89	0.72
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.24	0.72
5:B:798:TYR:HE2	6:C:62:PHE:CZ	2.07	0.72
6:C:47:ASP:HA	15:L:69:ALA:CB	2.17	0.72
4:A:446:ARG:HD3	4:A:480:ALA:HB2	1.71	0.72
5:B:190:TYR:CE2	13:J:62:ARG:HB3	2.24	0.72
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.70	0.72
5:B:737:THR:HG21	12:I:66:PRO:HA	1.71	0.72
5:B:1201:LYS:HE2	5:B:1205:GLN:OE1	1.89	0.72
7:D:130:LEU:C	7:D:132:GLN:H	1.97	0.72
11:H:81:PRO:CB	11:H:82:PRO:HD2	2.19	0.72
4:A:794:PRO:HG2	4:A:795:GLU:OE2	1.89	0.72
11:H:40:LEU:HD13	11:H:123:MET:HE3	1.70	0.72
4:A:590:ARG:NH2	4:A:620:LYS:HB3	2.05	0.72
5:B:911:ILE:HD11	5:B:941:LEU:HD13	1.70	0.72
7:D:18:VAL:O	7:D:19:GLU:HB2	1.89	0.72
5:B:791:THR:HG22	5:B:858:SER:O	1.88	0.72
6:C:212:PRO:HB3	6:C:213:PRO:HD2	1.70	0.72
4:A:50:ILE:C	4:A:52:GLY:H	1.96	0.72
5:B:613:VAL:HG22	5:B:628:THR:HA	1.70	0.72
5:B:810:GLU:HA	5:B:815:ARG:HH12	1.53	0.72
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.72	0.71
5:B:542:MET:CE	5:B:743:ILE:HG13	2.20	0.71
5:B:957:ASN:O	5:B:959:ASP:N	2.23	0.71
5:B:1001:PHE:CE1	5:B:1073:TYR:HB2	2.25	0.71
7:D:170:THR:CG2	7:D:172:LEU:HG	2.20	0.71
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:124:VAL:HG13	8:E:132:ILE:HB	1.71	0.71
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.70	0.71
5:B:980:PHE:HE1	5:B:990:ILE:HD11	1.53	0.71
3:P:8:A:O2'	3:P:9:G:H5'	1.91	0.71
4:A:798:GLY:HA2	4:A:815:PHE:CD1	2.25	0.71
1:T:16:DG:H4'	4:A:1403:GLU:OE2	1.91	0.71
4:A:34:LYS:HG2	4:A:36:ARG:HH21	1.54	0.71
4:A:244:PRO:HG2	4:A:245:PRO:HD3	1.71	0.71
4:A:1118:VAL:HG12	4:A:1327:ILE:HG13	1.73	0.71
5:B:996:ARG:HH22	6:C:175:ALA:H	1.35	0.71
7:D:35:LEU:H	7:D:35:LEU:HD12	1.55	0.71
1:T:23:DC:H2'	1:T:24:DT:C6	2.26	0.71
4:A:446:ARG:HB2	4:A:487:MET:SD	2.31	0.71
5:B:284:ILE:HD13	5:B:333:PHE:HD2	1.56	0.71
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.26	0.71
7:D:134:THR:HG22	7:D:135:GLY:N	2.06	0.71
11:H:81:PRO:HB2	11:H:82:PRO:HD2	1.71	0.71
13:J:64:ASN:HB3	13:J:65:PRO:HD3	1.71	0.71
13:J:64:ASN:HD22	13:J:65:PRO:HD3	1.54	0.71
4:A:164:ARG:HG3	4:A:165:GLY:H	1.56	0.71
5:B:295:GLY:H	5:B:298:LEU:HD23	1.55	0.71
5:B:515:HIS:H	5:B:518:HIS:CD2	2.09	0.71
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.73	0.71
10:G:115:MET:HB2	10:G:116:PRO:HD2	1.72	0.71
4:A:1279:ILE:HD11	4:A:1316:VAL:HG21	1.72	0.70
5:B:653:VAL:CG2	5:B:689:LEU:HB3	2.21	0.70
11:H:55:LEU:HD22	11:H:144:ILE:CG2	2.21	0.70
4:A:265:LYS:HD2	4:A:265:LYS:N	2.04	0.70
5:B:221:ASN:N	5:B:241:ARG:O	2.24	0.70
5:B:393:LYS:HA	5:B:393:LYS:HE3	1.71	0.70
6:C:36:VAL:HG21	6:C:251:LEU:HD22	1.72	0.70
9:F:97:ARG:O	9:F:101:ILE:HG13	1.91	0.70
10:G:143:ILE:HG22	10:G:144:ARG:N	2.06	0.70
11:H:15:VAL:HG22	11:H:26:ILE:HD11	1.73	0.70
4:A:450:LEU:H	4:A:450:LEU:HD12	1.55	0.70
4:A:666:ILE:HD12	4:A:667:GLY:H	1.57	0.70
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.74	0.70
5:B:168:GLY:H	5:B:450:ALA:HB1	1.56	0.70
7:D:9:GLN:NE2	7:D:38:ILE:HD12	2.07	0.70
7:D:170:THR:HG21	7:D:172:LEU:HG	1.73	0.70
4:A:68:GLN:C	4:A:70:CYS:H	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.73	0.70
4:A:590:ARG:HH21	4:A:620:LYS:HB2	1.55	0.70
4:A:351:THR:HB	5:B:1103:ILE:CD1	2.22	0.70
5:B:977:GLY:HA3	5:B:1099:VAL:HB	1.74	0.70
6:C:145:CYS:HA	13:J:2:ILE:HD11	1.73	0.70
6:C:179:GLU:HG2	6:C:180:TYR:N	2.07	0.70
9:F:82:THR:HG22	9:F:84:TYR:N	2.06	0.70
10:G:1:MET:SD	10:G:79:PHE:CD1	2.83	0.70
13:J:3:VAL:HG21	13:J:18:TRP:CB	2.22	0.70
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.22	0.70
4:A:981:LEU:HD21	4:A:1039:LYS:HA	1.73	0.70
10:G:145:VAL:HG12	10:G:146:LYS:N	2.05	0.70
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.55	0.70
4:A:567:LYS:NZ	11:H:46:LEU:HB2	2.07	0.70
4:A:714:PHE:HB2	12:I:97:MET:HE1	1.73	0.70
4:A:853:ASP:OD1	4:A:855:THR:HB	1.90	0.70
4:A:1283:VAL:HG12	4:A:1284:MET:N	2.07	0.70
4:A:1349:TYR:HB2	4:A:1372:VAL:HG21	1.74	0.70
5:B:1165:ILE:HG22	5:B:1166:CYS:H	1.57	0.70
13:J:1:MET:H1	13:J:56:LEU:N	1.90	0.70
14:K:12:LEU:H	14:K:12:LEU:HD12	1.57	0.70
4:A:92:HIS:O	4:A:94:GLY:N	2.25	0.69
4:A:1111:MET:HE2	4:A:1330:ASN:OD1	1.92	0.69
6:C:114:TYR:HB3	6:C:140:ASN:O	1.92	0.69
7:D:7:THR:HB	10:G:42:PHE:CZ	2.26	0.69
5:B:616:ILE:HD12	5:B:616:ILE:N	2.07	0.69
5:B:798:TYR:CE2	6:C:62:PHE:CE2	2.81	0.69
5:B:1097:HIS:H	5:B:1098:MET:HE2	1.55	0.69
6:C:209:TYR:HD1	6:C:209:TYR:H	1.39	0.69
11:H:111:LEU:HD23	11:H:127:GLY:O	1.93	0.69
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.28	0.69
4:A:590:ARG:NH2	4:A:620:LYS:CB	2.55	0.69
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.04	0.69
4:A:1373:ASP:HA	4:A:1376:THR:HG22	1.75	0.69
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.74	0.69
15:L:27:LEU:HD13	15:L:37:LYS:HE2	1.74	0.69
4:A:1329:THR:CG2	4:A:1331:SER:H	2.04	0.69
6:C:179:GLU:HG2	6:C:180:TYR:H	1.56	0.69
10:G:138:THR:CG2	10:G:139:ILE:H	1.92	0.69
4:A:855:THR:CG2	4:A:857:ARG:HE	2.01	0.69
4:A:1332:PHE:H	4:A:1332:PHE:HD2	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.57	0.69
4:A:416:ARG:C	4:A:417:TYR:HD2	2.00	0.69
5:B:950:ASP:O	5:B:951:GLN:HB2	1.91	0.69
6:C:66:ARG:HH21	13:J:5:VAL:HG23	1.57	0.69
4:A:567:LYS:HB3	11:H:96:VAL:N	2.07	0.69
4:A:567:LYS:HD3	11:H:95:TYR:CD2	2.27	0.69
4:A:567:LYS:HD2	4:A:568:PRO:HD2	1.74	0.69
5:B:411:PRO:O	5:B:414:ALA:HB3	1.93	0.69
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.75	0.69
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.74	0.69
7:D:7:THR:HB	10:G:42:PHE:CE2	2.28	0.69
11:H:4:THR:CA	11:H:60:ALA:HB2	2.22	0.69
14:K:47:ARG:HH11	14:K:47:ARG:CB	2.04	0.69
5:B:515:HIS:H	5:B:518:HIS:HD2	1.40	0.69
4:A:407:ARG:HB3	4:A:430:TRP:CE2	2.28	0.69
5:B:852:ARG:NH2	15:L:70:ARG:OXT	2.23	0.69
5:B:957:ASN:ND2	5:B:961:LEU:HD12	2.08	0.69
5:B:975:GLN:O	5:B:990:ILE:HD12	1.93	0.69
4:A:809:THR:H	4:A:812:GLU:HB2	1.58	0.68
4:A:1394:THR:HG21	4:A:1398:MET:SD	2.34	0.68
6:C:213:PRO:O	6:C:214:ASN:HB2	1.90	0.68
7:D:40:HIS:CE1	7:D:41:GLN:HG3	2.29	0.68
7:D:130:LEU:O	7:D:132:GLN:N	2.25	0.68
9:F:72:LYS:HD2	9:F:142:SER:HB3	1.75	0.68
4:A:7:SER:HB3	5:B:1193:GLN:NE2	2.08	0.68
4:A:679:ILE:HG12	4:A:732:LEU:HD12	1.75	0.68
5:B:1180:PHE:HB3	5:B:1191:ILE:CD1	2.23	0.68
6:C:244:VAL:O	6:C:248:ILE:HG13	1.94	0.68
4:A:913:LEU:HD12	4:A:914:GLU:H	1.58	0.68
5:B:882:THR:HB	5:B:934:LYS:O	1.94	0.68
6:C:226:ASP:O	6:C:227:THR:HB	1.92	0.68
14:K:63:VAL:HG23	14:K:63:VAL:O	1.94	0.68
4:A:463:ILE:CD1	4:A:469:ARG:HG3	2.23	0.68
4:A:546:VAL:O	4:A:550:LEU:HG	1.94	0.68
4:A:567:LYS:CB	11:H:95:TYR:HA	2.24	0.68
5:B:44:VAL:HG11	5:B:199:MET:HG2	1.74	0.68
5:B:745:PRO:O	5:B:748:ILE:HG12	1.93	0.68
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.75	0.68
5:B:1095:LEU:H	5:B:1095:LEU:HD12	1.58	0.68
6:C:164:ALA:HA	6:C:167:HIS:O	1.93	0.68
7:D:153:ARG:HB3	7:D:154:PHE:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:49:LEU:HG	10:G:76:ALA:HA	1.75	0.68
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.74	0.68
4:A:341:MET:HE2	4:A:843:LYS:NZ	2.07	0.68
5:B:542:MET:HG2	5:B:747:MET:HB3	1.74	0.68
5:B:603:LEU:HB3	5:B:609:ILE:CD1	2.23	0.68
5:B:642:ASP:O	5:B:644:GLU:N	2.26	0.68
7:D:53:SER:HB3	7:D:152:SER:CB	2.24	0.68
4:A:751:SER:O	4:A:752:LYS:HG2	1.94	0.68
10:G:35:GLU:OE2	10:G:48:VAL:HG23	1.94	0.68
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.19	0.68
4:A:475:THR:CG2	4:A:476:SER:H	2.03	0.68
4:A:524:VAL:HG12	4:A:525:GLN:N	2.08	0.68
4:A:1066:VAL:O	4:A:1070:GLN:HG3	1.94	0.68
11:H:17:PRO:HB3	11:H:24:CYS:SG	2.34	0.68
4:A:106:VAL:HG13	4:A:112:LYS:O	1.94	0.68
12:I:34:TYR:CD2	12:I:35:VAL:N	2.62	0.68
4:A:117:GLU:H	4:A:117:GLU:CD	2.01	0.67
5:B:658:ILE:HG22	5:B:662:MET:HE2	1.76	0.67
8:E:78:LEU:HD21	8:E:80:VAL:HG23	1.74	0.67
11:H:59:ILE:HG22	11:H:60:ALA:H	1.59	0.67
4:A:107:CYS:N	4:A:114:LEU:HD21	2.09	0.67
4:A:591:PHE:HA	4:A:595:THR:HG21	1.74	0.67
4:A:901:LEU:O	4:A:921:GLY:N	2.28	0.67
4:A:1438:THR:HB	5:B:1144:ALA:CB	2.19	0.67
5:B:254:LEU:HD23	5:B:381:MET:HE1	1.76	0.67
12:I:54:GLU:HB3	12:I:100:PHE:HE2	1.58	0.67
4:A:673:GLY:O	4:A:676:MET:HB2	1.95	0.67
5:B:65:GLU:HG3	5:B:66:ASP:H	1.59	0.67
5:B:184:ALA:HB1	5:B:188:ASP:HB3	1.76	0.67
5:B:516:ASN:HD22	5:B:516:ASN:H	1.39	0.67
5:B:693:ILE:HD13	5:B:701:ILE:HD13	1.76	0.67
5:B:705:MET:H	5:B:710:LEU:CD1	2.07	0.67
5:B:1166:CYS:HB2	5:B:1215:ARG:HH12	1.57	0.67
6:C:146:LYS:C	6:C:147:LEU:HD23	2.20	0.67
8:E:90:VAL:HG23	8:E:120:ALA:HA	1.76	0.67
8:E:198:ILE:HD11	8:E:212:ARG:HG3	1.75	0.67
15:L:32:ALA:HB3	15:L:55:ILE:CD1	2.21	0.67
4:A:107:CYS:SG	4:A:171:GLN:HG2	2.35	0.67
4:A:381:THR:HG23	4:A:383:TYR:H	1.59	0.67
4:A:1293:SER:OG	4:A:1294:PRO:HD2	1.94	0.67
4:A:1333:ILE:O	4:A:1337:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:CE1	5:B:1027:ILE:HG22	2.30	0.67
8:E:180:ARG:NH2	8:E:192:ARG:HB2	2.08	0.67
4:A:675:THR:O	4:A:679:ILE:HG13	1.95	0.67
4:A:1325:THR:O	8:E:148:GLU:HB2	1.94	0.67
5:B:800:GLN:HB3	13:J:52:THR:CG2	2.24	0.67
9:F:132:LEU:O	9:F:148:VAL:HG22	1.95	0.67
13:J:23:ASN:C	13:J:25:LEU:H	2.01	0.67
14:K:21:ILE:HG12	14:K:33:ILE:HG12	1.77	0.67
14:K:50:LEU:HD11	14:K:75:ILE:HD13	1.77	0.67
4:A:535:THR:CG2	4:A:616:VAL:HA	2.22	0.67
4:A:1299:VAL:HG12	4:A:1300:LYS:N	2.10	0.67
4:A:1324:PRO:HB2	8:E:142:VAL:HG11	1.76	0.67
5:B:199:MET:HE2	5:B:492:LEU:CD2	2.25	0.67
4:A:172:PRO:HD3	4:A:185:TRP:NE1	2.10	0.67
4:A:547:LEU:HD22	14:K:58:PHE:CD1	2.30	0.67
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.24	0.67
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.27	0.67
4:A:1323:ASP:C	4:A:1325:THR:H	2.03	0.67
4:A:1444:MET:CG	10:G:60:ARG:HA	2.25	0.67
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.75	0.67
4:A:984:LYS:O	4:A:988:LEU:HB2	1.94	0.67
4:A:1143:LEU:HD12	4:A:1146:VAL:HG23	1.75	0.67
10:G:51:TYR:C	10:G:51:TYR:CD2	2.72	0.67
4:A:1206:ASP:HB3	4:A:1274:ARG:HH12	1.60	0.66
5:B:240:ILE:CG2	5:B:254:LEU:HB3	2.25	0.66
6:C:43:THR:CG2	6:C:44:LEU:H	2.03	0.66
4:A:356:ASP:HB2	4:A:469:ARG:HH12	1.58	0.66
4:A:679:ILE:O	4:A:683:ILE:HG13	1.95	0.66
4:A:849:MET:CE	4:A:1061:GLY:HA2	2.25	0.66
2:N:3:DA:H2''	2:N:4:DG:OP2	1.95	0.66
4:A:1005:GLU:O	4:A:1009:ASN:HB2	1.95	0.66
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.77	0.66
5:B:69:LEU:HD13	5:B:432:MET:HE1	1.78	0.66
11:H:40:LEU:HD22	11:H:123:MET:HE3	1.77	0.66
5:B:756:ILE:O	5:B:759:PRO:HD3	1.96	0.66
9:F:125:LEU:HG	9:F:125:LEU:O	1.95	0.66
10:G:34:VAL:HG11	10:G:74:TYR:HE1	1.59	0.66
2:N:1:DC:H1'	2:N:2:DA:O5'	1.96	0.66
4:A:79:GLY:HA3	4:A:243:PRO:CG	2.26	0.66
4:A:225:ASN:ND2	4:A:228:PHE:H	1.90	0.66
4:A:567:LYS:HD3	11:H:95:TYR:CG	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:590:ARG:HG3	4:A:590:ARG:NH1	2.10	0.66
8:E:114:ASN:O	8:E:115:ASN:HB3	1.95	0.66
9:F:111:LEU:HD12	9:F:111:LEU:N	2.11	0.66
4:A:67:CYS:O	4:A:70:CYS:HB3	1.95	0.66
4:A:1121:GLU:HG2	4:A:1122:PRO:HD2	1.78	0.66
9:F:130:ILE:O	9:F:148:VAL:HG21	1.95	0.66
10:G:47:CYS:O	10:G:76:ALA:HB1	1.95	0.66
10:G:117:GLN:C	10:G:119:LEU:H	2.03	0.66
11:H:91:ASP:C	11:H:93:TYR:H	2.04	0.66
12:I:54:GLU:HB3	12:I:100:PHE:CE2	2.30	0.66
4:A:14:VAL:HG21	5:B:1216:LEU:HD12	1.78	0.66
4:A:499:ALA:O	4:A:503:GLN:HB2	1.96	0.66
5:B:37:PHE:CE1	5:B:41:LYS:HG3	2.31	0.66
6:C:67:LEU:HD11	6:C:155:LEU:CD1	2.26	0.66
7:D:128:VAL:O	7:D:132:GLN:HG3	1.96	0.66
4:A:92:HIS:HD2	4:A:304:MET:HE1	1.60	0.66
10:G:23:LYS:HG3	10:G:56:ILE:CD1	2.25	0.66
12:I:8:ARG:HG3	12:I:34:TYR:CE1	2.31	0.66
13:J:2:ILE:HG12	13:J:57:ILE:HD12	1.77	0.66
13:J:48:ARG:HD2	13:J:49:MET:N	2.10	0.66
14:K:6:ARG:O	14:K:9:LEU:HG	1.96	0.66
4:A:982:THR:HG22	4:A:984:LYS:H	1.60	0.66
12:I:62:ILE:O	12:I:62:ILE:HG12	1.94	0.66
14:K:10:PHE:N	14:K:10:PHE:CD2	2.64	0.66
4:A:265:LYS:HZ3	4:A:322:VAL:HG13	1.59	0.66
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.11	0.66
5:B:737:THR:CG2	12:I:66:PRO:HA	2.26	0.66
5:B:758:PHE:HB3	5:B:761:HIS:CD2	2.30	0.66
7:D:7:THR:O	7:D:9:GLN:N	2.29	0.66
7:D:52:LEU:HD21	7:D:147:TYR:CE2	2.31	0.66
5:B:121:ASN:HA	5:B:207:GLY:CA	2.26	0.65
5:B:798:TYR:CE2	6:C:62:PHE:HE2	2.15	0.65
6:C:73:GLN:HB3	6:C:131:HIS:H	1.61	0.65
4:A:248:PRO:O	4:A:260:ASP:HB2	1.95	0.65
4:A:376:TYR:OH	4:A:498:ARG:HD2	1.97	0.65
4:A:541:ILE:HG22	4:A:546:VAL:HG23	1.79	0.65
4:A:960:ILE:O	4:A:963:ILE:HG22	1.96	0.65
9:F:89:GLU:OE2	9:F:134:ILE:HG21	1.96	0.65
4:A:58:LEU:HD22	4:A:80:HIS:O	1.96	0.65
4:A:61:ILE:HG22	4:A:62:ASP:H	1.61	0.65
4:A:269:ILE:HD11	4:A:300:VAL:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1445:ILE:HD11	10:G:68:ALA:HB1	1.79	0.65
5:B:220:GLY:O	5:B:222:ILE:HG13	1.97	0.65
5:B:333:PHE:O	5:B:334:ILE:HG13	1.96	0.65
6:C:133:ILE:CD1	6:C:237:SER:HA	2.26	0.65
8:E:47:CYS:HA	8:E:52:ARG:O	1.97	0.65
13:J:3:VAL:HG21	13:J:18:TRP:CG	2.31	0.65
4:A:588:LEU:O	4:A:606:LEU:HA	1.95	0.65
4:A:858:ASN:C	4:A:858:ASN:HD22	2.04	0.65
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.32	0.65
5:B:872:GLU:CD	5:B:914:LYS:HE2	2.21	0.65
5:B:1099:VAL:CG1	5:B:1100:ASP:N	2.60	0.65
6:C:18:VAL:HG12	6:C:18:VAL:O	1.96	0.65
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.31	0.65
4:A:1224:LEU:HD12	4:A:1241:ARG:O	1.97	0.65
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.79	0.65
11:H:100:THR:HG22	11:H:101:ALA:N	2.12	0.65
13:J:44:TYR:HA	13:J:47:ARG:CB	2.24	0.65
14:K:101:LEU:O	14:K:101:LEU:HD23	1.96	0.65
4:A:107:CYS:H	4:A:114:LEU:HD21	1.61	0.65
4:A:384:ASN:CG	4:A:388:LEU:HD12	2.22	0.65
4:A:728:LYS:HA	4:A:731:ARG:HB2	1.79	0.65
5:B:1065:GLN:HB2	6:C:201:TRP:CZ3	2.32	0.65
6:C:183:TRP:O	6:C:185:LYS:N	2.29	0.65
15:L:70:ARG:HG2	15:L:70:ARG:HH11	1.62	0.65
4:A:298:PHE:HZ	4:A:314:ALA:HB2	1.61	0.65
4:A:306:ASN:HB2	4:A:324:SER:HB3	1.77	0.65
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.32	0.65
4:A:548:ASN:HA	14:K:60:ALA:HB1	1.79	0.65
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.77	0.65
5:B:902:GLY:O	15:L:65:VAL:HG11	1.97	0.65
5:B:916:THR:O	5:B:935:ARG:HG3	1.97	0.65
6:C:232:VAL:HG21	6:C:244:VAL:HG22	1.79	0.65
8:E:48:ASP:CG	8:E:49:SER:H	2.05	0.65
1:T:23:DC:H2''	1:T:24:DT:H5'	1.78	0.65
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.32	0.65
4:A:1100:ARG:NH2	4:A:1351:GLU:HG2	2.12	0.65
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.78	0.65
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.79	0.65
5:B:708:GLU:O	5:B:710:LEU:N	2.30	0.65
5:B:797:TYR:HB2	5:B:852:ARG:O	1.97	0.65
14:K:49:GLU:HG3	14:K:94:ILE:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:680:THR:HA	4:A:683:ILE:HD12	1.79	0.64
4:A:698:GLN:HA	12:I:97:MET:O	1.97	0.64
4:A:901:LEU:H	4:A:926:GLN:HE21	1.45	0.64
4:A:1227:ILE:HG22	4:A:1228:TRP:H	1.62	0.64
5:B:172:ILE:HG22	5:B:173:MET:N	2.12	0.64
5:B:233:PRO:HG2	5:B:234:ILE:CD1	2.26	0.64
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.79	0.64
15:L:40:LEU:HD13	15:L:44:ASP:HB3	1.79	0.64
4:A:54:ASN:HB3	4:A:247:ARG:HH12	1.63	0.64
4:A:172:PRO:HD3	4:A:185:TRP:HE1	1.62	0.64
4:A:903:ASN:HD22	4:A:903:ASN:C	2.04	0.64
5:B:684:LEU:H	5:B:684:LEU:HD12	1.61	0.64
5:B:1166:CYS:O	5:B:1168:LEU:N	2.28	0.64
5:B:1197:PRO:HG2	5:B:1200:ALA:HB2	1.78	0.64
14:K:29:ASN:O	14:K:76:GLN:HG3	1.98	0.64
1:T:20:DC:H4'	4:A:447:GLN:NE2	2.12	0.64
4:A:84:ILE:HD11	4:A:270:LEU:HD22	1.78	0.64
4:A:102:VAL:HG11	4:A:211:PHE:CE2	2.32	0.64
4:A:560:ILE:HG13	11:H:78:SER:HB2	1.78	0.64
5:B:185:THR:H	5:B:188:ASP:HB2	1.62	0.64
5:B:467:GLY:H	5:B:475:SER:CB	2.08	0.64
5:B:562:GLY:HA3	5:B:590:HIS:CE1	2.31	0.64
5:B:593:PRO:HG2	5:B:617:ARG:NH2	2.12	0.64
15:L:28:LYS:HB2	15:L:39:SER:HA	1.79	0.64
4:A:965:GLN:O	4:A:968:GLN:HB2	1.97	0.64
5:B:114:PRO:HG2	5:B:115:GLN:H	1.63	0.64
5:B:1065:GLN:HG3	5:B:1067:ARG:H	1.62	0.64
6:C:208:GLU:O	6:C:210:GLU:N	2.30	0.64
10:G:91:VAL:HG23	10:G:141:SER:O	1.97	0.64
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.79	0.64
4:A:1002:GLY:HA3	4:A:1007:ILE:HG21	1.79	0.64
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.12	0.64
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.79	0.64
6:C:214:ASN:HB3	6:C:217:ASP:OD2	1.98	0.64
4:A:605:MET:HE3	4:A:606:LEU:H	1.60	0.64
4:A:714:PHE:CB	12:I:97:MET:HE1	2.27	0.64
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.79	0.64
4:A:1100:ARG:HH21	4:A:1351:GLU:CG	2.11	0.64
4:A:1341:ILE:HG23	4:A:1342:GLU:H	1.62	0.64
6:C:98:VAL:C	6:C:99:LEU:HD23	2.22	0.64
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:325:ILE:HG22	5:B:1210:MET:HE2	1.79	0.64
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.10	0.64
13:J:8:PHE:H	13:J:49:MET:CE	2.11	0.64
13:J:36:LEU:HD12	13:J:47:ARG:NH1	2.13	0.64
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.24	0.64
4:A:1299:VAL:HG12	4:A:1300:LYS:H	1.63	0.64
4:A:1329:THR:HG22	4:A:1331:SER:N	2.13	0.64
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.33	0.64
4:A:114:LEU:O	4:A:115:LEU:HG	1.98	0.64
5:B:465:ASN:HD22	5:B:465:ASN:N	1.95	0.64
5:B:515:HIS:HD2	5:B:517:THR:H	1.44	0.64
6:C:76:ASP:O	6:C:79:GLN:HG2	1.97	0.64
6:C:166:GLU:HG3	14:K:10:PHE:CZ	2.24	0.64
6:C:251:LEU:O	6:C:251:LEU:HD12	1.98	0.64
13:J:14:VAL:HG12	13:J:50:ILE:HD11	1.78	0.64
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.63	0.64
5:B:1138:MET:HA	5:B:1138:MET:HE3	1.80	0.64
7:D:170:THR:HB	7:D:172:LEU:H	1.62	0.64
4:A:720:ARG:O	4:A:724:GLU:HB2	1.98	0.63
5:B:378:LEU:O	5:B:382:ILE:HG13	1.98	0.63
8:E:213:ILE:HG12	8:E:214:CYS:N	2.13	0.63
11:H:41:ASP:O	11:H:42:ILE:HG13	1.98	0.63
11:H:82:PRO:O	11:H:84:ALA:N	2.27	0.63
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.23	0.63
4:A:55:ASP:N	4:A:56:PRO:HD3	2.12	0.63
5:B:744:HIS:HD2	5:B:746:SER:OG	1.81	0.63
5:B:822:ASN:ND2	13:J:52:THR:HG21	2.12	0.63
5:B:1183:LYS:N	5:B:1183:LYS:HE3	2.13	0.63
7:D:8:PHE:CZ	7:D:40:HIS:HA	2.33	0.63
4:A:406:ILE:HG22	4:A:412:ARG:HA	1.81	0.63
4:A:1329:THR:CG2	4:A:1331:SER:HB3	2.28	0.63
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.64	0.63
5:B:822:ASN:HD22	13:J:52:THR:HG21	1.62	0.63
5:B:850:LEU:HD12	5:B:851:PHE:N	2.12	0.63
5:B:1152:MET:HE3	5:B:1157:ALA:HA	1.79	0.63
6:C:105:GLY:HA3	6:C:149:LYS:O	1.99	0.63
7:D:31:GLN:O	7:D:34:GLN:HG3	1.99	0.63
10:G:1:MET:SD	10:G:1:MET:C	2.81	0.63
10:G:3:PHE:CD1	10:G:80:LYS:NZ	2.65	0.63
1:T:23:DC:H2'	1:T:24:DT:H71	1.81	0.63
4:A:339:ASN:O	4:A:343:LYS:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1166:ASP:OD2	4:A:1239:ARG:HD2	1.98	0.63
4:A:1198:ASP:O	4:A:1202:MET:HG2	1.99	0.63
5:B:44:VAL:CG1	5:B:199:MET:HG2	2.28	0.63
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.64	0.63
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.33	0.63
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.81	0.63
11:H:42:ILE:HG23	11:H:95:TYR:CE1	2.30	0.63
4:A:35:ILE:HG22	4:A:84:ILE:HD12	1.81	0.63
4:A:1209:MET:SD	4:A:1236:LEU:HD22	2.38	0.63
4:A:1420:ASP:O	4:A:1421:CYS:HB2	1.98	0.63
5:B:65:GLU:HG3	5:B:66:ASP:N	2.14	0.63
5:B:95:ILE:HG13	5:B:130:VAL:HG22	1.80	0.63
5:B:345:LYS:O	5:B:347:LYS:HG2	1.98	0.63
5:B:879:ARG:HH11	5:B:883:LEU:CD2	2.06	0.63
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.08	0.63
5:B:773:MET:HE2	5:B:985:GLY:HA2	1.80	0.63
5:B:778:MET:HE2	5:B:1094:ARG:HG2	1.80	0.63
5:B:1197:PRO:HG2	5:B:1200:ALA:CB	2.28	0.63
7:D:35:LEU:CD2	7:D:173:HIS:HB3	2.28	0.63
7:D:47:LEU:HD12	7:D:48:ILE:H	1.62	0.63
4:A:144:THR:O	4:A:146:MET:HG3	1.98	0.63
4:A:356:ASP:OD2	14:K:65:HIS:HE1	1.82	0.63
4:A:438:ASP:O	4:A:439:ASN:HB2	1.97	0.63
4:A:1148:ILE:HG23	12:I:49:ILE:HB	1.80	0.63
9:F:111:LEU:C	9:F:113:GLY:N	2.53	0.63
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.34	0.63
12:I:25:LEU:HB3	12:I:38:ALA:HB2	1.79	0.63
4:A:90:VAL:CG1	4:A:297:GLN:HA	2.28	0.63
4:A:1329:THR:HG22	4:A:1331:SER:H	1.63	0.63
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.80	0.63
9:F:109:VAL:HG12	9:F:110:ASP:N	2.14	0.63
4:A:341:MET:CE	4:A:843:LYS:NZ	2.61	0.63
4:A:381:THR:CG2	4:A:383:TYR:H	2.12	0.63
4:A:450:LEU:HD12	4:A:450:LEU:N	2.14	0.63
4:A:993:LEU:HD22	4:A:1046:LEU:HD22	1.80	0.63
5:B:424:LEU:O	5:B:428:ILE:HG13	1.99	0.63
5:B:866:TYR:HD1	5:B:870:ILE:O	1.82	0.63
5:B:1096:ARG:O	5:B:1097:HIS:HB2	1.99	0.63
5:B:1224:PHE:CE2	8:E:171:LYS:HG3	2.31	0.63
12:I:80:SER:HB2	12:I:103:CYS:SG	2.39	0.63
13:J:64:ASN:HB3	13:J:65:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:600:PRO:C	4:A:602:ASP:H	2.05	0.62
4:A:857:ARG:HD3	4:A:861:GLY:O	1.99	0.62
4:A:870:GLU:HB2	8:E:204:THR:HG21	1.80	0.62
4:A:903:ASN:HD22	4:A:904:THR:H	1.47	0.62
5:B:324:ILE:HD13	5:B:330:ALA:HA	1.79	0.62
5:B:753:ALA:O	5:B:756:ILE:HG13	1.99	0.62
5:B:955:THR:HG22	5:B:956:THR:O	1.98	0.62
7:D:17:LYS:HE2	7:D:17:LYS:H	1.62	0.62
10:G:79:PHE:CE2	10:G:105:PRO:HD2	2.34	0.62
12:I:111:THR:CG2	12:I:112:SER:H	2.07	0.62
15:L:53:HIS:O	15:L:55:ILE:HG12	1.99	0.62
4:A:40:THR:CG2	4:A:41:MET:HG3	2.25	0.62
4:A:826:ASP:O	4:A:830:LYS:HB2	1.99	0.62
4:A:1370:LEU:O	4:A:1374:VAL:HG23	1.98	0.62
5:B:850:LEU:HD12	5:B:851:PHE:H	1.65	0.62
6:C:107:SER:C	6:C:109:SER:H	2.07	0.62
1:T:23:DC:H2''	1:T:24:DT:C5'	2.30	0.62
4:A:325:ILE:CG2	5:B:1210:MET:HE2	2.28	0.62
5:B:1081:LEU:HD12	5:B:1085:ILE:HD11	1.80	0.62
6:C:38:ILE:HA	6:C:173:ALA:CB	2.30	0.62
7:D:63:LEU:HD12	7:D:129:LEU:HG	1.81	0.62
1:T:19:DC:H2''	1:T:20:DC:O5'	1.99	0.62
3:P:2:U:C2'	3:P:3:U:O5'	2.48	0.62
4:A:7:SER:HB2	5:B:1175:LEU:HD22	1.81	0.62
4:A:382:PRO:CB	4:A:428:TYR:HE2	2.12	0.62
4:A:783:THR:HG21	4:A:815:PHE:CZ	2.35	0.62
4:A:901:LEU:HA	4:A:907:THR:OG1	1.99	0.62
5:B:400:HIS:O	5:B:402:GLY:N	2.32	0.62
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.80	0.62
10:G:1:MET:O	10:G:3:PHE:CE1	2.52	0.62
10:G:96:GLN:HG3	10:G:97:HIS:HD2	1.64	0.62
11:H:44:VAL:O	11:H:44:VAL:HG12	2.00	0.62
4:A:90:VAL:HG13	4:A:297:GLN:HA	1.81	0.62
4:A:93:VAL:HG23	4:A:304:MET:HE3	1.81	0.62
4:A:298:PHE:CZ	4:A:314:ALA:HB2	2.35	0.62
4:A:1206:ASP:HB3	4:A:1274:ARG:NH1	2.15	0.62
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.35	0.62
5:B:821:GLN:NE2	5:B:851:PHE:HA	2.14	0.62
6:C:100:THR:HG22	6:C:101:LEU:N	2.15	0.62
4:A:513:SER:HB2	4:A:520:CYS:HB3	1.80	0.62
4:A:782:ARG:NH2	5:B:699:GLU:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:856:THR:HB	4:A:865:GLN:HB2	1.81	0.62
5:B:579:ARG:HG2	5:B:579:ARG:HH11	1.65	0.62
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.35	0.62
7:D:134:THR:HG22	7:D:135:GLY:H	1.65	0.62
4:A:34:LYS:HB3	4:A:36:ARG:HE	1.65	0.62
4:A:746:MET:CE	5:B:1018:PRO:HG2	2.29	0.62
4:A:1208:THR:HG22	4:A:1210:GLY:N	2.14	0.62
5:B:217:ARG:HD2	5:B:217:ARG:C	2.24	0.62
5:B:899:ILE:CD1	5:B:911:ILE:HA	2.29	0.62
5:B:1008:PRO:HB2	5:B:1010:LEU:O	1.99	0.62
8:E:176:PRO:O	8:E:212:ARG:HA	1.99	0.62
1:T:11:DT:H2''	1:T:12:DA:H5'	1.81	0.62
4:A:17:VAL:HA	5:B:1215:ARG:O	1.99	0.62
4:A:23:SER:HA	4:A:233:TRP:CD1	2.35	0.62
4:A:1323:ASP:O	4:A:1325:THR:N	2.33	0.62
4:A:1454:MET:O	4:A:1454:MET:HG3	1.99	0.62
5:B:520:GLY:N	5:B:748:ILE:HG22	2.14	0.62
6:C:113:VAL:O	6:C:144:ILE:HB	2.00	0.62
10:G:79:PHE:CZ	10:G:106:MET:HE2	2.31	0.62
10:G:91:VAL:HA	10:G:101:VAL:HA	1.82	0.62
12:I:82:GLU:HB3	12:I:104:LEU:HD12	1.81	0.62
4:A:265:LYS:HE2	4:A:322:VAL:CG1	2.29	0.62
4:A:761:MET:HA	4:A:804:TYR:HB2	1.82	0.62
4:A:1017:LEU:HB3	8:E:205:SER:HA	1.82	0.62
5:B:557:PHE:C	5:B:557:PHE:CD2	2.77	0.62
5:B:1073:TYR:OH	6:C:179:GLU:HG3	1.99	0.62
7:D:33:PHE:CE1	10:G:80:LYS:HE3	2.35	0.62
11:H:142:LEU:C	11:H:143:LEU:HD12	2.25	0.62
4:A:71:GLN:C	4:A:73:GLY:H	2.08	0.61
4:A:1124:HIS:HB3	4:A:1130:GLN:HG2	1.82	0.61
5:B:766:ARG:HH22	5:B:1020:ARG:HH11	1.48	0.61
5:B:794:ASN:C	5:B:795:ILE:HD12	2.25	0.61
5:B:847:ASP:C	5:B:849:GLY:H	2.07	0.61
6:C:101:LEU:HD22	6:C:118:LEU:HD21	1.81	0.61
7:D:14:ARG:O	7:D:16:LYS:HD3	2.00	0.61
4:A:663:SER:OG	4:A:664:THR:N	2.32	0.61
4:A:903:ASN:ND2	4:A:904:THR:N	2.46	0.61
5:B:1084:GLN:NE2	5:B:1084:GLN:H	1.98	0.61
6:C:66:ARG:NH2	13:J:5:VAL:HG23	2.15	0.61
7:D:153:ARG:NH2	7:D:184:ALA:HA	2.15	0.61
8:E:134:THR:C	8:E:135:PHE:HD1	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:195:VAL:HG22	8:E:213:ILE:HG13	1.81	0.61
5:B:807:ARG:HG2	5:B:1045:SER:OG	1.99	0.61
8:E:157:SER:OG	8:E:160:GLU:HG3	2.01	0.61
4:A:728:LYS:O	4:A:732:LEU:HG	2.00	0.61
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.00	0.61
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.66	0.61
4:A:1356:ILE:HD13	4:A:1363:VAL:HG21	1.81	0.61
5:B:69:LEU:HD13	5:B:429:PHE:HD1	1.65	0.61
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.35	0.61
7:D:47:LEU:CD1	7:D:48:ILE:H	2.13	0.61
10:G:153:GLN:HG2	10:G:154:VAL:HG23	1.82	0.61
4:A:19:PHE:HB3	4:A:1413:GLY:HA2	1.81	0.61
4:A:718:VAL:HG12	4:A:722:LEU:HD11	1.82	0.61
4:A:1039:LYS:HE3	4:A:1043:ASP:OD2	2.01	0.61
5:B:37:PHE:CD1	5:B:41:LYS:HG3	2.36	0.61
5:B:705:MET:N	5:B:710:LEU:HD12	2.14	0.61
7:D:5:THR:HG23	10:G:9:LEU:HD13	1.82	0.61
11:H:61:SER:O	11:H:62:SER:HB3	2.01	0.61
4:A:21:LEU:HD11	4:A:1414:ALA:HA	1.83	0.61
4:A:138:ILE:CD1	4:A:222:LEU:HD23	2.31	0.61
4:A:269:ILE:HD13	4:A:300:VAL:HG22	1.81	0.61
4:A:321:PRO:O	4:A:322:VAL:CB	2.48	0.61
4:A:784:LEU:HD11	4:A:815:PHE:CE2	2.35	0.61
5:B:1102:LYS:O	5:B:1103:ILE:C	2.44	0.61
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	1.99	0.61
9:F:108:PHE:HE1	9:F:131:PRO:HG3	1.66	0.61
10:G:128:PRO:O	10:G:138:THR:HG23	2.01	0.61
4:A:29:ALA:HB1	5:B:1184:GLY:CA	2.31	0.61
4:A:87:ALA:CB	4:A:276:LEU:HD23	2.31	0.61
4:A:168:GLY:O	4:A:169:ASN:C	2.44	0.61
4:A:353:ILE:HG21	4:A:487:MET:CE	2.31	0.61
4:A:470:LEU:HD22	4:A:487:MET:CE	2.30	0.61
4:A:870:GLU:HG2	8:E:208:TYR:CG	2.35	0.61
4:A:1035:TYR:O	4:A:1037:LEU:N	2.34	0.61
5:B:295:GLY:N	5:B:298:LEU:HD23	2.16	0.61
6:C:147:LEU:HD23	6:C:147:LEU:N	2.14	0.61
3:P:2:U:H2'	3:P:3:U:O5'	2.00	0.61
4:A:172:PRO:HB3	4:A:185:TRP:CE2	2.35	0.61
4:A:1444:MET:HG2	10:G:60:ARG:CA	2.29	0.61
5:B:359:GLU:O	5:B:362:PRO:HD3	2.00	0.61
5:B:658:ILE:CG2	5:B:662:MET:HE2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1165:ILE:CG2	5:B:1166:CYS:N	2.61	0.61
6:C:186:LEU:HD21	6:C:224:GLN:O	2.01	0.61
4:A:4:GLN:O	4:A:5:GLN:HB2	2.00	0.61
4:A:896:ARG:NH2	4:A:1030:ARG:NH2	2.49	0.61
5:B:508:LEU:O	5:B:509:ALA:CB	2.49	0.61
5:B:654:ARG:HH11	5:B:654:ARG:HG3	1.65	0.61
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.48	0.61
6:C:238:ILE:HG22	6:C:243:VAL:HG23	1.83	0.61
6:C:241:ASP:O	6:C:245:VAL:HG23	2.00	0.61
7:D:7:THR:HG21	7:D:32:GLU:CD	2.25	0.61
1:T:11:DT:O2	2:N:7:DG:N2	2.33	0.61
4:A:384:ASN:O	4:A:385:ILE:C	2.43	0.61
4:A:427:GLN:HG3	4:A:430:TRP:CE2	2.36	0.61
4:A:1373:ASP:HA	4:A:1376:THR:CG2	2.30	0.61
4:A:1450:LEU:O	4:A:1450:LEU:HG	2.01	0.61
5:B:121:ASN:HA	5:B:207:GLY:HA2	1.83	0.61
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.28	0.61
7:D:17:LYS:H	7:D:17:LYS:CE	2.14	0.61
8:E:15:ALA:O	8:E:19:VAL:HG23	2.01	0.61
4:A:337:ARG:HD3	5:B:1132:GLU:OE1	2.00	0.60
4:A:345:VAL:HG23	4:A:346:ASP:O	2.01	0.60
4:A:1094:VAL:HG13	4:A:1113:THR:CG2	2.21	0.60
5:B:955:THR:CG2	5:B:956:THR:N	2.64	0.60
6:C:100:THR:HG22	6:C:101:LEU:H	1.65	0.60
8:E:22:MET:CE	8:E:26:ARG:HH21	2.14	0.60
9:F:143:PHE:C	9:F:143:PHE:HD1	2.09	0.60
4:A:152:VAL:HG13	4:A:153:PRO:HD2	1.82	0.60
4:A:269:ILE:CD1	4:A:300:VAL:HA	2.30	0.60
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.83	0.60
5:B:948:ILE:HG22	5:B:949:VAL:O	2.02	0.60
10:G:145:VAL:CG1	10:G:146:LYS:N	2.64	0.60
4:A:590:ARG:O	4:A:591:PHE:HB2	2.00	0.60
4:A:694:THR:O	4:A:698:GLN:HG3	2.02	0.60
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.42	0.60
5:B:842:ASN:ND2	5:B:845:SER:OG	2.35	0.60
8:E:10:SER:O	8:E:14:ARG:HG3	2.00	0.60
13:J:9:SER:HB2	13:J:45:CYS:HB2	1.83	0.60
2:N:2:DA:OP1	2:N:2:DA:H3'	2.01	0.60
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	1.84	0.60
4:A:50:ILE:O	4:A:52:GLY:N	2.32	0.60
4:A:882:SER:HB3	4:A:953:ASN:OD1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:124:VAL:HA	8:E:132:ILE:HD12	1.82	0.60
9:F:119:ARG:HH11	9:F:119:ARG:HG3	1.66	0.60
13:J:44:TYR:CD2	13:J:44:TYR:N	2.68	0.60
4:A:896:ARG:HD3	4:A:897:TYR:CE1	2.36	0.60
4:A:1121:GLU:CG	4:A:1122:PRO:HD2	2.31	0.60
8:E:135:PHE:HD2	8:E:140:LEU:HD21	1.66	0.60
3:P:3:U:O2'	4:A:320:ARG:NH2	2.35	0.60
4:A:49:LYS:HZ1	4:A:61:ILE:N	1.99	0.60
4:A:1030:ARG:HG3	4:A:1034:GLU:OE2	2.00	0.60
5:B:582:VAL:HG23	5:B:626:ILE:HB	1.82	0.60
5:B:1182:CYS:O	5:B:1183:LYS:O	2.20	0.60
11:H:81:PRO:CB	11:H:82:PRO:CD	2.80	0.60
4:A:377:PRO:HG3	4:A:493:GLN:HG3	1.83	0.60
4:A:384:ASN:OD1	4:A:388:LEU:HD12	2.01	0.60
4:A:590:ARG:HG3	4:A:590:ARG:HH11	1.65	0.60
4:A:672:ASP:HB2	4:A:736:ASN:OD1	2.01	0.60
4:A:958:VAL:HG11	4:A:1049:ILE:HG23	1.83	0.60
4:A:1410:PHE:HA	5:B:1212:ILE:CD1	2.31	0.60
5:B:601:ARG:O	5:B:605:ARG:HG3	2.01	0.60
5:B:611:PRO:HG2	5:B:685:LEU:HD21	1.83	0.60
5:B:912:ILE:HB	5:B:939:THR:OG1	2.01	0.60
8:E:78:LEU:HD23	8:E:78:LEU:C	2.27	0.60
4:A:1290:LYS:O	4:A:1291:VAL:HG23	2.02	0.60
4:A:1323:ASP:OD1	4:A:1325:THR:HB	2.02	0.60
5:B:294:ASP:O	5:B:296:GLU:N	2.31	0.60
5:B:570:VAL:CG2	5:B:573:GLN:HB3	2.31	0.60
5:B:597:MET:HE2	5:B:601:ARG:HG3	1.83	0.60
5:B:825:VAL:CG1	5:B:826:ALA:N	2.65	0.60
5:B:1115:THR:O	5:B:1116:ARG:HB2	2.02	0.60
5:B:882:THR:HG21	5:B:884:ARG:HB2	1.84	0.60
5:B:1163:CYS:SG	5:B:1165:ILE:HB	2.41	0.60
10:G:45:ILE:O	10:G:45:ILE:HG22	2.02	0.60
15:L:38:LEU:O	15:L:39:SER:HB3	2.02	0.60
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.84	0.59
4:A:466:SER:HA	14:K:2:ASN:HD22	1.67	0.59
4:A:781:ASP:O	4:A:789:LYS:HA	2.02	0.59
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.01	0.59
4:A:1102:LYS:HG2	4:A:1106:ASN:HD21	1.65	0.59
5:B:522:VAL:HG11	5:B:537:LYS:HB3	1.82	0.59
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.36	0.59
5:B:799:PRO:HB3	5:B:818:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:124:LEU:O	6:C:127:ARG:HG2	2.02	0.59
7:D:172:LEU:HD22	7:D:176:GLU:OE1	2.01	0.59
4:A:841:LEU:O	4:A:845:LEU:HG	2.02	0.59
4:A:960:ILE:HA	4:A:963:ILE:CG2	2.32	0.59
4:A:1102:LYS:HG2	4:A:1106:ASN:ND2	2.16	0.59
4:A:1149:ALA:HB2	12:I:47:GLU:HA	1.83	0.59
6:C:66:ARG:NH2	13:J:3:VAL:O	2.35	0.59
7:D:176:GLU:C	7:D:178:ALA:H	2.10	0.59
8:E:14:ARG:NH2	8:E:141:VAL:HG12	2.13	0.59
10:G:91:VAL:HB	10:G:139:ILE:O	2.01	0.59
14:K:21:ILE:HG23	14:K:31:VAL:HG11	1.84	0.59
15:L:31:CYS:SG	15:L:34:CYS:SG	3.00	0.59
4:A:53:LEU:HD22	4:A:54:ASN:HD22	1.66	0.59
4:A:1151:GLU:HA	12:I:44:TYR:O	2.01	0.59
4:A:1317:MET:O	4:A:1322:ILE:HD11	2.01	0.59
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.82	0.59
5:B:192:LEU:O	5:B:193:LYS:HB2	2.02	0.59
5:B:408:LEU:O	5:B:411:PRO:HD2	2.02	0.59
8:E:161:LYS:HD2	8:E:195:VAL:HG23	1.84	0.59
11:H:40:LEU:HD13	11:H:123:MET:HB2	1.85	0.59
12:I:55:THR:HG22	12:I:58:VAL:HG21	1.84	0.59
4:A:86:LEU:HG	4:A:237:THR:O	2.03	0.59
4:A:1153:TYR:CE1	12:I:42:LEU:HD13	2.36	0.59
7:D:63:LEU:HD13	7:D:133:THR:OG1	2.02	0.59
8:E:17:ARG:O	8:E:21:GLU:HG3	2.02	0.59
10:G:27:LYS:O	10:G:30:LEU:HB3	2.02	0.59
10:G:34:VAL:HG11	10:G:74:TYR:CE1	2.37	0.59
10:G:51:TYR:O	10:G:54:ILE:HG13	2.02	0.59
10:G:119:LEU:HD12	10:G:131:GLN:O	2.03	0.59
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.84	0.59
4:A:869:GLY:O	8:E:204:THR:HG21	2.01	0.59
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.43	0.59
4:A:1445:ILE:H	4:A:1445:ILE:CD1	2.00	0.59
5:B:57:TYR:N	5:B:57:TYR:HD1	2.01	0.59
5:B:167:ILE:HG22	5:B:453:ILE:HD12	1.84	0.59
5:B:347:LYS:HG3	5:B:348:ARG:H	1.67	0.59
12:I:55:THR:CG2	12:I:58:VAL:HG21	2.33	0.59
12:I:106:CYS:O	12:I:107:SER:HB2	2.01	0.59
15:L:55:ILE:O	15:L:56:LEU:HB2	2.02	0.59
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.27	0.59
4:A:816:HIS:HE2	5:B:764:SER:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1116:LEU:HD11	4:A:1118:VAL:HG13	1.84	0.59
4:A:1343:ALA:HB2	8:E:150:VAL:HG22	1.83	0.59
5:B:824:ILE:HG23	5:B:1087:PHE:HE2	1.67	0.59
5:B:1000:PRO:O	5:B:1007:VAL:HG23	2.02	0.59
8:E:144:ILE:HG13	8:E:145:THR:N	2.17	0.59
4:A:829:VAL:C	4:A:831:THR:H	2.10	0.59
4:A:1114:PRO:HB2	4:A:1311:VAL:HG23	1.84	0.59
5:B:542:MET:HE3	5:B:636:PRO:HG2	1.85	0.59
9:F:130:ILE:O	9:F:148:VAL:CG2	2.51	0.59
4:A:37:PHE:N	4:A:37:PHE:CD1	2.69	0.59
4:A:42:ASP:HA	4:A:46:THR:O	2.03	0.59
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.01	0.59
4:A:1341:ILE:CG2	4:A:1342:GLU:N	2.66	0.59
5:B:589:VAL:HG12	5:B:590:HIS:N	2.03	0.59
6:C:77:ILE:HG23	6:C:161:LYS:HE3	1.85	0.59
4:A:252:PHE:O	4:A:253:ASN:HB2	2.03	0.59
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	1.85	0.59
4:A:1349:TYR:CA	4:A:1372:VAL:HG21	2.32	0.59
5:B:35:SER:O	5:B:39:ARG:HG3	2.03	0.59
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.37	0.59
6:C:69:LEU:N	6:C:69:LEU:HD12	2.18	0.59
8:E:178:ILE:HG22	8:E:213:ILE:O	2.03	0.59
1:T:13:DC:H2'	1:T:14:DT:H71	1.85	0.59
4:A:49:LYS:HZ3	4:A:61:ILE:HG13	1.63	0.59
4:A:63:ARG:HA	4:A:74:MET:SD	2.43	0.59
4:A:401:GLY:C	4:A:435:HIS:CD2	2.81	0.59
4:A:503:GLN:NE2	9:F:90:ARG:HH21	2.00	0.59
4:A:511:ILE:HA	4:A:521:MET:HE3	1.84	0.59
4:A:596:THR:O	4:A:598:LEU:N	2.35	0.59
4:A:954:TRP:HB3	4:A:955:PRO:HD2	1.85	0.59
5:B:542:MET:HB3	5:B:636:PRO:HD2	1.85	0.59
5:B:918:ILE:HG21	5:B:935:ARG:NH1	2.17	0.59
4:A:84:ILE:CD1	4:A:270:LEU:HD22	2.32	0.58
4:A:222:LEU:O	4:A:224:PHE:N	2.36	0.58
4:A:1313:LEU:HD23	4:A:1338:VAL:HG21	1.85	0.58
5:B:39:ARG:HH21	5:B:665:GLU:CD	2.11	0.58
5:B:309:GLN:CD	12:I:52:ILE:HD11	2.28	0.58
5:B:502:ILE:H	5:B:502:ILE:HD12	1.68	0.58
5:B:642:ASP:HB3	5:B:649:LYS:CD	2.32	0.58
6:C:8:VAL:HG12	6:C:9:LYS:N	2.18	0.58
10:G:106:MET:CG	10:G:107:LYS:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:741:ASN:HD21	4:A:743:VAL:HB	1.68	0.58
4:A:774:ARG:HB2	4:A:797:LYS:O	2.02	0.58
4:A:890:ASP:H	4:A:1296:GLY:HA3	1.68	0.58
4:A:1130:GLN:HE21	4:A:1134:ILE:HD11	1.67	0.58
4:A:1410:PHE:HD2	5:B:1212:ILE:HD12	1.69	0.58
5:B:168:GLY:N	5:B:450:ALA:HB1	2.17	0.58
5:B:326:ASP:OD2	5:B:328:GLU:HB2	2.02	0.58
11:H:83:GLN:O	11:H:85:GLY:N	2.36	0.58
15:L:40:LEU:HD22	15:L:44:ASP:CB	2.34	0.58
4:A:547:LEU:HD22	14:K:58:PHE:CE1	2.38	0.58
4:A:774:ARG:O	4:A:775:ILE:C	2.46	0.58
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.39	0.58
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.85	0.58
5:B:792:MET:HG3	5:B:855:PHE:HE1	1.68	0.58
11:H:93:TYR:CD2	11:H:143:LEU:HB3	2.38	0.58
13:J:14:VAL:HG12	13:J:14:VAL:O	2.03	0.58
13:J:45:CYS:O	13:J:48:ARG:HG3	2.03	0.58
4:A:185:TRP:HZ3	4:A:200:ARG:HG2	1.65	0.58
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.99	0.58
6:C:66:ARG:NH1	13:J:2:ILE:CG2	2.67	0.58
6:C:174:ALA:O	6:C:175:ALA:HB3	2.04	0.58
10:G:18:PHE:HA	10:G:22:MET:HE2	1.85	0.58
10:G:49:LEU:HD21	10:G:77:VAL:HG23	1.85	0.58
10:G:149:GLY:O	10:G:159:ALA:HB1	2.02	0.58
13:J:44:TYR:HD2	13:J:44:TYR:N	1.99	0.58
14:K:53:ASP:OD1	14:K:55:LYS:HB2	2.02	0.58
5:B:293:PRO:HG2	5:B:296:GLU:HB3	1.86	0.58
9:F:111:LEU:O	9:F:113:GLY:N	2.34	0.58
14:K:31:VAL:HG12	14:K:32:VAL:N	2.17	0.58
4:A:369:SER:HB2	14:K:2:ASN:OD1	2.03	0.58
4:A:541:ILE:HG21	4:A:549:MET:CE	2.33	0.58
4:A:785:PRO:HG2	4:A:786:HIS:HD2	1.68	0.58
4:A:910:PRO:HB3	4:A:917:SER:H	1.68	0.58
4:A:1114:PRO:O	4:A:1115:SER:O	2.21	0.58
5:B:20:ASP:O	5:B:22:SER:N	2.37	0.58
6:C:29:MET:HE2	14:K:98:LEU:CD2	2.33	0.58
6:C:31:ASN:O	6:C:34:ARG:HB3	2.04	0.58
9:F:143:PHE:C	9:F:143:PHE:CD1	2.78	0.58
13:J:27:GLU:C	13:J:29:GLU:H	2.12	0.58
14:K:6:ARG:O	14:K:8:GLU:N	2.37	0.58
1:T:22:DC:OP1	5:B:1122:ARG:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:401:GLY:C	4:A:435:HIS:HD2	2.10	0.58
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.86	0.58
4:A:858:ASN:ND2	4:A:861:GLY:H	2.01	0.58
5:B:265:SER:O	5:B:266:ALA:HB3	2.03	0.58
5:B:345:LYS:O	5:B:347:LYS:N	2.35	0.58
5:B:563:MET:HE2	5:B:587:HIS:C	2.29	0.58
5:B:1006:ILE:HG23	13:J:45:CYS:SG	2.44	0.58
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.34	0.58
7:D:52:LEU:C	7:D:54:GLU:H	2.11	0.58
8:E:177:ARG:HD3	8:E:215:MET:CG	2.31	0.58
4:A:63:ARG:HA	4:A:74:MET:CE	2.34	0.58
4:A:130:ASP:O	4:A:131:SER:C	2.47	0.58
4:A:152:VAL:CG1	4:A:153:PRO:HD2	2.33	0.58
4:A:1017:LEU:CB	8:E:205:SER:HA	2.34	0.58
4:A:1334:ASP:O	4:A:1337:GLU:N	2.36	0.58
5:B:828:ALA:HB2	5:B:1085:ILE:HG23	1.85	0.58
5:B:863:GLU:OE2	5:B:873:THR:HA	2.03	0.58
7:D:145:MET:O	7:D:149:THR:HB	2.03	0.58
12:I:55:THR:HG22	12:I:55:THR:O	2.02	0.58
1:T:21:DT:H2''	1:T:22:DC:O5'	2.03	0.58
4:A:372:LYS:HA	4:A:435:HIS:ND1	2.19	0.58
4:A:675:THR:OG1	4:A:736:ASN:ND2	2.37	0.58
4:A:1313:LEU:HD23	4:A:1338:VAL:CG2	2.34	0.58
5:B:449:ASN:C	5:B:451:LYS:H	2.12	0.58
5:B:980:PHE:CA	5:B:1095:LEU:HD11	2.34	0.58
4:A:224:PHE:CZ	4:A:234:MET:HE2	2.39	0.58
4:A:347:PHE:HE2	4:A:375:THR:HG23	1.69	0.58
4:A:445:ASN:HB2	4:A:454:SER:O	2.03	0.58
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.37	0.58
5:B:1038:SER:C	5:B:1040:ASN:H	2.10	0.58
6:C:249:ASP:O	6:C:252:GLN:HB3	2.04	0.58
9:F:89:GLU:O	9:F:93:ILE:HG13	2.04	0.58
11:H:22:LYS:O	11:H:23:VAL:HG23	2.04	0.58
4:A:416:ARG:C	4:A:417:TYR:CD2	2.81	0.57
4:A:494:SER:O	4:A:497:THR:N	2.37	0.57
4:A:1116:LEU:CD1	4:A:1118:VAL:HG13	2.34	0.57
5:B:172:ILE:HD13	5:B:178:ASN:CB	2.25	0.57
8:E:145:THR:HG21	8:E:187:TYR:CD2	2.39	0.57
13:J:1:MET:N	13:J:56:LEU:H	2.00	0.57
13:J:64:ASN:CB	13:J:65:PRO:CD	2.78	0.57
15:L:27:LEU:HB3	15:L:37:LYS:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:42:ASP:C	4:A:44:THR:H	2.12	0.57
4:A:49:LYS:HE2	4:A:61:ILE:HD12	1.84	0.57
4:A:685:GLU:HG3	4:A:686:ALA:N	2.18	0.57
5:B:54:PHE:HA	5:B:58:THR:HB	1.85	0.57
5:B:57:TYR:N	5:B:57:TYR:CD1	2.69	0.57
5:B:525:ALA:O	5:B:768:THR:HG23	2.05	0.57
5:B:576:ASP:HA	5:B:622:LYS:NZ	2.20	0.57
10:G:106:MET:HG2	10:G:107:LYS:N	2.19	0.57
4:A:577:ILE:O	4:A:580:VAL:HG23	2.04	0.57
4:A:626:ASN:O	4:A:631:HIS:CD2	2.57	0.57
4:A:701:LEU:HD21	12:I:114:GLN:HB2	1.86	0.57
5:B:758:PHE:HZ	5:B:1031:LEU:HD22	1.69	0.57
5:B:1031:LEU:HD11	5:B:1042:GLY:HA3	1.85	0.57
5:B:1176:ASN:C	5:B:1178:ASN:H	2.10	0.57
7:D:54:GLU:O	7:D:58:VAL:HG23	2.03	0.57
12:I:2:THR:O	12:I:3:THR:C	2.46	0.57
4:A:382:PRO:HB3	4:A:428:TYR:CE2	2.38	0.57
4:A:863:VAL:HG11	4:A:866:PHE:CD2	2.38	0.57
4:A:1447:GLU:OE2	10:G:23:LYS:HB2	2.04	0.57
5:B:100:PRO:HD2	5:B:180:TYR:CE1	2.40	0.57
7:D:137:ASN:C	7:D:137:ASN:HD22	2.13	0.57
8:E:101:GLN:NE2	8:E:127:ILE:HG21	2.19	0.57
10:G:79:PHE:HE2	10:G:105:PRO:HG2	1.69	0.57
11:H:58:THR:HB	11:H:143:LEU:HD13	1.86	0.57
13:J:47:ARG:HG2	13:J:47:ARG:HH11	1.69	0.57
14:K:65:HIS:CD2	14:K:67:PHE:HB2	2.39	0.57
4:A:34:LYS:HG2	4:A:36:ARG:NH2	2.19	0.57
4:A:102:VAL:O	4:A:105:CYS:HB2	2.04	0.57
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.39	0.57
4:A:1313:LEU:O	4:A:1315:GLU:N	2.37	0.57
4:A:1341:ILE:O	4:A:1344:GLY:N	2.38	0.57
9:F:118:LEU:HD12	9:F:118:LEU:O	2.05	0.57
13:J:1:MET:H2	13:J:57:ILE:N	1.88	0.57
4:A:138:ILE:HD13	4:A:222:LEU:HD23	1.86	0.57
4:A:157:ASP:C	4:A:159:THR:H	2.12	0.57
4:A:215:SER:O	4:A:218:ASP:HB2	2.04	0.57
4:A:565:ILE:O	4:A:570:PRO:HA	2.05	0.57
4:A:647:GLY:O	4:A:651:LYS:HG3	2.04	0.57
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.35	0.57
7:D:175:PHE:HZ	10:G:85:GLU:HG3	1.68	0.57
9:F:90:ARG:HD3	9:F:155:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:1:MET:H1	13:J:56:LEU:H	1.51	0.57
4:A:34:LYS:CG	4:A:36:ARG:HH21	2.18	0.57
4:A:50:ILE:C	4:A:52:GLY:N	2.60	0.57
4:A:844:ALA:O	4:A:845:LEU:HD23	2.04	0.57
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.03	0.57
5:B:579:ARG:N	5:B:589:VAL:HG13	2.18	0.57
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.38	0.57
6:C:213:PRO:HG2	6:C:214:ASN:H	1.69	0.57
7:D:52:LEU:O	7:D:54:GLU:N	2.36	0.57
8:E:94:LYS:CE	8:E:98:ILE:HD11	2.30	0.57
9:F:90:ARG:HG3	9:F:91:ALA:N	2.18	0.57
10:G:143:ILE:CG2	10:G:144:ARG:N	2.67	0.57
4:A:477:PRO:HG2	4:A:521:MET:HG2	1.87	0.57
4:A:1364:ASN:O	4:A:1365:TYR:C	2.47	0.57
5:B:955:THR:HG22	5:B:956:THR:N	2.20	0.57
5:B:1069:PHE:H	5:B:1069:PHE:HD1	1.52	0.57
6:C:263:THR:C	6:C:265:MET:H	2.12	0.57
4:A:385:ILE:HG22	4:A:386:ASP:N	2.20	0.57
5:B:357:GLN:O	5:B:366:GLN:HA	2.04	0.57
5:B:594:ALA:CA	5:B:617:ARG:HH12	2.15	0.57
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.35	0.57
11:H:126:GLU:C	11:H:130:ARG:HH22	2.13	0.57
4:A:477:PRO:CG	4:A:521:MET:HG2	2.35	0.57
4:A:1116:LEU:H	4:A:1308:THR:HG22	1.69	0.57
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.51	0.57
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.82	0.57
5:B:25:ILE:HD11	5:B:653:VAL:C	2.29	0.57
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.40	0.57
5:B:190:TYR:HD2	13:J:62:ARG:O	1.88	0.57
5:B:1099:VAL:O	5:B:1101:ASP:N	2.38	0.57
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.85	0.57
7:D:17:LYS:O	7:D:17:LYS:HG2	2.04	0.57
9:F:77:ASP:C	9:F:79:ARG:H	2.12	0.57
10:G:1:MET:SD	10:G:1:MET:O	2.63	0.57
14:K:61:TYR:C	14:K:61:TYR:CD2	2.80	0.57
4:A:44:THR:O	4:A:45:GLN:HB2	2.04	0.56
4:A:93:VAL:CG2	4:A:304:MET:HE3	2.34	0.56
4:A:115:LEU:CB	4:A:122:MET:HE2	2.33	0.56
4:A:442:VAL:O	4:A:457:ALA:HA	2.05	0.56
4:A:590:ARG:HB3	4:A:605:MET:N	2.20	0.56
5:B:552:MET:HA	5:B:555:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:34:CYS:SG	15:L:34:CYS:O	2.63	0.56
4:A:93:VAL:HG11	4:A:305:ASP:HB3	1.86	0.56
4:A:444:PHE:CB	4:A:458:HIS:HD2	2.17	0.56
4:A:886:ILE:CG2	4:A:887:GLY:N	2.67	0.56
4:A:946:VAL:HG13	8:E:201:LYS:HB3	1.85	0.56
5:B:642:ASP:HB3	5:B:649:LYS:HD2	1.87	0.56
6:C:70:ILE:HG12	6:C:142:VAL:HG11	1.87	0.56
7:D:191:ALA:C	7:D:193:THR:H	2.12	0.56
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.41	0.56
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.35	0.56
4:A:1259:MET:C	4:A:1261:LYS:H	2.12	0.56
5:B:310:MET:HE1	5:B:383:ASN:OD1	2.06	0.56
5:B:603:LEU:HD13	5:B:608:ASP:CB	2.33	0.56
5:B:616:ILE:HG23	5:B:700:SER:OG	2.06	0.56
5:B:635:ARG:NH2	5:B:742:GLU:OE2	2.38	0.56
5:B:792:MET:HA	5:B:856:PHE:O	2.06	0.56
5:B:912:ILE:O	5:B:938:SER:HB3	2.05	0.56
6:C:73:GLN:NE2	6:C:75:MET:HB2	2.20	0.56
6:C:181:ASP:OD1	6:C:186:LEU:HD13	2.05	0.56
8:E:55:ARG:HD2	8:E:83:CYS:O	2.05	0.56
9:F:135:ARG:HD3	9:F:143:PHE:CD2	2.39	0.56
10:G:25:TYR:HE2	10:G:29:LYS:HD2	1.70	0.56
11:H:110:ASP:O	11:H:128:ASN:ND2	2.38	0.56
12:I:14:LEU:HA	12:I:28:GLU:O	2.06	0.56
13:J:21:TYR:CE1	13:J:36:LEU:HD21	2.40	0.56
4:A:282:ASN:O	4:A:284:ALA:N	2.38	0.56
5:B:20:ASP:C	5:B:22:SER:H	2.14	0.56
5:B:97:VAL:HG12	5:B:178:ASN:HD21	1.70	0.56
5:B:1183:LYS:HA	5:B:1186:ASP:HA	1.88	0.56
6:C:77:ILE:HA	6:C:129:ILE:HD11	1.88	0.56
10:G:74:TYR:H	10:G:74:TYR:HD2	1.51	0.56
11:H:89:LEU:O	11:H:91:ASP:N	2.36	0.56
14:K:49:GLU:HG3	14:K:94:ILE:CG1	2.35	0.56
4:A:42:ASP:HB3	4:A:45:GLN:H	1.70	0.56
5:B:195:CYS:SG	5:B:196:PRO:HD2	2.46	0.56
5:B:880:THR:O	5:B:881:ASN:HB2	2.05	0.56
6:C:40:GLU:HA	6:C:163:ILE:HG21	1.87	0.56
7:D:34:GLN:C	7:D:36:LYS:H	2.14	0.56
7:D:195:ILE:HG22	7:D:198:LEU:HG	1.85	0.56
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.71	0.56
4:A:860:LEU:CD1	4:A:1393:ASN:HB2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:94:LYS:HG2	5:B:95:ILE:N	2.20	0.56
5:B:225:VAL:HG12	5:B:238:ALA:HB2	1.88	0.56
5:B:839:MET:HG3	5:B:1010:LEU:HD11	1.86	0.56
5:B:1085:ILE:HD12	5:B:1085:ILE:H	1.70	0.56
6:C:254:LYS:O	6:C:258:ILE:HD13	2.05	0.56
11:H:23:VAL:HG13	11:H:42:ILE:O	2.05	0.56
4:A:75:ASN:O	4:A:76:GLU:CB	2.54	0.56
4:A:965:GLN:HA	4:A:968:GLN:HG3	1.87	0.56
5:B:39:ARG:NH2	5:B:665:GLU:HG2	2.20	0.56
5:B:258:LEU:HG	5:B:258:LEU:O	2.05	0.56
5:B:620:ARG:NH2	12:I:89:GLN:NE2	2.54	0.56
5:B:707:PRO:O	5:B:711:GLU:HG3	2.06	0.56
5:B:906:SER:O	5:B:941:LEU:HD23	2.05	0.56
7:D:160:VAL:O	7:D:164:ILE:HG13	2.06	0.56
13:J:64:ASN:ND2	13:J:65:PRO:HD3	2.21	0.56
4:A:55:ASP:C	4:A:57:ARG:N	2.52	0.56
4:A:262:LEU:O	4:A:264:PHE:N	2.39	0.56
4:A:1341:ILE:CG2	4:A:1342:GLU:H	2.18	0.56
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.41	0.56
5:B:640:VAL:O	5:B:641:GLU:C	2.49	0.56
5:B:981:ALA:HB2	5:B:987:LYS:HA	1.87	0.56
10:G:117:GLN:O	10:G:119:LEU:N	2.37	0.56
4:A:68:GLN:O	4:A:70:CYS:N	2.34	0.56
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.86	0.56
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.88	0.56
5:B:176:SER:O	5:B:182:SER:HB3	2.05	0.56
5:B:299:GLU:HB3	5:B:571:PRO:HG3	1.87	0.56
5:B:365:THR:HG23	5:B:367:LEU:N	2.13	0.56
5:B:1099:VAL:C	5:B:1101:ASP:H	2.14	0.56
9:F:138:LEU:HB3	9:F:139:PRO:HD2	1.87	0.56
14:K:10:PHE:N	14:K:10:PHE:HD2	2.03	0.56
14:K:46:ILE:O	14:K:50:LEU:HB2	2.04	0.56
1:T:12:DA:H2''	1:T:13:DC:O5'	2.05	0.56
4:A:442:VAL:HB	4:A:489:LEU:HD11	1.87	0.56
4:A:903:ASN:C	4:A:903:ASN:ND2	2.63	0.56
4:A:947:PHE:HD2	4:A:954:TRP:CZ2	2.24	0.56
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.69	0.56
4:A:1164:PRO:HG2	4:A:1165:GLU:H	1.71	0.56
5:B:260:GLY:O	5:B:267:ARG:HD3	2.06	0.56
5:B:305:VAL:O	5:B:305:VAL:HG12	2.05	0.56
5:B:405:ARG:CZ	5:B:632:ARG:HG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:731:VAL:HG12	5:B:732:SER:N	2.20	0.56
5:B:1087:PHE:HD2	5:B:1088:GLY:N	2.04	0.56
6:C:203:GLN:HG2	6:C:207:CYS:SG	2.46	0.56
6:C:248:ILE:HD13	14:K:101:LEU:HD22	1.88	0.56
8:E:3:GLN:HG3	8:E:4:GLU:N	2.20	0.56
9:F:81:THR:HB	9:F:136:ARG:HH11	1.70	0.56
9:F:111:LEU:H	9:F:111:LEU:CD1	2.15	0.56
11:H:89:LEU:C	11:H:91:ASP:N	2.63	0.56
12:I:33:SER:O	12:I:35:VAL:HG23	2.06	0.56
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	2.21	0.55
4:A:577:ILE:C	4:A:579:SER:N	2.62	0.55
4:A:1149:ALA:CB	12:I:47:GLU:HA	2.36	0.55
4:A:1214:GLU:O	4:A:1218:GLN:HG2	2.05	0.55
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.14	0.55
5:B:637:LEU:HD21	5:B:742:GLU:OE2	2.05	0.55
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.40	0.55
5:B:861:ASP:OD1	5:B:862:GLN:N	2.39	0.55
11:H:135:LEU:HD13	11:H:137:GLN:HE21	1.71	0.55
12:I:85:PHE:CD1	12:I:99:LEU:HD13	2.41	0.55
14:K:42:LEU:HD21	14:K:46:ILE:HD11	1.88	0.55
14:K:45:LEU:HG	14:K:94:ILE:CD1	2.33	0.55
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.87	0.55
1:T:12:DA:C2	2:N:6:DA:C2	2.94	0.55
4:A:44:THR:O	4:A:44:THR:HG22	2.06	0.55
4:A:482:PHE:O	5:B:989:THR:HG23	2.06	0.55
4:A:605:MET:HE2	4:A:607:ILE:CG1	2.37	0.55
4:A:849:MET:HE3	4:A:1061:GLY:CA	2.36	0.55
5:B:222:ILE:O	5:B:240:ILE:HA	2.06	0.55
5:B:259:TYR:HB2	5:B:268:THR:HG23	1.88	0.55
5:B:310:MET:O	5:B:313:MET:HB2	2.06	0.55
5:B:906:SER:HA	5:B:946:ASN:HB2	1.88	0.55
5:B:1196:ILE:HB	5:B:1197:PRO:HD2	1.88	0.55
6:C:152:GLU:HG2	6:C:153:LEU:H	1.72	0.55
10:G:14:HIS:CD2	10:G:16:SER:HB2	2.41	0.55
3:P:2:U:O2'	3:P:3:U:H5'	2.06	0.55
4:A:709:THR:HG21	12:I:93:LYS:O	2.06	0.55
4:A:768:GLN:CG	4:A:816:HIS:HA	2.36	0.55
4:A:867:ILE:HG22	4:A:872:GLY:N	2.22	0.55
4:A:1125:ALA:C	4:A:1127:ASP:H	2.14	0.55
5:B:226:PHE:HA	5:B:395:GLN:HG3	1.86	0.55
5:B:515:HIS:CD2	5:B:517:THR:H	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1065:GLN:HE21	5:B:1067:ARG:HG2	1.72	0.55
8:E:198:ILE:CD1	8:E:212:ARG:HG3	2.36	0.55
10:G:9:LEU:HG	10:G:10:ASN:N	2.20	0.55
11:H:116:TYR:HE2	11:H:140:ALA:CB	2.19	0.55
4:A:22:PHE:CE1	5:B:1213:THR:HG22	2.42	0.55
4:A:69:THR:C	4:A:71:GLN:N	2.61	0.55
4:A:278:THR:O	4:A:278:THR:HG22	2.07	0.55
4:A:416:ARG:O	4:A:417:TYR:HD2	1.89	0.55
5:B:44:VAL:O	5:B:45:SER:C	2.49	0.55
5:B:332:ASP:O	5:B:334:ILE:N	2.37	0.55
5:B:446:LEU:O	5:B:447:ALA:HB3	2.06	0.55
5:B:1135:ARG:O	5:B:1139:ILE:HG13	2.07	0.55
8:E:124:VAL:HG13	8:E:132:ILE:CB	2.35	0.55
12:I:71:SER:OG	12:I:83:ASN:HB2	2.07	0.55
4:A:34:LYS:CB	4:A:36:ARG:HE	2.18	0.55
4:A:69:THR:C	4:A:71:GLN:H	2.15	0.55
4:A:567:LYS:HB3	11:H:95:TYR:CA	2.35	0.55
4:A:1260:LEU:O	4:A:1260:LEU:HG	2.07	0.55
10:G:44:TYR:O	10:G:78:VAL:HG12	2.07	0.55
4:A:317:LYS:O	4:A:318:SER:CB	2.55	0.55
4:A:1349:TYR:CB	4:A:1372:VAL:HG21	2.36	0.55
4:A:1402:PHE:CE1	4:A:1403:GLU:HG3	2.42	0.55
4:A:1445:ILE:HD12	10:G:59:GLY:O	2.07	0.55
5:B:94:LYS:O	5:B:130:VAL:HG13	2.07	0.55
5:B:778:MET:CE	5:B:1094:ARG:CD	2.85	0.55
7:D:153:ARG:C	7:D:154:PHE:CD1	2.85	0.55
11:H:127:GLY:O	11:H:128:ASN:HB2	2.06	0.55
4:A:154:SER:HB3	4:A:162:VAL:HG21	1.89	0.55
4:A:590:ARG:HH11	4:A:590:ARG:CG	2.19	0.55
4:A:816:HIS:CD2	5:B:764:SER:HB2	2.42	0.55
4:A:843:LYS:HD3	4:A:846:GLU:OE2	2.07	0.55
4:A:845:LEU:HD22	4:A:1374:VAL:HG21	1.89	0.55
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	2.06	0.55
4:A:1265:ASN:C	4:A:1267:MET:N	2.64	0.55
5:B:358:LYS:HA	5:B:366:GLN:HB3	1.89	0.55
5:B:637:LEU:O	5:B:690:VAL:HG13	2.06	0.55
5:B:705:MET:HE2	5:B:745:PRO:HB3	1.89	0.55
6:C:31:ASN:O	6:C:34:ARG:N	2.40	0.55
2:N:1:DC:H1'	2:N:2:DA:C5'	2.37	0.55
4:A:10:PRO:O	5:B:1193:GLN:HB3	2.06	0.55
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:767:GLN:HB2	4:A:799:PHE:HD1	1.71	0.55
4:A:785:PRO:HG2	4:A:786:HIS:CD2	2.41	0.55
4:A:942:PHE:C	4:A:942:PHE:CD2	2.85	0.55
4:A:1035:TYR:O	4:A:1037:LEU:HD23	2.07	0.55
5:B:361:LEU:N	5:B:362:PRO:CD	2.70	0.55
5:B:797:TYR:C	5:B:798:TYR:HD2	2.15	0.55
5:B:806:THR:CG2	5:B:808:ALA:HB3	2.37	0.55
15:L:25:ALA:O	15:L:26:THR:HB	2.07	0.55
4:A:265:LYS:HE2	4:A:322:VAL:HG13	1.89	0.55
4:A:308:ILE:HG22	4:A:309:ALA:H	1.71	0.55
4:A:709:THR:HB	4:A:712:GLU:HG3	1.88	0.55
4:A:873:MET:C	4:A:1058:VAL:HG23	2.31	0.55
4:A:981:LEU:HD23	4:A:1039:LYS:HA	1.87	0.55
5:B:215:GLN:HA	5:B:215:GLN:NE2	2.21	0.55
5:B:351:TYR:CE1	5:B:355:ILE:HD11	2.42	0.55
5:B:866:TYR:O	5:B:868:MET:N	2.40	0.55
6:C:45:ALA:O	6:C:159:ALA:HA	2.07	0.55
6:C:147:LEU:HD12	6:C:151:GLN:O	2.07	0.55
6:C:187:LYS:C	6:C:189:THR:H	2.15	0.55
9:F:76:LYS:O	9:F:79:ARG:HD3	2.07	0.55
4:A:853:ASP:OD1	4:A:855:THR:CB	2.55	0.55
5:B:69:LEU:HD22	5:B:429:PHE:HE1	1.71	0.55
5:B:473:MET:O	5:B:475:SER:N	2.40	0.55
5:B:640:VAL:O	5:B:640:VAL:HG12	2.07	0.55
5:B:758:PHE:CE1	5:B:1027:ILE:CG2	2.90	0.55
5:B:874:PHE:HA	5:B:913:GLY:O	2.06	0.55
5:B:1172:ILE:HG22	5:B:1172:ILE:O	2.07	0.55
10:G:73:LYS:HE2	10:G:74:TYR:O	2.07	0.55
4:A:598:LEU:O	4:A:599:SER:C	2.49	0.54
5:B:953:LEU:CD2	5:B:965:LYS:HB2	2.35	0.54
5:B:1099:VAL:HG12	5:B:1100:ASP:H	1.71	0.54
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.42	0.54
12:I:52:ILE:HG13	12:I:52:ILE:O	2.06	0.54
12:I:59:VAL:C	12:I:61:ASP:H	2.15	0.54
15:L:30:ILE:O	15:L:56:LEU:HA	2.07	0.54
15:L:49:LYS:O	15:L:50:ASP:CB	2.54	0.54
15:L:58:LYS:O	15:L:58:LYS:HG2	2.06	0.54
1:T:20:DC:H4'	4:A:447:GLN:HE22	1.71	0.54
4:A:19:PHE:HE1	4:A:1396:ALA:HB3	1.71	0.54
4:A:718:VAL:O	4:A:721:PHE:HB2	2.08	0.54
4:A:1191:TRP:CD1	4:A:1256:GLU:HB2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1291:VAL:HG13	4:A:1292:PRO:CD	2.35	0.54
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.22	0.54
5:B:180:TYR:HD1	5:B:180:TYR:H	1.54	0.54
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.88	0.54
12:I:60:GLN:NE2	12:I:107:SER:OG	2.40	0.54
13:J:5:VAL:O	13:J:6:ARG:O	2.26	0.54
14:K:53:ASP:C	14:K:55:LYS:H	2.16	0.54
4:A:3:GLY:O	4:A:4:GLN:CB	2.56	0.54
4:A:61:ILE:HG22	4:A:62:ASP:N	2.23	0.54
4:A:244:PRO:CG	4:A:245:PRO:HD3	2.38	0.54
4:A:767:GLN:NE2	4:A:774:ARG:HB3	2.22	0.54
4:A:808:LEU:HG	4:A:812:GLU:HB3	1.89	0.54
4:A:1441:PHE:CE2	9:F:89:GLU:HG2	2.42	0.54
5:B:865:LYS:HE2	5:B:871:THR:OG1	2.06	0.54
5:B:1006:ILE:HD13	13:J:44:TYR:CE2	2.43	0.54
5:B:1223:ASP:O	5:B:1224:PHE:HB2	2.08	0.54
7:D:56:ARG:HD3	7:D:149:THR:HA	1.88	0.54
8:E:124:VAL:HG13	8:E:132:ILE:HD12	1.88	0.54
1:T:12:DA:H2''	1:T:13:DC:C5'	2.37	0.54
1:T:18:DC:P	1:T:18:DC:H3'	2.48	0.54
4:A:219:PHE:O	4:A:222:LEU:O	2.25	0.54
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.35	0.54
5:B:459:TYR:CE1	5:B:469:GLN:HG2	2.42	0.54
6:C:73:GLN:HE21	6:C:75:MET:N	2.05	0.54
8:E:22:MET:HE3	8:E:26:ARG:HH21	1.72	0.54
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.34	0.54
4:A:840:ARG:O	4:A:841:LEU:C	2.51	0.54
4:A:979:SER:OG	4:A:980:ASP:N	2.41	0.54
4:A:1074:GLU:N	4:A:1075:PRO:HD2	2.23	0.54
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.08	0.54
7:D:209:ARG:O	7:D:212:LYS:HB2	2.08	0.54
9:F:119:ARG:HG3	9:F:119:ARG:NH1	2.23	0.54
4:A:3:GLY:O	4:A:4:GLN:HB2	2.08	0.54
4:A:182:VAL:HG22	4:A:201:VAL:HA	1.89	0.54
4:A:779:PHE:O	4:A:780:VAL:C	2.51	0.54
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.06	0.54
5:B:825:VAL:HG12	5:B:826:ALA:N	2.21	0.54
7:D:40:HIS:HB2	10:G:73:LYS:HZ2	1.69	0.54
14:K:47:ARG:C	14:K:47:ARG:HD2	2.32	0.54
4:A:265:LYS:NZ	4:A:322:VAL:HG13	2.23	0.54
4:A:316:GLN:O	4:A:317:LYS:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:MET:HE2	4:A:607:ILE:HG13	1.89	0.54
4:A:1346:ALA:HB3	8:E:149:LEU:HD13	1.89	0.54
5:B:796:LEU:HD12	5:B:852:ARG:O	2.08	0.54
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.07	0.54
7:D:39:ASN:ND2	7:D:41:GLN:HB2	2.23	0.54
12:I:51:ASN:O	12:I:54:GLU:HG3	2.08	0.54
15:L:39:SER:O	15:L:40:LEU:HG	2.08	0.54
4:A:41:MET:HB3	4:A:48:ALA:O	2.08	0.54
4:A:774:ARG:NH2	4:A:797:LYS:HB2	2.23	0.54
4:A:831:THR:HG23	4:A:832:ALA:N	2.21	0.54
5:B:130:VAL:HB	5:B:167:ILE:CD1	2.38	0.54
5:B:185:THR:O	5:B:188:ASP:HB2	2.07	0.54
5:B:205:ILE:N	5:B:205:ILE:HD12	2.23	0.54
5:B:1152:MET:HE1	5:B:1157:ALA:HA	1.89	0.54
6:C:8:VAL:HG12	6:C:9:LYS:H	1.73	0.54
6:C:46:ILE:HD12	6:C:67:LEU:HB3	1.89	0.54
7:D:167:LEU:O	7:D:170:THR:OG1	2.26	0.54
8:E:85:GLU:HB2	8:E:88:VAL:HG22	1.89	0.54
11:H:102:TYR:N	11:H:102:TYR:CD2	2.76	0.54
14:K:65:HIS:HD2	14:K:67:PHE:N	2.05	0.54
4:A:417:TYR:O	4:A:418:SER:C	2.50	0.54
4:A:910:PRO:HB3	4:A:917:SER:N	2.22	0.54
5:B:576:ASP:HA	5:B:622:LYS:HZ2	1.73	0.54
5:B:653:VAL:HG22	5:B:689:LEU:HD13	1.90	0.54
5:B:658:ILE:HG22	5:B:659:ALA:N	2.22	0.54
5:B:843:GLN:O	5:B:844:SER:C	2.51	0.54
5:B:948:ILE:O	5:B:968:VAL:HG13	2.08	0.54
5:B:1099:VAL:HG12	5:B:1100:ASP:N	2.23	0.54
6:C:116:LYS:HD3	6:C:140:ASN:CB	2.27	0.54
12:I:103:CYS:HB3	12:I:106:CYS:SG	2.48	0.54
14:K:15:GLY:O	14:K:16:GLU:HG3	2.08	0.54
4:A:144:THR:O	4:A:146:MET:HE2	2.08	0.53
4:A:172:PRO:HG3	4:A:185:TRP:CZ2	2.43	0.53
4:A:472:LEU:O	4:A:475:THR:HG22	2.07	0.53
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.38	0.53
4:A:1254:ALA:O	4:A:1255:GLU:HB2	2.07	0.53
4:A:1329:THR:HG23	4:A:1331:SER:H	1.73	0.53
5:B:1001:PHE:CD2	6:C:34:ARG:NH2	2.76	0.53
5:B:1183:LYS:C	5:B:1185:CYS:H	2.16	0.53
7:D:7:THR:HG21	7:D:32:GLU:OE2	2.08	0.53
7:D:39:ASN:HD22	7:D:41:GLN:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:89:GLU:HB3	9:F:134:ILE:CD1	2.39	0.53
11:H:99:GLY:HA3	11:H:118:PHE:HA	1.89	0.53
4:A:130:ASP:O	4:A:133:LYS:N	2.39	0.53
4:A:714:PHE:O	4:A:718:VAL:HG23	2.08	0.53
4:A:806:ARG:HH12	5:B:729:ILE:CD1	2.20	0.53
5:B:39:ARG:HG2	5:B:39:ARG:HH11	1.73	0.53
5:B:1084:GLN:OE1	6:C:189:THR:CG2	2.57	0.53
6:C:259:LEU:HD13	14:K:91:CYS:HB2	1.90	0.53
11:H:58:THR:HG22	11:H:59:ILE:N	2.23	0.53
13:J:1:MET:H1	13:J:56:LEU:HB2	1.73	0.53
4:A:167:CYS:O	4:A:167:CYS:SG	2.66	0.53
4:A:347:PHE:CE2	4:A:375:THR:HG23	2.43	0.53
4:A:940:ARG:HG2	4:A:940:ARG:HH11	1.72	0.53
4:A:1225:PHE:HE2	4:A:1227:ILE:HD11	1.72	0.53
5:B:485:ARG:NH2	5:B:782:LEU:HD11	2.23	0.53
5:B:1162:ILE:O	5:B:1171:VAL:HG21	2.08	0.53
6:C:142:VAL:H	13:J:16:ASP:HB3	1.72	0.53
10:G:88:ASP:OD2	10:G:88:ASP:N	2.42	0.53
11:H:5:LEU:HD22	11:H:133:ASN:O	2.09	0.53
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.90	0.53
4:A:846:GLU:OE1	4:A:1425:SER:OG	2.27	0.53
4:A:858:ASN:HD22	4:A:861:GLY:H	1.56	0.53
5:B:563:MET:HE1	5:B:580:VAL:HB	1.89	0.53
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.74	0.53
6:C:35:ARG:NH1	14:K:41:THR:H	2.06	0.53
6:C:101:LEU:HD13	6:C:118:LEU:HD23	1.90	0.53
6:C:125:MET:HB2	6:C:127:ARG:NH2	2.23	0.53
8:E:124:VAL:HG13	8:E:132:ILE:CG1	2.39	0.53
10:G:61:ILE:HG23	10:G:66:GLY:O	2.08	0.53
11:H:56:THR:HB	11:H:145:ARG:HG2	1.90	0.53
11:H:62:SER:O	11:H:63:LEU:C	2.52	0.53
14:K:110:ASN:C	14:K:112:GLN:H	2.16	0.53
4:A:504:LEU:HD12	4:A:504:LEU:N	2.24	0.53
4:A:921:GLY:O	4:A:922:ASP:C	2.51	0.53
7:D:49:ALA:HB2	7:D:174:PRO:CB	2.37	0.53
7:D:53:SER:HB3	7:D:152:SER:HB2	1.91	0.53
10:G:102:GLN:HG3	10:G:106:MET:O	2.08	0.53
11:H:128:ASN:CG	11:H:128:ASN:O	2.51	0.53
12:I:34:TYR:CD2	12:I:34:TYR:C	2.87	0.53
14:K:50:LEU:HD11	14:K:75:ILE:CD1	2.37	0.53
4:A:68:GLN:HE22	4:A:80:HIS:CG	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:84:ILE:O	4:A:84:ILE:HG23	2.07	0.53
4:A:332:LYS:O	4:A:333:GLU:HB2	2.09	0.53
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.91	0.53
4:A:665:GLY:HA2	5:B:1026:LEU:HD22	1.91	0.53
4:A:971:PHE:CE2	4:A:1040:GLN:HG2	2.44	0.53
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.73	0.53
6:C:215:GLU:O	6:C:216:GLY:C	2.51	0.53
8:E:207:ARG:CB	8:E:207:ARG:HH11	2.20	0.53
12:I:85:PHE:CD2	12:I:85:PHE:N	2.74	0.53
13:J:44:TYR:CA	13:J:47:ARG:HB2	2.33	0.53
4:A:658:LEU:HD13	5:B:831:SER:HA	1.90	0.53
4:A:786:HIS:CD2	4:A:786:HIS:N	2.74	0.53
4:A:1372:VAL:O	4:A:1376:THR:HG22	2.07	0.53
5:B:483:LEU:HD11	5:B:491:THR:CG2	2.32	0.53
9:F:86:THR:HG23	9:F:89:GLU:OE1	2.09	0.53
15:L:48:CYS:HB3	15:L:51:CYS:O	2.08	0.53
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.72	0.53
4:A:503:GLN:HE21	9:F:90:ARG:HH21	1.55	0.53
4:A:1120:LEU:CD1	4:A:1120:LEU:H	2.22	0.53
4:A:1198:ASP:HB3	4:A:1201:ALA:HB3	1.90	0.53
4:A:1283:VAL:CG1	4:A:1284:MET:H	2.17	0.53
4:A:1289:ARG:NH1	4:A:1326:ARG:NH1	2.56	0.53
5:B:287:ARG:NH1	5:B:324:ILE:O	2.41	0.53
5:B:745:PRO:O	5:B:747:MET:N	2.41	0.53
8:E:78:LEU:HD21	8:E:80:VAL:CG2	2.37	0.53
10:G:34:VAL:CG1	10:G:45:ILE:HG21	2.36	0.53
11:H:15:VAL:HG22	11:H:26:ILE:CD1	2.39	0.53
11:H:103:LYS:HG2	11:H:104:PHE:N	2.24	0.53
14:K:55:LYS:HB3	14:K:81:TYR:CD1	2.44	0.53
4:A:262:LEU:C	4:A:264:PHE:N	2.66	0.53
4:A:289:ILE:C	4:A:291:GLU:H	2.17	0.53
4:A:682:THR:CG2	4:A:728:LYS:HE3	2.37	0.53
5:B:126:SER:O	5:B:169:ARG:HA	2.09	0.53
5:B:286:PHE:CD1	5:B:297:ILE:HG23	2.44	0.53
5:B:744:HIS:ND1	5:B:745:PRO:HD2	2.24	0.53
6:C:22:LEU:HD13	6:C:230:MET:HE1	1.90	0.53
8:E:207:ARG:HH11	8:E:207:ARG:HB3	1.74	0.53
10:G:85:GLU:HG2	10:G:86:VAL:N	2.24	0.53
13:J:7:CYS:SG	13:J:46:CYS:HA	2.49	0.53
1:T:19:DC:H2''	1:T:20:DC:C5'	2.39	0.53
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:909:ASP:C	4:A:911:SER:H	2.16	0.53
4:A:1140:HIS:CE1	4:A:1272:THR:HG23	2.43	0.53
4:A:1325:THR:HG23	8:E:146:HIS:O	2.08	0.53
5:B:1001:PHE:CE2	6:C:34:ARG:NE	2.77	0.53
6:C:144:ILE:O	6:C:145:CYS:HB3	2.09	0.53
8:E:22:MET:HE3	8:E:26:ARG:NH2	2.24	0.53
12:I:13:MET:CE	12:I:14:LEU:H	2.22	0.53
14:K:82:ASP:OD1	14:K:84:LYS:N	2.41	0.53
4:A:341:MET:CE	4:A:843:LYS:HZ3	2.21	0.52
4:A:352:VAL:O	4:A:467:THR:HB	2.09	0.52
4:A:524:VAL:CG1	4:A:525:GLN:H	2.21	0.52
4:A:665:GLY:HA2	5:B:1026:LEU:CD2	2.39	0.52
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.90	0.52
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.74	0.52
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.90	0.52
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	1.90	0.52
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.36	0.52
5:B:112:LEU:HD12	5:B:113:TYR:H	1.73	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.52
5:B:999:MET:HB3	5:B:1007:VAL:HG21	1.91	0.52
10:G:13:LEU:CD2	10:G:17:PHE:HB2	2.34	0.52
13:J:27:GLU:O	13:J:29:GLU:N	2.39	0.52
15:L:52:GLY:O	15:L:53:HIS:C	2.51	0.52
4:A:18:GLN:O	5:B:1215:ARG:HG2	2.10	0.52
4:A:24:PRO:HD2	4:A:233:TRP:HE1	1.74	0.52
4:A:79:GLY:HA3	4:A:243:PRO:HG3	1.91	0.52
4:A:523:ILE:CD1	4:A:649:ILE:HG21	2.38	0.52
4:A:527:THR:CG2	4:A:650:GLN:HA	2.40	0.52
4:A:1120:LEU:CD1	4:A:1120:LEU:N	2.72	0.52
4:A:1409:LEU:CD1	5:B:1207:LEU:HD21	2.39	0.52
6:C:53:THR:O	6:C:153:LEU:HA	2.09	0.52
7:D:151:PHE:CD1	7:D:151:PHE:N	2.77	0.52
8:E:83:CYS:HG	8:E:110:PHE:HZ	1.54	0.52
8:E:192:ARG:HH11	8:E:192:ARG:HG3	1.73	0.52
10:G:34:VAL:HG12	10:G:45:ILE:CG2	2.34	0.52
4:A:92:HIS:O	4:A:93:VAL:C	2.52	0.52
4:A:997:LEU:N	4:A:997:LEU:HD23	2.23	0.52
5:B:464:GLY:HA2	5:B:479:VAL:O	2.09	0.52
5:B:705:MET:HA	5:B:705:MET:HE3	1.91	0.52
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.29	0.52
9:F:118:LEU:O	9:F:122:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:143:ILE:HG23	10:G:169:GLY:O	2.09	0.52
14:K:6:ARG:C	14:K:8:GLU:H	2.16	0.52
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.39	0.52
4:A:811:GLN:O	4:A:812:GLU:C	2.53	0.52
4:A:1329:THR:HG21	4:A:1331:SER:HB3	1.92	0.52
5:B:130:VAL:HB	5:B:167:ILE:HD12	1.91	0.52
5:B:558:LEU:HD21	5:B:600:LEU:HD11	1.91	0.52
5:B:811:TYR:N	5:B:811:TYR:CD1	2.78	0.52
5:B:847:ASP:C	5:B:849:GLY:N	2.67	0.52
5:B:880:THR:HB	5:B:934:LYS:HD2	1.92	0.52
8:E:16:PHE:CE2	8:E:20:LYS:HE2	2.44	0.52
9:F:116:ASP:O	9:F:120:ILE:HG13	2.10	0.52
10:G:66:GLY:O	10:G:67:SER:C	2.52	0.52
10:G:117:GLN:C	10:G:119:LEU:N	2.67	0.52
11:H:12:VAL:HA	11:H:28:ALA:HB2	1.92	0.52
13:J:48:ARG:HE	13:J:49:MET:HE2	1.74	0.52
4:A:63:ARG:HA	4:A:74:MET:HE2	1.91	0.52
4:A:255:SER:OG	5:B:918:ILE:HG23	2.09	0.52
4:A:567:LYS:HD2	4:A:568:PRO:CD	2.40	0.52
4:A:699:ALA:HB3	4:A:701:LEU:HG	1.91	0.52
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.09	0.52
4:A:1377:THR:O	4:A:1379:GLY:N	2.42	0.52
5:B:860:MET:HG2	5:B:861:ASP:N	2.25	0.52
5:B:1095:LEU:H	5:B:1095:LEU:CD1	2.19	0.52
6:C:252:GLN:HG3	14:K:95:ILE:HG23	1.92	0.52
7:D:66:ARG:O	7:D:70:PHE:HB2	2.09	0.52
1:T:16:DG:N2	2:N:2:DA:C2	2.78	0.52
4:A:298:PHE:CD2	4:A:299:HIS:N	2.78	0.52
4:A:626:ASN:C	4:A:628:GLY:H	2.16	0.52
4:A:853:ASP:OD2	4:A:855:THR:CG2	2.58	0.52
4:A:996:ASN:C	4:A:998:LEU:HD12	2.35	0.52
4:A:1445:ILE:HD12	4:A:1445:ILE:N	2.07	0.52
5:B:638:PHE:HB3	5:B:651:LEU:HD22	1.90	0.52
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.92	0.52
5:B:1031:LEU:CD2	5:B:1044:ALA:HB2	2.40	0.52
4:A:254:GLU:O	4:A:256:GLN:N	2.41	0.52
4:A:1436:ILE:O	4:A:1437:GLY:C	2.51	0.52
6:C:52:GLU:CD	6:C:154:LYS:HD2	2.34	0.52
9:F:75:PRO:HG2	9:F:78:GLN:HB2	1.92	0.52
10:G:7:LEU:HB2	10:G:74:TYR:HE2	1.67	0.52
10:G:83:LYS:HG2	10:G:149:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:36:CYS:HA	11:H:126:GLU:O	2.09	0.52
12:I:7:CYS:HB3	12:I:14:LEU:HD21	1.90	0.52
4:A:40:THR:HG22	4:A:41:MET:CG	2.28	0.52
4:A:262:LEU:HD12	4:A:328:ARG:NH2	2.24	0.52
4:A:438:ASP:OD1	4:A:461:LYS:HA	2.10	0.52
4:A:623:GLY:C	4:A:625:SER:H	2.17	0.52
4:A:873:MET:C	4:A:1058:VAL:CG2	2.83	0.52
4:A:982:THR:N	4:A:985:ASP:HB2	2.25	0.52
4:A:1021:LEU:O	4:A:1025:ARG:HG2	2.10	0.52
4:A:1313:LEU:HB3	4:A:1338:VAL:HG21	1.92	0.52
5:B:29:ASP:OD1	5:B:658:ILE:HD13	2.10	0.52
5:B:846:ILE:HA	5:B:850:LEU:HB3	1.91	0.52
5:B:899:ILE:CG2	5:B:949:VAL:HG21	2.40	0.52
5:B:983:ARG:HD2	5:B:1091:TYR:HB3	1.92	0.52
11:H:107:VAL:O	11:H:108:SER:O	2.28	0.52
13:J:23:ASN:C	13:J:25:LEU:N	2.66	0.52
4:A:767:GLN:HE21	4:A:774:ARG:HB3	1.75	0.52
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.25	0.52
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.92	0.52
5:B:516:ASN:N	5:B:516:ASN:ND2	2.47	0.52
5:B:616:ILE:HG13	5:B:697:GLU:HG3	1.92	0.52
5:B:782:LEU:HD12	5:B:788:ARG:NH1	2.20	0.52
5:B:806:THR:HB	5:B:809:MET:HG3	1.92	0.52
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.45	0.52
6:C:161:LYS:O	6:C:170:TRP:NE1	2.42	0.52
7:D:210:ILE:O	7:D:214:LEU:HG	2.10	0.52
11:H:58:THR:HG22	11:H:59:ILE:H	1.74	0.52
11:H:113:ALA:HB2	11:H:126:GLU:HG3	1.91	0.52
15:L:28:LYS:HB2	15:L:39:SER:CA	2.39	0.52
1:T:23:DC:H2'	1:T:24:DT:H6	1.71	0.52
4:A:148:CYS:O	4:A:168:GLY:HA2	2.09	0.52
5:B:843:GLN:HB2	5:B:993:THR:HB	1.91	0.52
6:C:86:CYS:O	6:C:88:CYS:N	2.41	0.52
6:C:175:ALA:CB	13:J:43:ARG:HH12	2.23	0.52
6:C:175:ALA:CB	13:J:43:ARG:NH1	2.72	0.52
8:E:157:SER:C	8:E:159:ASP:N	2.68	0.52
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.92	0.52
11:H:104:PHE:CE2	11:H:136:LYS:HG2	2.45	0.52
12:I:6:PHE:HA	12:I:14:LEU:HG	1.92	0.52
12:I:82:GLU:HB3	12:I:104:LEU:CD1	2.39	0.52
14:K:41:THR:HG22	14:K:42:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:230:ARG:H	4:A:233:TRP:HE3	1.52	0.51
4:A:360:GLU:HG3	4:A:459:ARG:HH12	1.73	0.51
4:A:825:ILE:O	4:A:829:VAL:HG23	2.10	0.51
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.92	0.51
4:A:961:ARG:HG3	4:A:961:ARG:NH1	2.24	0.51
4:A:1168:GLU:O	4:A:1172:LEU:HG	2.10	0.51
5:B:368:GLU:O	5:B:370:PHE:N	2.42	0.51
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.40	0.51
5:B:899:ILE:HD11	5:B:910:VAL:O	2.10	0.51
5:B:945:GLU:O	5:B:946:ASN:HB3	2.10	0.51
5:B:992:ILE:HG12	5:B:993:THR:N	2.25	0.51
5:B:1180:PHE:O	5:B:1181:GLU:O	2.27	0.51
12:I:4:PHE:CD1	12:I:4:PHE:C	2.88	0.51
12:I:110:PHE:H	12:I:110:PHE:HD2	1.58	0.51
4:A:320:ARG:NH1	4:A:320:ARG:HG3	2.25	0.51
4:A:451:HIS:CD2	4:A:1074:GLU:HG3	2.45	0.51
4:A:471:ASN:OD1	4:A:472:LEU:N	2.43	0.51
4:A:765:VAL:HG23	4:A:802:ASN:O	2.10	0.51
4:A:958:VAL:HG22	4:A:1052:GLN:HB3	1.92	0.51
4:A:1205:LYS:O	4:A:1206:ASP:C	2.54	0.51
5:B:29:ASP:CG	5:B:658:ILE:HD13	2.35	0.51
5:B:189:LEU:O	5:B:192:LEU:N	2.39	0.51
5:B:360:PHE:C	5:B:360:PHE:CD2	2.88	0.51
5:B:549:THR:HB	5:B:628:THR:OG1	2.10	0.51
5:B:687:GLU:O	5:B:689:LEU:HG	2.11	0.51
5:B:843:GLN:O	5:B:846:ILE:N	2.43	0.51
5:B:1201:LYS:HE2	5:B:1205:GLN:CD	2.35	0.51
6:C:29:MET:HE2	14:K:98:LEU:HG	1.92	0.51
6:C:59:ALA:O	6:C:62:PHE:HB3	2.10	0.51
6:C:99:LEU:HA	6:C:119:VAL:O	2.10	0.51
7:D:24:ALA:C	7:D:26:THR:H	2.18	0.51
15:L:28:LYS:HB2	15:L:39:SER:CB	2.41	0.51
1:T:19:DC:C4	1:T:20:DC:N4	2.79	0.51
4:A:35:ILE:HD13	4:A:241:VAL:HG11	1.93	0.51
4:A:511:ILE:O	4:A:519:PRO:HA	2.10	0.51
4:A:567:LYS:CE	11:H:46:LEU:HB2	2.40	0.51
4:A:730:GLY:O	4:A:732:LEU:N	2.43	0.51
6:C:248:ILE:HG23	14:K:98:LEU:HD22	1.92	0.51
7:D:17:LYS:H	7:D:17:LYS:CD	2.23	0.51
7:D:185:CYS:CB	7:D:211:LEU:HD22	2.40	0.51
8:E:175:LEU:HD23	8:E:176:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:6:DA:C2'	2:N:7:DG:OP2	2.55	0.51
4:A:18:GLN:HB2	5:B:1215:ARG:HB2	1.93	0.51
4:A:69:THR:O	4:A:71:GLN:N	2.43	0.51
4:A:853:ASP:OD2	4:A:855:THR:HG22	2.10	0.51
5:B:957:ASN:O	5:B:958:GLN:C	2.53	0.51
6:C:77:ILE:C	6:C:79:GLN:H	2.18	0.51
7:D:21:GLU:HB2	7:D:22:GLU:OE1	2.11	0.51
7:D:156:ASP:C	7:D:158:GLU:H	2.19	0.51
11:H:40:LEU:HD22	11:H:123:MET:CE	2.40	0.51
1:T:18:DC:H3'	1:T:18:DC:OP1	2.11	0.51
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.46	0.51
4:A:244:PRO:O	4:A:246:VAL:N	2.43	0.51
4:A:261:ASP:O	4:A:264:PHE:HB2	2.11	0.51
4:A:388:LEU:O	4:A:392:VAL:HG23	2.10	0.51
4:A:567:LYS:HE3	11:H:46:LEU:HB2	1.93	0.51
4:A:1208:THR:O	4:A:1212:VAL:HG23	2.10	0.51
4:A:1280:GLU:O	4:A:1281:ARG:C	2.53	0.51
5:B:288:ALA:HA	5:B:331:LEU:HD12	1.91	0.51
5:B:610:ASN:O	5:B:612:GLU:N	2.44	0.51
5:B:1045:SER:O	5:B:1046:PRO:O	2.27	0.51
6:C:253:LYS:O	6:C:256:ALA:HB3	2.10	0.51
11:H:47:PHE:CD2	11:H:95:TYR:HD1	2.28	0.51
4:A:34:LYS:HD3	4:A:34:LYS:H	1.75	0.51
4:A:68:GLN:C	4:A:70:CYS:N	2.68	0.51
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.36	0.51
4:A:320:ARG:HG3	4:A:320:ARG:HH11	1.74	0.51
4:A:349:ALA:C	5:B:1128:LEU:HD11	2.35	0.51
4:A:470:LEU:HD12	4:A:471:ASN:O	2.11	0.51
4:A:831:THR:CG2	4:A:832:ALA:N	2.72	0.51
5:B:1085:ILE:N	5:B:1085:ILE:CD1	2.69	0.51
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.43	0.51
5:B:1142:GLY:C	5:B:1144:ALA:H	2.18	0.51
8:E:22:MET:HE3	8:E:26:ARG:CZ	2.40	0.51
9:F:116:ASP:HB3	9:F:119:ARG:HB2	1.93	0.51
13:J:48:ARG:HD2	13:J:48:ARG:C	2.35	0.51
4:A:367:PRO:HD3	4:A:467:THR:O	2.10	0.51
4:A:913:LEU:HD12	4:A:914:GLU:N	2.23	0.51
4:A:1209:MET:CE	4:A:1236:LEU:HB3	2.40	0.51
4:A:1332:PHE:CD2	4:A:1332:PHE:N	2.74	0.51
5:B:33:VAL:HG12	5:B:681:TRP:HZ3	1.76	0.51
5:B:792:MET:H	5:B:857:ARG:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.46	0.51
7:D:47:LEU:HD12	7:D:48:ILE:N	2.25	0.51
4:A:65:LEU:O	4:A:66:LYS:C	2.53	0.51
4:A:108:MET:N	4:A:108:MET:SD	2.84	0.51
4:A:276:LEU:HD13	4:A:293:GLU:HA	1.93	0.51
4:A:567:LYS:CG	4:A:568:PRO:CD	2.83	0.51
4:A:567:LYS:CB	4:A:568:PRO:CD	2.88	0.51
4:A:596:THR:C	4:A:598:LEU:N	2.69	0.51
4:A:666:ILE:HD11	5:B:1067:ARG:O	2.11	0.51
4:A:1144:LYS:HB2	4:A:1268:LEU:O	2.11	0.51
5:B:102:VAL:CG2	5:B:112:LEU:HD22	2.41	0.51
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.93	0.51
11:H:82:PRO:C	11:H:84:ALA:H	2.15	0.51
4:A:224:PHE:HZ	4:A:234:MET:HE2	1.73	0.51
4:A:317:LYS:O	4:A:318:SER:HB3	2.11	0.51
5:B:197:PHE:CZ	5:B:816:GLU:HG2	2.46	0.51
5:B:882:THR:CB	5:B:934:LYS:O	2.59	0.51
5:B:996:ARG:NH2	6:C:175:ALA:N	2.56	0.51
5:B:1011:ILE:O	5:B:1011:ILE:HG22	2.10	0.51
7:D:134:THR:CG2	7:D:135:GLY:N	2.74	0.51
8:E:28:TYR:CE1	8:E:78:LEU:HD13	2.46	0.51
11:H:130:ARG:HD2	11:H:130:ARG:N	2.21	0.51
12:I:34:TYR:HD2	12:I:35:VAL:N	2.08	0.51
4:A:227:VAL:HG21	7:D:14:ARG:HH12	1.76	0.51
4:A:382:PRO:CA	4:A:428:TYR:HE2	2.24	0.51
4:A:466:SER:HB2	5:B:1099:VAL:HG11	1.93	0.51
4:A:541:ILE:HD13	4:A:549:MET:CE	2.22	0.51
4:A:852:TYR:CD1	9:F:136:ARG:HB3	2.45	0.51
5:B:39:ARG:NH2	5:B:665:GLU:CD	2.69	0.51
5:B:516:ASN:H	5:B:516:ASN:ND2	2.08	0.51
5:B:521:LEU:HD13	5:B:633:VAL:CG1	2.41	0.51
5:B:1002:THR:O	5:B:1004:GLU:N	2.44	0.51
6:C:259:LEU:HD13	14:K:91:CYS:CB	2.41	0.51
8:E:83:CYS:SG	8:E:110:PHE:HZ	2.34	0.51
1:T:13:DC:H2''	1:T:14:DT:O5'	2.11	0.50
4:A:37:PHE:HD1	4:A:37:PHE:H	1.58	0.50
4:A:166:GLY:O	4:A:167:CYS:SG	2.69	0.50
4:A:849:MET:HB3	4:A:1063:MET:SD	2.50	0.50
4:A:1076:ALA:HA	4:A:1079:MET:CE	2.38	0.50
4:A:1315:GLU:C	4:A:1317:MET:H	2.18	0.50
5:B:234:ILE:HD12	5:B:234:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:680:THR:O	5:B:684:LEU:HD12	2.11	0.50
5:B:859:TYR:CZ	5:B:941:LEU:HD12	2.46	0.50
5:B:894:ASP:HB2	15:L:58:LYS:NZ	2.25	0.50
5:B:957:ASN:O	5:B:960:GLY:N	2.44	0.50
5:B:1050:ILE:HG22	5:B:1051:THR:N	2.25	0.50
4:A:7:SER:HB3	5:B:1193:GLN:HE21	1.76	0.50
4:A:89:PRO:O	4:A:204:THR:HG21	2.10	0.50
4:A:283:GLY:O	4:A:285:PRO:CD	2.58	0.50
4:A:852:TYR:CD2	4:A:1060:PRO:CB	2.95	0.50
4:A:870:GLU:HG2	8:E:208:TYR:CD2	2.46	0.50
4:A:878:ILE:HG21	4:A:955:PRO:HB2	1.93	0.50
4:A:1143:LEU:O	4:A:1146:VAL:HG23	2.12	0.50
5:B:205:ILE:O	5:B:207:GLY:N	2.44	0.50
5:B:284:ILE:HG23	5:B:324:ILE:HD12	1.93	0.50
5:B:579:ARG:HG2	5:B:579:ARG:NH1	2.26	0.50
5:B:1198:TYR:O	5:B:1201:LYS:HB3	2.10	0.50
6:C:101:LEU:HD22	6:C:118:LEU:CD2	2.41	0.50
11:H:138:GLU:O	11:H:139:ASN:C	2.53	0.50
13:J:43:ARG:HG2	13:J:46:CYS:SG	2.52	0.50
15:L:46:VAL:O	15:L:46:VAL:HG12	2.10	0.50
4:A:346:ASP:CG	5:B:1108:ARG:HA	2.36	0.50
4:A:537:ARG:NH1	11:H:120:GLY:O	2.43	0.50
4:A:605:MET:HE1	4:A:612:ILE:HG23	1.94	0.50
4:A:907:THR:HG23	4:A:908:LEU:N	2.26	0.50
5:B:593:PRO:O	5:B:594:ALA:C	2.53	0.50
5:B:657:HIS:CE1	5:B:689:LEU:HD11	2.47	0.50
5:B:661:LEU:HD23	5:B:679:TYR:O	2.11	0.50
5:B:893:LEU:HD22	5:B:897:GLY:C	2.36	0.50
11:H:76:THR:O	11:H:76:THR:HG22	2.10	0.50
15:L:40:LEU:HD13	15:L:44:ASP:CB	2.40	0.50
4:A:18:GLN:CB	5:B:1215:ARG:HB2	2.42	0.50
4:A:446:ARG:HB3	4:A:478:TYR:HB3	1.93	0.50
4:A:474:VAL:C	4:A:477:PRO:HD2	2.35	0.50
4:A:492:PRO:O	4:A:493:GLN:NE2	2.45	0.50
5:B:446:LEU:N	5:B:446:LEU:HD23	2.26	0.50
8:E:198:ILE:HD11	8:E:212:ARG:CG	2.42	0.50
4:A:106:VAL:HG13	4:A:112:LYS:N	2.26	0.50
4:A:146:MET:HB3	4:A:171:GLN:O	2.12	0.50
4:A:172:PRO:HB3	4:A:185:TRP:CD2	2.46	0.50
4:A:471:ASN:O	4:A:474:VAL:HG12	2.11	0.50
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1116:LEU:N	4:A:1308:THR:CG2	2.69	0.50
4:A:1343:ALA:O	4:A:1346:ALA:HB3	2.12	0.50
4:A:1445:ILE:HD11	10:G:68:ALA:CB	2.39	0.50
5:B:841:MET:HE1	5:B:980:PHE:CE1	2.47	0.50
5:B:885:MET:HA	5:B:936:ASP:HB2	1.94	0.50
5:B:1162:ILE:HG22	5:B:1163:CYS:H	1.76	0.50
6:C:22:LEU:HD13	6:C:230:MET:CE	2.41	0.50
6:C:66:ARG:NH1	6:C:144:ILE:O	2.43	0.50
9:F:99:LEU:HD12	9:F:103:MET:HG3	1.94	0.50
11:H:103:LYS:HG2	11:H:104:PHE:H	1.75	0.50
4:A:146:MET:HA	4:A:171:GLN:HB2	1.91	0.50
4:A:218:ASP:O	4:A:219:PHE:C	2.53	0.50
4:A:470:LEU:HD22	4:A:487:MET:HE3	1.91	0.50
4:A:600:PRO:HG2	4:A:601:LYS:H	1.75	0.50
4:A:1006:ILE:CD1	8:E:163:GLU:HG3	2.42	0.50
4:A:1152:ILE:HG13	12:I:44:TYR:HD2	1.76	0.50
5:B:69:LEU:HD13	5:B:429:PHE:CD1	2.47	0.50
5:B:190:TYR:HE2	13:J:62:ARG:HB3	1.72	0.50
5:B:240:ILE:HG23	5:B:240:ILE:O	2.10	0.50
5:B:750:GLY:O	5:B:751:VAL:C	2.54	0.50
5:B:780:VAL:HG21	13:J:56:LEU:HD11	1.92	0.50
5:B:956:THR:CG2	5:B:960:GLY:HA2	2.42	0.50
6:C:174:ALA:O	6:C:175:ALA:CB	2.59	0.50
7:D:56:ARG:HA	7:D:148:LEU:HD13	1.94	0.50
10:G:80:LYS:O	10:G:80:LYS:HG2	2.12	0.50
4:A:204:THR:O	4:A:206:GLU:N	2.45	0.50
4:A:265:LYS:NZ	4:A:322:VAL:HG22	2.27	0.50
4:A:331:GLY:O	4:A:332:LYS:O	2.30	0.50
4:A:335:ARG:HA	4:A:339:ASN:HD22	1.76	0.50
4:A:738:LYS:C	4:A:740:LEU:H	2.19	0.50
4:A:982:THR:O	4:A:985:ASP:HB2	2.12	0.50
4:A:1146:VAL:HG11	4:A:1207:LEU:HD12	1.94	0.50
4:A:1323:ASP:C	4:A:1325:THR:N	2.70	0.50
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	2.26	0.50
7:D:29:LEU:O	7:D:30:GLY:C	2.52	0.50
8:E:20:LYS:NZ	8:E:60:PHE:CE1	2.79	0.50
10:G:4:ILE:HG12	10:G:77:VAL:HG22	1.92	0.50
12:I:101:PHE:N	12:I:101:PHE:CD1	2.79	0.50
15:L:27:LEU:HD13	15:L:37:LYS:CE	2.41	0.50
4:A:37:PHE:N	4:A:37:PHE:HD1	2.09	0.50
4:A:241:VAL:HG13	4:A:266:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LYS:CE	4:A:322:VAL:HG13	2.42	0.50
4:A:325:ILE:HG21	5:B:1210:MET:HG3	1.93	0.50
4:A:670:ILE:HG23	4:A:805:LEU:CD2	2.40	0.50
4:A:888:GLY:O	4:A:940:ARG:NH2	2.45	0.50
4:A:901:LEU:N	4:A:926:GLN:NE2	2.52	0.50
4:A:1431:GLY:HA3	5:B:1152:MET:SD	2.52	0.50
5:B:25:ILE:HG23	5:B:658:ILE:CD1	2.41	0.50
5:B:172:ILE:CG2	5:B:173:MET:N	2.75	0.50
5:B:299:GLU:OE2	5:B:572:HIS:HE1	1.94	0.50
5:B:546:SER:OG	5:B:631:GLY:N	2.38	0.50
5:B:1020:ARG:HB2	5:B:1022:THR:HG22	1.94	0.50
6:C:167:HIS:HA	14:K:6:ARG:HH12	1.76	0.50
6:C:242:GLN:HB3	6:C:246:ARG:HG3	1.94	0.50
8:E:17:ARG:O	8:E:20:LYS:HB2	2.11	0.50
8:E:42:PHE:HZ	8:E:58:MET:HE3	1.75	0.50
10:G:17:PHE:N	10:G:17:PHE:CD2	2.78	0.50
14:K:60:ALA:O	14:K:73:LEU:HD12	2.11	0.50
4:A:98:LYS:O	4:A:102:VAL:HG23	2.12	0.50
4:A:119:ASN:O	4:A:122:MET:HB3	2.11	0.50
4:A:351:THR:HG22	5:B:1103:ILE:HA	1.94	0.50
4:A:605:MET:HE3	4:A:606:LEU:N	2.27	0.50
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.52	0.50
4:A:816:HIS:CD2	5:B:764:SER:H	2.29	0.50
4:A:1277:GLU:C	4:A:1279:ILE:H	2.20	0.50
5:B:117:ALA:HA	5:B:122:LEU:HD12	1.93	0.50
5:B:347:LYS:HG3	5:B:348:ARG:N	2.27	0.50
5:B:582:VAL:HA	5:B:626:ILE:O	2.12	0.50
5:B:1038:SER:C	5:B:1040:ASN:N	2.70	0.50
5:B:1106:ARG:HD3	5:B:1126:GLY:O	2.12	0.50
7:D:34:GLN:C	7:D:36:LYS:N	2.67	0.50
8:E:205:SER:O	8:E:207:ARG:N	2.45	0.50
10:G:1:MET:CE	10:G:80:LYS:O	2.60	0.50
12:I:86:PHE:CE1	12:I:100:PHE:HB2	2.47	0.50
14:K:46:ILE:HG21	14:K:87:LEU:HD11	1.94	0.50
4:A:58:LEU:O	4:A:59:GLY:O	2.30	0.49
4:A:88:LYS:HE3	4:A:280:GLU:OE2	2.12	0.49
4:A:345:VAL:HG11	5:B:1130:PHE:HB2	1.95	0.49
4:A:973:ILE:HD13	4:A:1036:ARG:O	2.11	0.49
4:A:1062:GLU:OE2	9:F:88:TYR:OH	2.30	0.49
5:B:311:LEU:O	5:B:312:GLU:C	2.55	0.49
5:B:824:ILE:CG2	5:B:1087:PHE:CE2	2.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HA	5:B:999:MET:HE3	1.93	0.49
6:C:251:LEU:O	6:C:255:VAL:HG23	2.11	0.49
12:I:26:LEU:CD2	12:I:37:GLU:HA	2.39	0.49
13:J:14:VAL:CG1	13:J:50:ILE:HD11	2.41	0.49
14:K:7:PHE:O	14:K:11:LEU:HB2	2.12	0.49
15:L:36:SER:O	15:L:37:LYS:C	2.55	0.49
4:A:28:ARG:O	4:A:29:ALA:C	2.55	0.49
4:A:49:LYS:NZ	4:A:61:ILE:CG1	2.71	0.49
4:A:92:HIS:CD2	4:A:304:MET:HE1	2.45	0.49
5:B:378:LEU:O	5:B:378:LEU:HD12	2.12	0.49
5:B:621:GLU:HG3	5:B:621:GLU:O	2.12	0.49
5:B:745:PRO:C	5:B:747:MET:N	2.69	0.49
5:B:894:ASP:HB2	15:L:58:LYS:HZ3	1.77	0.49
5:B:903:VAL:HG12	5:B:904:ARG:N	2.26	0.49
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.42	0.49
10:G:38:CYS:SG	10:G:44:TYR:CE1	3.03	0.49
11:H:91:ASP:C	11:H:93:TYR:N	2.70	0.49
11:H:116:TYR:HB2	11:H:123:MET:HB3	1.95	0.49
4:A:244:PRO:HG2	4:A:245:PRO:CD	2.41	0.49
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.94	0.49
4:A:696:GLU:OE2	4:A:702:LEU:HD21	2.13	0.49
4:A:844:ALA:C	4:A:845:LEU:HD23	2.38	0.49
4:A:1164:PRO:HG2	4:A:1165:GLU:HG3	1.94	0.49
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.93	0.49
5:B:977:GLY:HA3	5:B:1099:VAL:CB	2.42	0.49
6:C:31:ASN:O	6:C:32:SER:C	2.55	0.49
6:C:73:GLN:HE21	6:C:75:MET:H	1.59	0.49
6:C:259:LEU:HD21	14:K:92:ASN:CG	2.38	0.49
8:E:12:LEU:HD21	8:E:58:MET:SD	2.53	0.49
8:E:55:ARG:C	8:E:57:MET:H	2.19	0.49
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.46	0.49
14:K:17:SER:O	14:K:18:LYS:C	2.54	0.49
4:A:231:PRO:C	4:A:233:TRP:H	2.20	0.49
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.27	0.49
5:B:171:PRO:HD2	5:B:457:LEU:HD13	1.95	0.49
5:B:658:ILE:O	5:B:661:LEU:HB2	2.11	0.49
5:B:846:ILE:CG2	5:B:974:PRO:HG2	2.41	0.49
5:B:918:ILE:HG21	5:B:935:ARG:HH11	1.76	0.49
5:B:1161:HIS:HB3	5:B:1171:VAL:HG11	1.95	0.49
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.93	0.49
8:E:79:TRP:CD1	8:E:96:PHE:HE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:168:TYR:HB3	8:E:170:LEU:HG	1.94	0.49
9:F:103:MET:HE1	10:G:65:ASP:HB2	1.95	0.49
13:J:7:CYS:HB3	13:J:10:CYS:SG	2.51	0.49
14:K:58:PHE:HE2	14:K:74:ARG:HE	1.57	0.49
4:A:108:MET:HE3	4:A:210:ILE:CD1	2.41	0.49
4:A:302:THR:HA	4:A:305:ASP:O	2.12	0.49
4:A:417:TYR:CD2	4:A:417:TYR:N	2.80	0.49
4:A:527:THR:HG21	4:A:650:GLN:HA	1.95	0.49
4:A:590:ARG:HB2	4:A:605:MET:HB3	1.94	0.49
4:A:920:LEU:HD23	4:A:920:LEU:C	2.37	0.49
4:A:929:LEU:CD2	4:A:983:ILE:HG21	2.42	0.49
5:B:35:SER:HA	5:B:811:TYR:CE2	2.37	0.49
5:B:121:ASN:ND2	5:B:207:GLY:HA3	2.28	0.49
5:B:175:ARG:HG2	5:B:175:ARG:NH1	2.24	0.49
5:B:882:THR:HG22	5:B:884:ARG:HB2	1.93	0.49
6:C:27:LEU:O	6:C:28:ALA:C	2.56	0.49
6:C:137:LYS:HB3	6:C:138:GLU:OE1	2.13	0.49
10:G:96:GLN:HA	10:G:121:PHE:CE2	2.48	0.49
11:H:40:LEU:HD12	11:H:122:LEU:O	2.12	0.49
11:H:58:THR:HB	11:H:143:LEU:HB2	1.95	0.49
4:A:2:VAL:HG21	5:B:1157:ALA:O	2.11	0.49
4:A:1317:MET:HG3	4:A:1327:ILE:HG21	1.93	0.49
5:B:224:GLN:O	5:B:238:ALA:HA	2.12	0.49
5:B:237:VAL:HG22	5:B:257:LYS:HA	1.95	0.49
5:B:1166:CYS:HB2	5:B:1215:ARG:HH11	1.75	0.49
7:D:37:GLN:CD	10:G:5:LYS:HZ2	2.17	0.49
10:G:1:MET:O	10:G:3:PHE:CD1	2.65	0.49
4:A:54:ASN:HB3	4:A:247:ARG:HH22	1.78	0.49
4:A:412:ARG:HH22	5:B:1108:ARG:HH22	1.61	0.49
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.44	0.49
4:A:541:ILE:HG21	4:A:549:MET:HE3	1.94	0.49
4:A:590:ARG:NH2	4:A:620:LYS:HB2	2.22	0.49
4:A:744:LYS:HG2	4:A:748:MET:HE2	1.94	0.49
4:A:798:GLY:HA2	4:A:815:PHE:HD1	1.72	0.49
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.94	0.49
4:A:1111:MET:CE	4:A:1330:ASN:OD1	2.60	0.49
4:A:1189:SER:OG	4:A:1190:PRO:HD2	2.13	0.49
4:A:1334:ASP:O	4:A:1336:MET:N	2.45	0.49
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.27	0.49
5:B:31:TRP:CZ3	5:B:34:ILE:HD12	2.48	0.49
6:C:26:ASP:O	6:C:27:LEU:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:70:ILE:HD11	6:C:144:ILE:CG1	2.43	0.49
6:C:70:ILE:HD13	6:C:115:SER:HB3	1.94	0.49
6:C:184:ASN:HD21	6:C:187:LYS:HA	1.77	0.49
6:C:193:TYR:C	6:C:193:TYR:CD1	2.90	0.49
7:D:27:LEU:HD13	7:D:173:HIS:HD2	1.78	0.49
8:E:135:PHE:CB	8:E:140:LEU:HD11	2.37	0.49
4:A:55:ASP:N	4:A:56:PRO:CD	2.76	0.49
4:A:262:LEU:C	4:A:264:PHE:H	2.21	0.49
4:A:648:ASN:O	4:A:649:ILE:C	2.55	0.49
5:B:364:ILE:HG12	5:B:585:VAL:CG1	2.36	0.49
6:C:208:GLU:C	6:C:210:GLU:H	2.21	0.49
8:E:24:LYS:HB3	8:E:30:ILE:HD12	1.95	0.49
12:I:100:PHE:N	12:I:100:PHE:CD1	2.81	0.49
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.47	0.49
4:A:537:ARG:HH12	11:H:122:LEU:HG	1.77	0.49
4:A:711:ARG:NH1	12:I:95:THR:HB	2.27	0.49
4:A:1001:ARG:O	4:A:1002:GLY:O	2.31	0.49
4:A:1273:LEU:HD12	4:A:1273:LEU:N	2.28	0.49
5:B:519:TRP:C	5:B:519:TRP:CD1	2.91	0.49
5:B:654:ARG:H	5:B:657:HIS:HD2	1.61	0.49
5:B:758:PHE:CZ	5:B:1031:LEU:HD22	2.48	0.49
5:B:806:THR:HG22	5:B:808:ALA:CB	2.43	0.49
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.95	0.49
5:B:1156:ASP:HB3	5:B:1197:PRO:HA	1.95	0.49
6:C:191:TYR:CD2	6:C:201:TRP:CD1	3.01	0.49
6:C:258:ILE:HD12	6:C:258:ILE:N	2.28	0.49
4:A:157:ASP:C	4:A:159:THR:N	2.70	0.49
4:A:474:VAL:HG22	4:A:478:TYR:HE1	1.77	0.49
4:A:597:LEU:HD12	4:A:597:LEU:N	2.28	0.49
4:A:699:ALA:O	4:A:700:ASN:HB3	2.13	0.49
4:A:767:GLN:OE1	4:A:799:PHE:HB2	2.13	0.49
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.28	0.49
5:B:661:LEU:HD11	5:B:684:LEU:HD21	1.93	0.49
5:B:796:LEU:HD21	5:B:821:GLN:HE21	1.77	0.49
5:B:824:ILE:HG12	13:J:48:ARG:HH12	1.77	0.49
5:B:1068:GLY:O	5:B:1069:PHE:O	2.31	0.49
5:B:1202:LEU:HD23	5:B:1206:GLU:HG3	1.93	0.49
5:B:1216:LEU:C	5:B:1217:TYR:HD1	2.21	0.49
6:C:40:GLU:HA	6:C:163:ILE:CG2	2.43	0.49
7:D:47:LEU:HD11	10:G:3:PHE:CD2	2.48	0.49
7:D:202:ILE:CG2	7:D:207:LEU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:100:PHE:N	12:I:100:PHE:HD1	2.11	0.49
2:N:5:DT:H2''	2:N:6:DA:OP2	2.13	0.48
4:A:18:GLN:HB3	5:B:1215:ARG:HG3	1.93	0.48
4:A:105:CYS:O	4:A:114:LEU:HG	2.13	0.48
4:A:150:THR:HG22	4:A:150:THR:O	2.13	0.48
4:A:416:ARG:HG3	4:A:417:TYR:CD2	2.48	0.48
4:A:655:PHE:O	4:A:658:LEU:HB3	2.13	0.48
5:B:181:LEU:HD22	5:B:189:LEU:HD22	1.95	0.48
5:B:652:LYS:HB3	5:B:689:LEU:CD2	2.43	0.48
5:B:745:PRO:C	5:B:747:MET:H	2.21	0.48
5:B:996:ARG:NH1	6:C:38:ILE:HG23	2.27	0.48
6:C:113:VAL:HG23	6:C:147:LEU:HD21	1.95	0.48
6:C:183:TRP:CE2	6:C:207:CYS:HB3	2.47	0.48
8:E:42:PHE:HZ	8:E:58:MET:CE	2.25	0.48
9:F:109:VAL:HG12	9:F:110:ASP:H	1.78	0.48
13:J:57:ILE:HA	13:J:60:PHE:CD2	2.34	0.48
15:L:52:GLY:O	15:L:54:ARG:N	2.46	0.48
15:L:70:ARG:HG2	15:L:70:ARG:NH1	2.27	0.48
4:A:35:ILE:HG22	4:A:35:ILE:O	2.11	0.48
4:A:244:PRO:O	4:A:247:ARG:N	2.42	0.48
4:A:266:LEU:HD21	4:A:303:TYR:CE1	2.48	0.48
4:A:285:PRO:CG	4:A:288:ALA:HB3	2.43	0.48
4:A:353:ILE:HB	4:A:470:LEU:HD23	1.96	0.48
4:A:722:LEU:HD21	4:A:794:PRO:HB3	1.95	0.48
4:A:912:LEU:O	4:A:979:SER:N	2.44	0.48
4:A:1210:GLY:O	4:A:1214:GLU:HG2	2.13	0.48
5:B:253:THR:HG22	5:B:254:LEU:N	2.27	0.48
5:B:265:SER:O	5:B:266:ALA:CB	2.61	0.48
5:B:435:THR:CG2	5:B:437:GLU:HB2	2.43	0.48
5:B:661:LEU:C	5:B:663:ALA:H	2.20	0.48
5:B:1034:VAL:HG12	5:B:1035:ALA:N	2.27	0.48
7:D:51:ASN:O	7:D:52:LEU:O	2.31	0.48
7:D:59:ILE:HG21	7:D:145:MET:SD	2.53	0.48
7:D:219:THR:HG22	7:D:220:LEU:O	2.13	0.48
8:E:168:TYR:CB	8:E:170:LEU:HG	2.43	0.48
10:G:1:MET:HE1	10:G:80:LYS:O	2.13	0.48
10:G:25:TYR:CE2	10:G:29:LYS:HD2	2.48	0.48
11:H:127:GLY:HA3	11:H:130:ARG:NH2	2.28	0.48
12:I:55:THR:HG22	12:I:58:VAL:CG2	2.44	0.48
14:K:47:ARG:HD2	14:K:47:ARG:O	2.13	0.48
1:T:24:DT:H2''	1:T:25:DC:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:26:DA:H2''	1:T:27:DT:O5'	2.11	0.48
4:A:23:SER:O	4:A:24:PRO:C	2.53	0.48
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.42	0.48
5:B:615:MET:C	5:B:616:ILE:HD12	2.36	0.48
5:B:840:ILE:HD13	5:B:994:TYR:CE1	2.49	0.48
5:B:942:ARG:O	5:B:944:THR:N	2.46	0.48
7:D:47:LEU:CD1	10:G:3:PHE:HD2	2.26	0.48
7:D:144:THR:HG21	10:G:46:LEU:HD13	1.95	0.48
9:F:81:THR:HB	9:F:136:ARG:NH1	2.28	0.48
12:I:78:CYS:SG	12:I:103:CYS:SG	2.99	0.48
4:A:441:PRO:HD2	4:A:498:ARG:CZ	2.43	0.48
4:A:444:PHE:HB3	4:A:458:HIS:CD2	2.49	0.48
4:A:1115:SER:O	4:A:1311:VAL:HG22	2.14	0.48
4:A:1441:PHE:CZ	9:F:89:GLU:HA	2.48	0.48
5:B:56:ASP:CB	5:B:57:TYR:HD1	2.26	0.48
5:B:769:TYR:O	5:B:772:ALA:N	2.45	0.48
5:B:806:THR:C	5:B:808:ALA:N	2.69	0.48
5:B:827:ILE:O	5:B:1085:ILE:HG23	2.13	0.48
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.13	0.48
6:C:132:PRO:O	6:C:134:ILE:HG13	2.14	0.48
11:H:139:ASN:O	11:H:140:ALA:HB2	2.13	0.48
12:I:13:MET:HE3	12:I:14:LEU:H	1.78	0.48
14:K:87:LEU:O	14:K:88:LYS:C	2.56	0.48
4:A:41:MET:O	4:A:50:ILE:HG13	2.14	0.48
4:A:44:THR:O	4:A:45:GLN:CB	2.62	0.48
4:A:567:LYS:HD3	11:H:95:TYR:HA	1.95	0.48
4:A:663:SER:HA	5:B:1014:PRO:HB3	1.95	0.48
4:A:1007:ILE:O	4:A:1010:ALA:N	2.46	0.48
4:A:1193:LEU:HD21	4:A:1267:MET:HE2	1.96	0.48
4:A:1437:GLY:HA3	9:F:88:TYR:CD2	2.49	0.48
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.49	0.48
6:C:142:VAL:O	6:C:142:VAL:HG12	2.13	0.48
7:D:12:ARG:HH21	7:D:12:ARG:CB	2.22	0.48
11:H:8:ASP:HB3	11:H:10:PHE:CE1	2.49	0.48
12:I:29:CYS:SG	12:I:32:CYS:SG	3.12	0.48
13:J:1:MET:H1	13:J:56:LEU:CB	2.25	0.48
4:A:427:GLN:O	4:A:428:TYR:C	2.56	0.48
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.21	0.48
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.29	0.48
5:B:65:GLU:HG3	5:B:66:ASP:OD1	2.13	0.48
5:B:843:GLN:O	5:B:846:ILE:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1072:MET:HE3	5:B:1085:ILE:HD13	1.96	0.48
6:C:184:ASN:ND2	6:C:187:LYS:HA	2.29	0.48
8:E:39:LEU:O	8:E:42:PHE:HB3	2.12	0.48
9:F:97:ARG:HG3	9:F:101:ILE:HD11	1.95	0.48
10:G:88:ASP:HB3	10:G:144:ARG:HA	1.95	0.48
12:I:15:TYR:N	12:I:15:TYR:CD1	2.82	0.48
14:K:53:ASP:C	14:K:55:LYS:N	2.70	0.48
4:A:116:ASP:C	4:A:118:HIS:N	2.70	0.48
4:A:116:ASP:O	4:A:118:HIS:N	2.47	0.48
4:A:1134:ILE:O	4:A:1138:ILE:HG13	2.13	0.48
5:B:51:PHE:CD2	5:B:173:MET:HB3	2.48	0.48
5:B:521:LEU:HD13	5:B:633:VAL:HG12	1.95	0.48
5:B:563:MET:HE2	5:B:587:HIS:O	2.14	0.48
5:B:589:VAL:CG1	5:B:590:HIS:H	2.04	0.48
5:B:654:ARG:HG3	5:B:654:ARG:NH1	2.28	0.48
5:B:1002:THR:O	5:B:1005:GLY:N	2.43	0.48
7:D:156:ASP:C	7:D:158:GLU:N	2.71	0.48
10:G:14:HIS:CD2	10:G:16:SER:CB	2.96	0.48
11:H:101:ALA:HB2	11:H:116:TYR:CE1	2.49	0.48
14:K:85:ASP:O	14:K:88:LYS:HB2	2.13	0.48
15:L:33:GLU:OE2	15:L:55:ILE:HD11	2.14	0.48
4:A:19:PHE:HB3	4:A:1413:GLY:CA	2.43	0.48
4:A:666:ILE:HD12	4:A:667:GLY:N	2.26	0.48
4:A:836:TYR:CD2	4:A:840:ARG:HD2	2.49	0.48
4:A:886:ILE:HG13	4:A:943:LEU:CD1	2.43	0.48
4:A:1389:PHE:CD1	4:A:1390:ASN:N	2.82	0.48
5:B:309:GLN:O	5:B:312:GLU:HB3	2.13	0.48
5:B:1156:ASP:O	5:B:1157:ALA:O	2.32	0.48
7:D:16:LYS:HD3	7:D:16:LYS:H	1.78	0.48
11:H:44:VAL:HG13	11:H:48:PRO:HA	1.96	0.48
3:P:8:A:C2'	3:P:9:G:H5'	2.44	0.48
4:A:35:ILE:HD12	4:A:83:HIS:O	2.13	0.48
4:A:699:ALA:O	4:A:700:ASN:CB	2.61	0.48
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.46	0.48
4:A:1206:ASP:C	4:A:1274:ARG:NH1	2.71	0.48
4:A:1279:ILE:HD11	4:A:1316:VAL:HG22	1.95	0.48
5:B:261:ARG:NH1	5:B:261:ARG:HB3	2.29	0.48
5:B:314:LEU:O	5:B:317:CYS:HB3	2.14	0.48
5:B:552:MET:C	5:B:554:ILE:H	2.22	0.48
5:B:683:SER:O	5:B:687:GLU:HB2	2.14	0.48
5:B:785:TYR:CD1	5:B:785:TYR:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1174:LYS:O	5:B:1176:ASN:N	2.47	0.48
6:C:6:PRO:CB	6:C:25:VAL:HG12	2.41	0.48
12:I:50:THR:HG22	12:I:52:ILE:H	1.79	0.48
13:J:31:ASP:O	13:J:32:GLU:C	2.57	0.48
3:P:5:A:H2'	3:P:6:G:C8	2.49	0.48
4:A:224:PHE:CE1	4:A:231:PRO:HG3	2.49	0.48
4:A:622:VAL:O	4:A:622:VAL:HG13	2.14	0.48
4:A:939:ASP:OD2	4:A:1020:CYS:HA	2.14	0.48
4:A:1120:LEU:N	4:A:1120:LEU:HD12	2.29	0.48
4:A:1162:VAL:HG11	12:I:41:PRO:HG3	1.96	0.48
5:B:166:PHE:C	5:B:167:ILE:HG13	2.39	0.48
5:B:280:ILE:CG2	5:B:285:ILE:HG13	2.43	0.48
5:B:863:GLU:O	5:B:961:LEU:HD22	2.14	0.48
5:B:1183:LYS:N	5:B:1183:LYS:CE	2.76	0.48
7:D:151:PHE:CE2	10:G:89:GLY:HA2	2.49	0.48
14:K:7:PHE:HA	14:K:10:PHE:HE2	1.76	0.48
4:A:22:PHE:HB2	5:B:1211:ASN:ND2	2.28	0.47
4:A:72:GLU:O	4:A:73:GLY:O	2.32	0.47
4:A:148:CYS:HB3	4:A:168:GLY:HA2	1.96	0.47
4:A:218:ASP:HA	4:A:221:SER:OG	2.14	0.47
4:A:474:VAL:HG22	4:A:474:VAL:O	2.13	0.47
4:A:596:THR:C	4:A:598:LEU:H	2.22	0.47
4:A:600:PRO:C	4:A:602:ASP:N	2.72	0.47
4:A:809:THR:O	4:A:813:PHE:N	2.37	0.47
4:A:1094:VAL:HG12	4:A:1095:THR:N	2.29	0.47
5:B:25:ILE:HG23	5:B:658:ILE:HD11	1.96	0.47
5:B:806:THR:HG22	5:B:808:ALA:HB3	1.96	0.47
5:B:1183:LYS:HE3	5:B:1183:LYS:O	2.14	0.47
6:C:107:SER:C	6:C:109:SER:N	2.72	0.47
6:C:166:GLU:O	6:C:167:HIS:HB2	2.14	0.47
11:H:40:LEU:CD1	11:H:123:MET:HB2	2.44	0.47
15:L:28:LYS:HG3	15:L:39:SER:OG	2.13	0.47
15:L:40:LEU:CD1	15:L:44:ASP:HB3	2.44	0.47
4:A:89:PRO:C	4:A:204:THR:HG21	2.39	0.47
4:A:361:LEU:HD12	4:A:474:VAL:HB	1.96	0.47
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.96	0.47
4:A:1019:CYS:O	4:A:1022:LEU:N	2.47	0.47
5:B:190:TYR:CD2	13:J:62:ARG:HB3	2.49	0.47
5:B:300:HIS:O	5:B:303:TYR:HE2	1.97	0.47
5:B:611:PRO:CB	5:B:685:LEU:HD11	2.41	0.47
6:C:112:ASN:HB2	6:C:114:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:55:ARG:C	8:E:57:MET:N	2.69	0.47
11:H:4:THR:HG22	11:H:5:LEU:H	1.79	0.47
11:H:118:PHE:N	11:H:118:PHE:CD1	2.82	0.47
11:H:135:LEU:HD13	11:H:137:GLN:NE2	2.28	0.47
1:T:16:DG:H5''	4:A:1403:GLU:HG2	1.95	0.47
4:A:335:ARG:NH1	5:B:1202:LEU:HD22	2.30	0.47
4:A:365:GLY:O	4:A:468:PHE:HA	2.13	0.47
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.49	0.47
4:A:399:HIS:CB	4:A:400:PRO:CD	2.86	0.47
4:A:626:ASN:O	4:A:631:HIS:HD2	1.97	0.47
4:A:946:VAL:HG22	8:E:201:LYS:HD2	1.95	0.47
4:A:1316:VAL:O	4:A:1316:VAL:HG12	2.13	0.47
5:B:37:PHE:CD1	5:B:37:PHE:C	2.92	0.47
5:B:269:ILE:HG22	5:B:282:ILE:HG23	1.94	0.47
5:B:604:ARG:NH2	5:B:613:VAL:O	2.48	0.47
5:B:1081:LEU:O	5:B:1082:MET:C	2.57	0.47
6:C:16:ASP:C	6:C:17:ASN:ND2	2.71	0.47
6:C:175:ALA:HB1	13:J:43:ARG:NH1	2.30	0.47
6:C:209:TYR:CD1	6:C:209:TYR:N	2.76	0.47
7:D:4:SER:C	7:D:5:THR:OG1	2.56	0.47
12:I:105:SER:O	12:I:106:CYS:HB3	2.14	0.47
13:J:7:CYS:HA	13:J:49:MET:HE3	1.96	0.47
13:J:16:ASP:O	13:J:18:TRP:N	2.47	0.47
2:N:6:DA:O5'	2:N:6:DA:H2'	2.14	0.47
4:A:1030:ARG:NH1	4:A:1035:TYR:OH	2.48	0.47
4:A:1220:PHE:CE2	4:A:1263:ILE:HG23	2.49	0.47
4:A:1409:LEU:HD13	5:B:1207:LEU:CD2	2.43	0.47
5:B:90:ILE:CD1	5:B:432:MET:SD	3.02	0.47
5:B:293:PRO:HG2	5:B:296:GLU:CB	2.44	0.47
5:B:796:LEU:HD11	5:B:821:GLN:NE2	2.29	0.47
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.96	0.47
7:D:176:GLU:O	7:D:178:ALA:N	2.48	0.47
8:E:43:LYS:O	8:E:45:LYS:N	2.45	0.47
8:E:60:PHE:C	8:E:60:PHE:CD2	2.91	0.47
9:F:77:ASP:C	9:F:79:ARG:N	2.72	0.47
9:F:93:ILE:HD11	9:F:134:ILE:CD1	2.37	0.47
10:G:44:TYR:O	10:G:78:VAL:HA	2.13	0.47
10:G:138:THR:HG22	10:G:139:ILE:HG13	1.96	0.47
12:I:92:ARG:HG2	12:I:94:ASP:OD1	2.14	0.47
4:A:961:ARG:HG2	4:A:965:GLN:HE21	1.79	0.47
4:A:1261:LYS:O	4:A:1264:GLU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.44	0.47
5:B:401:PHE:HB2	5:B:517:THR:OG1	2.14	0.47
5:B:781:PHE:HE2	5:B:793:ALA:HB1	1.79	0.47
7:D:191:ALA:O	7:D:193:THR:N	2.47	0.47
8:E:19:VAL:HG11	8:E:80:VAL:HG11	1.96	0.47
12:I:49:ILE:HG22	12:I:49:ILE:O	2.13	0.47
12:I:80:SER:CB	12:I:103:CYS:SG	3.02	0.47
15:L:38:LEU:HD11	15:L:49:LYS:HE2	1.95	0.47
1:T:20:DC:H2''	1:T:21:DT:C5'	2.44	0.47
4:A:24:PRO:HD2	4:A:233:TRP:NE1	2.29	0.47
4:A:404:TYR:HB2	4:A:433:GLU:HB2	1.97	0.47
4:A:444:PHE:HB2	4:A:458:HIS:HD2	1.80	0.47
4:A:466:SER:CA	14:K:2:ASN:HD22	2.28	0.47
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.96	0.47
4:A:853:ASP:OD1	4:A:855:THR:N	2.47	0.47
5:B:37:PHE:CE2	5:B:542:MET:HA	2.50	0.47
5:B:575:PRO:HG2	5:B:576:ASP:H	1.78	0.47
5:B:680:THR:O	5:B:684:LEU:CD1	2.63	0.47
5:B:1202:LEU:HD22	5:B:1206:GLU:CD	2.40	0.47
7:D:19:GLU:O	7:D:21:GLU:N	2.48	0.47
12:I:83:ASN:HA	12:I:102:VAL:O	2.14	0.47
4:A:15:LYS:HD3	5:B:1220:ARG:HH21	1.80	0.47
4:A:23:SER:O	4:A:25:GLU:N	2.47	0.47
4:A:310:GLY:O	4:A:312:PRO:HD2	2.14	0.47
4:A:573:SER:O	4:A:574:GLY:C	2.57	0.47
4:A:591:PHE:HA	4:A:595:THR:CG2	2.44	0.47
4:A:808:LEU:HD23	4:A:813:PHE:CA	2.40	0.47
4:A:899:VAL:CG2	4:A:908:LEU:HD21	2.45	0.47
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.02	0.47
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.95	0.47
4:A:1280:GLU:O	4:A:1282:VAL:HG23	2.15	0.47
4:A:1364:ASN:HD22	4:A:1365:TYR:N	2.13	0.47
4:A:1373:ASP:CA	4:A:1376:THR:HG22	2.44	0.47
4:A:1389:PHE:CZ	4:A:1402:PHE:CE2	3.02	0.47
5:B:465:ASN:N	5:B:465:ASN:ND2	2.63	0.47
5:B:742:GLU:O	5:B:743:ILE:C	2.58	0.47
5:B:763:GLN:O	5:B:764:SER:C	2.58	0.47
5:B:857:ARG:HD2	5:B:945:GLU:OE1	2.15	0.47
5:B:909:ASP:OD1	5:B:909:ASP:N	2.47	0.47
5:B:953:LEU:HD23	5:B:953:LEU:O	2.14	0.47
6:C:105:GLY:O	6:C:149:LYS:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:174:ALA:HA	13:J:10:CYS:O	2.15	0.47
10:G:1:MET:HG2	10:G:85:GLU:OE1	2.14	0.47
10:G:101:VAL:CG1	10:G:102:GLN:N	2.77	0.47
11:H:100:THR:HG1	11:H:138:GLU:HG3	1.78	0.47
12:I:4:PHE:C	12:I:4:PHE:HD1	2.22	0.47
4:A:244:PRO:CB	4:A:245:PRO:HD3	2.45	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.97	0.47
4:A:547:LEU:HD22	14:K:58:PHE:HD1	1.76	0.47
4:A:574:GLY:O	4:A:575:LYS:C	2.58	0.47
4:A:577:ILE:O	4:A:578:LEU:C	2.55	0.47
5:B:824:ILE:HG22	5:B:824:ILE:O	2.14	0.47
5:B:970:THR:HG22	5:B:971:THR:N	2.30	0.47
9:F:82:THR:CG2	9:F:84:TYR:H	2.18	0.47
12:I:106:CYS:O	12:I:107:SER:CB	2.62	0.47
14:K:57:LEU:HD12	14:K:77:THR:O	2.15	0.47
15:L:38:LEU:CD1	15:L:49:LYS:HE2	2.45	0.47
4:A:14:VAL:HG21	5:B:1216:LEU:CD1	2.44	0.47
4:A:377:PRO:HD3	4:A:493:GLN:OE1	2.14	0.47
4:A:384:ASN:O	4:A:386:ASP:N	2.47	0.47
4:A:472:LEU:O	4:A:475:THR:HB	2.15	0.47
4:A:528:LEU:HD23	4:A:751:SER:HA	1.96	0.47
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.33	0.47
5:B:798:TYR:CD2	5:B:798:TYR:N	2.82	0.47
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.96	0.47
6:C:69:LEU:N	6:C:69:LEU:CD1	2.78	0.47
6:C:80:LEU:HD11	6:C:95:CYS:C	2.40	0.47
8:E:157:SER:C	8:E:159:ASP:H	2.23	0.47
10:G:125:SER:OG	10:G:128:PRO:HA	2.14	0.47
11:H:100:THR:CG2	11:H:101:ALA:N	2.76	0.47
13:J:8:PHE:N	13:J:49:MET:HE3	2.25	0.47
4:A:351:THR:CB	5:B:1103:ILE:HD12	2.44	0.47
4:A:418:SER:C	4:A:420:ARG:N	2.72	0.47
4:A:618:GLU:O	4:A:621:THR:N	2.36	0.47
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.69	0.47
4:A:871:ASP:OD2	4:A:873:MET:HB2	2.15	0.47
4:A:1362:TYR:CD1	4:A:1363:VAL:N	2.83	0.47
5:B:118:ARG:HH11	5:B:204:ILE:HD11	1.80	0.47
5:B:844:SER:O	5:B:847:ASP:HB2	2.14	0.47
5:B:986:GLN:OE1	5:B:986:GLN:HA	2.13	0.47
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.45	0.47
5:B:1160:VAL:CG1	5:B:1161:HIS:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:94:LYS:HG3	8:E:98:ILE:HD11	1.97	0.47
11:H:11:GLN:HA	11:H:53:ASP:O	2.15	0.47
14:K:83:PRO:O	14:K:84:LYS:C	2.58	0.47
15:L:40:LEU:HB3	15:L:41:SER:H	1.52	0.47
4:A:247:ARG:HH11	4:A:247:ARG:HG3	1.81	0.46
4:A:252:PHE:O	4:A:253:ASN:CB	2.63	0.46
4:A:757:ASN:HA	5:B:1021:MET:SD	2.55	0.46
4:A:862:ASN:HA	8:E:174:GLN:HB3	1.97	0.46
4:A:1173:HIS:C	4:A:1174:PHE:CD1	2.93	0.46
4:A:1438:THR:HG22	9:F:92:ARG:HD2	1.97	0.46
5:B:90:ILE:HD11	5:B:432:MET:SD	2.55	0.46
5:B:230:ALA:N	5:B:231:PRO:HD2	2.30	0.46
5:B:293:PRO:CG	5:B:296:GLU:OE1	2.63	0.46
5:B:661:LEU:C	5:B:663:ALA:N	2.73	0.46
5:B:1138:MET:HA	5:B:1138:MET:CE	2.45	0.46
5:B:1177:HIS:C	5:B:1179:GLN:H	2.24	0.46
8:E:90:VAL:O	8:E:90:VAL:HG22	2.15	0.46
8:E:94:LYS:HG3	8:E:98:ILE:CD1	2.45	0.46
8:E:164:LEU:HD11	8:E:211:TYR:CE1	2.50	0.46
11:H:24:CYS:HB2	11:H:44:VAL:HG21	1.96	0.46
12:I:5:ARG:HG2	12:I:6:PHE:O	2.15	0.46
12:I:8:ARG:CG	12:I:34:TYR:HE1	2.26	0.46
4:A:315:LEU:HD13	5:B:471:LYS:HB3	1.97	0.46
4:A:469:ARG:HH11	4:A:469:ARG:HB3	1.80	0.46
4:A:1029:ARG:HH11	4:A:1029:ARG:HG3	1.80	0.46
5:B:38:PHE:CD1	5:B:811:TYR:CD2	3.04	0.46
5:B:40:GLU:HG2	5:B:40:GLU:O	2.14	0.46
5:B:181:LEU:HD22	5:B:189:LEU:CD2	2.45	0.46
5:B:388:CYS:O	5:B:391:ASP:N	2.43	0.46
5:B:616:ILE:N	5:B:616:ILE:CD1	2.76	0.46
5:B:1072:MET:HE1	5:B:1085:ILE:HB	1.95	0.46
10:G:79:PHE:HE2	10:G:105:PRO:CG	2.28	0.46
10:G:87:VAL:HG21	10:G:103:VAL:HG11	1.97	0.46
11:H:33:GLN:C	11:H:35:GLN:H	2.22	0.46
1:T:11:DT:C2'	1:T:12:DA:H5'	2.46	0.46
4:A:252:PHE:HB2	4:A:256:GLN:CD	2.40	0.46
4:A:332:LYS:H	4:A:337:ARG:HB3	1.79	0.46
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.15	0.46
4:A:629:LEU:O	4:A:633:VAL:HG23	2.15	0.46
4:A:665:GLY:O	4:A:667:GLY:N	2.48	0.46
4:A:726:ARG:O	4:A:729:ALA:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1072:ILE:HD11	4:A:1368:MET:HG2	1.97	0.46
5:B:43:LEU:HD11	5:B:811:TYR:O	2.15	0.46
5:B:94:LYS:HG2	5:B:95:ILE:H	1.78	0.46
5:B:121:ASN:OD1	5:B:963:PHE:HZ	1.99	0.46
5:B:212:LEU:HD12	5:B:409:ALA:HB1	1.98	0.46
5:B:603:LEU:HB3	5:B:609:ILE:CG1	2.46	0.46
5:B:664:THR:HG23	5:B:678:GLU:N	2.29	0.46
5:B:1001:PHE:CE2	6:C:34:ARG:CZ	2.99	0.46
5:B:1034:VAL:HG21	5:B:1055:ILE:HG23	1.96	0.46
6:C:43:THR:CG2	6:C:44:LEU:N	2.64	0.46
6:C:66:ARG:CZ	13:J:2:ILE:HG21	2.44	0.46
6:C:75:MET:HE2	6:C:239:PRO:CG	2.46	0.46
8:E:29:PHE:O	8:E:30:ILE:HG13	2.15	0.46
11:H:83:GLN:C	11:H:85:GLY:N	2.60	0.46
4:A:713:SER:O	4:A:717:ASN:ND2	2.49	0.46
4:A:971:PHE:HE2	4:A:1040:GLN:HG2	1.81	0.46
4:A:1385:THR:C	4:A:1387:HIS:H	2.23	0.46
4:A:1385:THR:C	4:A:1387:HIS:N	2.72	0.46
5:B:580:VAL:HG13	5:B:624:LEU:HB3	1.97	0.46
5:B:1125:ASP:O	5:B:1126:GLY:O	2.34	0.46
5:B:1167:GLY:H	5:B:1217:TYR:HE1	1.64	0.46
5:B:1202:LEU:O	5:B:1203:LEU:C	2.57	0.46
6:C:6:PRO:HB3	6:C:25:VAL:CG1	2.41	0.46
6:C:27:LEU:O	6:C:30:ALA:N	2.49	0.46
6:C:69:LEU:CD1	6:C:69:LEU:H	2.28	0.46
6:C:236:GLY:C	6:C:238:ILE:N	2.71	0.46
8:E:85:GLU:O	8:E:88:VAL:HG23	2.15	0.46
12:I:29:CYS:SG	12:I:31:THR:HB	2.56	0.46
12:I:59:VAL:C	12:I:61:ASP:N	2.73	0.46
4:A:208:LEU:HD23	4:A:208:LEU:C	2.40	0.46
4:A:210:ILE:O	4:A:214:ILE:HG13	2.14	0.46
4:A:253:ASN:HB3	5:B:935:ARG:NH2	2.31	0.46
4:A:264:PHE:O	4:A:267:ALA:HB3	2.15	0.46
4:A:528:LEU:HD23	4:A:751:SER:CA	2.46	0.46
4:A:854:ASN:HB2	4:A:1000:LEU:HD21	1.96	0.46
4:A:858:ASN:ND2	4:A:858:ASN:C	2.74	0.46
4:A:1162:VAL:O	4:A:1162:VAL:HG12	2.14	0.46
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.98	0.46
5:B:558:LEU:C	5:B:560:GLU:N	2.74	0.46
5:B:871:THR:HG22	5:B:872:GLU:N	2.30	0.46
5:B:1147:LEU:O	5:B:1148:LYS:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1166:CYS:O	5:B:1166:CYS:SG	2.74	0.46
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.96	0.46
6:C:189:THR:HG22	6:C:190:ASP:N	2.31	0.46
9:F:75:PRO:O	9:F:77:ASP:O	2.32	0.46
4:A:65:LEU:O	4:A:66:LYS:O	2.34	0.46
4:A:206:GLU:O	4:A:210:ILE:HG13	2.16	0.46
4:A:512:VAL:HA	4:A:519:PRO:HA	1.97	0.46
4:A:516:SER:O	4:A:517:ASN:C	2.58	0.46
4:A:608:ILE:HD12	4:A:613:ILE:CD1	2.45	0.46
4:A:1000:LEU:HD23	4:A:1000:LEU:HA	1.81	0.46
4:A:1349:TYR:N	4:A:1372:VAL:HG21	2.31	0.46
5:B:31:TRP:CE3	5:B:31:TRP:HA	2.50	0.46
5:B:102:VAL:O	5:B:109:THR:HA	2.16	0.46
5:B:283:VAL:O	5:B:286:PHE:N	2.49	0.46
5:B:555:ILE:HD11	5:B:587:HIS:CE1	2.51	0.46
5:B:797:TYR:O	13:J:1:MET:HG2	2.15	0.46
5:B:1034:VAL:O	5:B:1037:LEU:N	2.45	0.46
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.41	0.46
8:E:93:MET:SD	8:E:97:VAL:HG23	2.55	0.46
10:G:15:PRO:O	10:G:16:SER:C	2.59	0.46
10:G:26:LEU:O	10:G:27:LYS:C	2.59	0.46
11:H:4:THR:O	11:H:5:LEU:HD23	2.16	0.46
4:A:53:LEU:O	4:A:54:ASN:C	2.59	0.46
4:A:108:MET:HE3	4:A:210:ILE:HD13	1.98	0.46
4:A:265:LYS:HE2	4:A:322:VAL:HG11	1.98	0.46
4:A:730:GLY:C	4:A:732:LEU:N	2.73	0.46
4:A:1437:GLY:CA	9:F:88:TYR:CD2	2.99	0.46
5:B:165:VAL:HG11	5:B:448:ILE:CD1	2.46	0.46
5:B:361:LEU:HD11	5:B:377:PHE:CD2	2.50	0.46
5:B:903:VAL:O	5:B:948:ILE:HG23	2.16	0.46
6:C:77:ILE:CG2	6:C:161:LYS:HE3	2.45	0.46
6:C:125:MET:HB2	6:C:127:ARG:HH21	1.81	0.46
11:H:128:ASN:O	11:H:128:ASN:OD1	2.34	0.46
14:K:107:THR:O	14:K:111:LEU:HG	2.16	0.46
4:A:75:ASN:O	4:A:76:GLU:HB3	2.15	0.46
4:A:416:ARG:HG3	4:A:417:TYR:CE2	2.51	0.46
4:A:556:TRP:CZ3	4:A:558:GLY:HA2	2.51	0.46
4:A:806:ARG:NH1	5:B:729:ILE:HG13	2.31	0.46
4:A:1239:ARG:NH1	4:A:1239:ARG:HB3	2.31	0.46
4:A:1364:ASN:C	4:A:1364:ASN:ND2	2.73	0.46
5:B:34:ILE:O	5:B:35:SER:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:CD	5:B:1084:GLN:N	2.74	0.46
7:D:7:THR:HB	10:G:42:PHE:HZ	1.77	0.46
7:D:27:LEU:HD13	7:D:173:HIS:CD2	2.50	0.46
7:D:185:CYS:HB2	7:D:211:LEU:HD22	1.96	0.46
8:E:46:TYR:CD2	8:E:58:MET:HG2	2.51	0.46
10:G:14:HIS:HD1	10:G:15:PRO:HD2	1.76	0.46
14:K:5:ASP:O	14:K:6:ARG:C	2.58	0.46
4:A:61:ILE:CG2	4:A:62:ASP:H	2.22	0.46
4:A:298:PHE:O	4:A:299:HIS:C	2.59	0.46
4:A:351:THR:HB	5:B:1103:ILE:HD11	1.97	0.46
4:A:845:LEU:O	4:A:846:GLU:C	2.59	0.46
4:A:909:ASP:O	4:A:911:SER:N	2.49	0.46
4:A:1142:THR:O	4:A:1145:SER:OG	2.34	0.46
5:B:227:LYS:HB2	5:B:395:GLN:OE1	2.16	0.46
5:B:383:ASN:O	5:B:384:ARG:C	2.58	0.46
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.98	0.46
5:B:980:PHE:HE2	5:B:1094:ARG:HB2	1.81	0.46
7:D:153:ARG:HB3	7:D:154:PHE:CD1	2.51	0.46
8:E:20:LYS:NZ	8:E:60:PHE:HE1	2.13	0.46
8:E:163:GLU:O	8:E:164:LEU:C	2.58	0.46
12:I:69:PRO:HG2	12:I:85:PHE:CD2	2.50	0.46
4:A:10:PRO:HD2	5:B:1191:ILE:O	2.16	0.46
4:A:128:ILE:O	4:A:134:ARG:HG3	2.16	0.46
4:A:236:LEU:HD11	4:A:304:MET:HE1	1.98	0.46
4:A:259:GLU:OE1	4:A:263:THR:HG21	2.16	0.46
4:A:298:PHE:HD2	4:A:299:HIS:N	2.13	0.46
4:A:683:ILE:HG21	4:A:801:GLU:CG	2.45	0.46
4:A:711:ARG:O	4:A:714:PHE:HB3	2.15	0.46
4:A:960:ILE:CA	4:A:963:ILE:HG22	2.41	0.46
4:A:1007:ILE:C	4:A:1009:ASN:N	2.73	0.46
4:A:1423:GLY:O	4:A:1424:VAL:C	2.59	0.46
5:B:221:ASN:OD1	5:B:242:SER:HA	2.16	0.46
5:B:228:LYS:O	5:B:229:ALA:O	2.34	0.46
5:B:412:LEU:HB3	5:B:466:TRP:CZ2	2.51	0.46
5:B:555:ILE:HG22	5:B:556:THR:N	2.31	0.46
5:B:591:ARG:O	5:B:593:PRO:HD3	2.16	0.46
5:B:780:VAL:HG21	13:J:56:LEU:CD1	2.46	0.46
5:B:825:VAL:HG21	5:B:1092:TYR:HE1	1.80	0.46
5:B:883:LEU:O	5:B:885:MET:N	2.49	0.46
5:B:895:ASP:C	5:B:897:GLY:N	2.74	0.46
5:B:975:GLN:HG2	5:B:976:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:204:SER:C	6:C:206:ASN:N	2.73	0.46
7:D:138:ASN:OD1	7:D:141:LEU:HB2	2.15	0.46
10:G:1:MET:HG2	10:G:85:GLU:CD	2.41	0.46
12:I:12:ASN:HB3	12:I:13:MET:H	1.55	0.46
14:K:55:LYS:HB3	14:K:81:TYR:CE1	2.51	0.46
2:N:1:DC:H1'	2:N:2:DA:H5'	1.98	0.45
2:N:3:DA:H1'	2:N:4:DG:H5'	1.97	0.45
4:A:92:HIS:O	4:A:95:PHE:N	2.46	0.45
4:A:254:GLU:HB2	5:B:935:ARG:HH12	1.80	0.45
4:A:1007:ILE:C	4:A:1009:ASN:H	2.24	0.45
5:B:118:ARG:CG	5:B:204:ILE:HD13	2.46	0.45
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.98	0.45
5:B:764:SER:HB3	5:B:765:PRO:CD	2.46	0.45
5:B:863:GLU:OE1	5:B:962:LYS:HD2	2.16	0.45
10:G:1:MET:O	10:G:1:MET:CE	2.64	0.45
11:H:31:THR:O	11:H:31:THR:HG22	2.16	0.45
12:I:80:SER:OG	12:I:105:SER:HB2	2.16	0.45
15:L:43:THR:C	15:L:45:ALA:H	2.22	0.45
4:A:252:PHE:O	4:A:256:GLN:NE2	2.49	0.45
4:A:254:GLU:HB2	5:B:935:ARG:HH22	1.81	0.45
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.47	0.45
4:A:573:SER:O	4:A:576:GLN:HB2	2.14	0.45
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.45	0.45
4:A:1397:LEU:HB2	4:A:1426:GLU:OE1	2.16	0.45
5:B:240:ILE:HG22	5:B:254:LEU:HB3	1.98	0.45
5:B:324:ILE:CG2	5:B:325:GLN:N	2.79	0.45
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.93	0.45
5:B:878:GLN:O	5:B:879:ARG:C	2.58	0.45
5:B:1040:ASN:O	5:B:1042:GLY:N	2.50	0.45
7:D:12:ARG:O	7:D:14:ARG:HG3	2.16	0.45
2:N:2:DA:H2''	2:N:3:DA:OP2	2.15	0.45
4:A:203:SER:OG	4:A:206:GLU:HB2	2.17	0.45
4:A:347:PHE:H	5:B:1107:ALA:HA	1.80	0.45
4:A:464:PRO:O	4:A:465:TYR:O	2.35	0.45
4:A:577:ILE:O	4:A:579:SER:N	2.48	0.45
4:A:913:LEU:HD21	4:A:915:SER:OG	2.15	0.45
4:A:971:PHE:O	4:A:972:HIS:C	2.59	0.45
4:A:1347:ALA:O	4:A:1348:LEU:C	2.59	0.45
4:A:1443:VAL:C	4:A:1444:MET:HG3	2.40	0.45
5:B:126:SER:CB	5:B:172:ILE:HD11	2.45	0.45
5:B:521:LEU:HB3	5:B:633:VAL:CG1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.45	0.45
5:B:814:PHE:C	5:B:816:GLU:N	2.73	0.45
5:B:1004:GLU:HB2	5:B:1006:ILE:HG13	1.97	0.45
5:B:1161:HIS:NE2	5:B:1175:LEU:HD21	2.31	0.45
5:B:1162:ILE:HD11	5:B:1194:ILE:CD1	2.43	0.45
10:G:30:LEU:HD22	10:G:72:VAL:HG11	1.97	0.45
10:G:99:PHE:CD1	10:G:99:PHE:C	2.95	0.45
13:J:1:MET:N	13:J:57:ILE:N	2.58	0.45
14:K:12:LEU:HD12	14:K:12:LEU:N	2.29	0.45
1:T:18:DC:H5'	4:A:832:ALA:O	2.17	0.45
4:A:335:ARG:O	4:A:336:ILE:C	2.60	0.45
4:A:399:HIS:O	4:A:401:GLY:N	2.49	0.45
4:A:650:GLN:HB3	4:A:654:ASN:HD21	1.82	0.45
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.52	0.45
4:A:1095:THR:HG21	4:A:1103:GLU:OE1	2.16	0.45
5:B:32:ALA:O	5:B:35:SER:HB2	2.16	0.45
5:B:39:ARG:HG2	5:B:39:ARG:NH1	2.31	0.45
5:B:895:ASP:C	5:B:897:GLY:H	2.24	0.45
5:B:1002:THR:O	5:B:1003:ALA:C	2.59	0.45
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.16	0.45
6:C:242:GLN:C	6:C:244:VAL:N	2.72	0.45
10:G:132:SER:HB3	10:G:135:ASP:HB2	1.97	0.45
11:H:95:TYR:CE2	11:H:97:MET:HG3	2.52	0.45
13:J:19:GLU:O	13:J:23:ASN:HB2	2.16	0.45
4:A:552:TRP:NE1	14:K:62:LYS:HB3	2.31	0.45
4:A:1438:THR:CB	5:B:1144:ALA:HB3	2.27	0.45
5:B:830:TYR:O	5:B:831:SER:C	2.59	0.45
5:B:844:SER:O	5:B:847:ASP:N	2.46	0.45
6:C:252:GLN:CG	14:K:95:ILE:HG23	2.46	0.45
7:D:176:GLU:C	7:D:178:ALA:N	2.72	0.45
10:G:108:VAL:HG13	10:G:159:ALA:O	2.17	0.45
12:I:32:CYS:SG	12:I:33:SER:N	2.89	0.45
14:K:31:VAL:CG1	14:K:32:VAL:N	2.80	0.45
14:K:58:PHE:CE2	14:K:74:ARG:NE	2.76	0.45
1:T:23:DC:H2''	1:T:24:DT:O5'	2.16	0.45
4:A:73:GLY:O	4:A:75:ASN:N	2.50	0.45
4:A:313:GLN:O	4:A:314:ALA:HB3	2.16	0.45
4:A:666:ILE:HD12	4:A:666:ILE:N	2.32	0.45
4:A:889:SER:HB3	4:A:1297:GLU:HG2	1.98	0.45
4:A:935:GLN:O	4:A:936:LEU:C	2.59	0.45
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:131:ASP:HA	5:B:164:LYS:HB3	1.97	0.45
5:B:189:LEU:HD12	5:B:196:PRO:HA	1.99	0.45
5:B:212:LEU:HD12	5:B:409:ALA:CB	2.47	0.45
5:B:449:ASN:O	5:B:451:LYS:N	2.50	0.45
5:B:610:ASN:C	5:B:612:GLU:H	2.25	0.45
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.32	0.45
6:C:76:ASP:OD2	6:C:128:ASN:N	2.48	0.45
6:C:143:LEU:HD21	6:C:146:LYS:CE	2.47	0.45
7:D:195:ILE:CG2	7:D:198:LEU:HG	2.46	0.45
8:E:48:ASP:CG	8:E:49:SER:N	2.71	0.45
8:E:102:GLU:C	8:E:104:ASN:N	2.71	0.45
10:G:45:ILE:HD13	10:G:78:VAL:HG13	1.98	0.45
14:K:53:ASP:HB3	14:K:56:VAL:CG2	2.35	0.45
14:K:88:LYS:O	14:K:91:CYS:HB2	2.17	0.45
3:P:5:A:H2'	3:P:6:G:H8	1.82	0.45
4:A:1146:VAL:HG11	4:A:1207:LEU:CD1	2.47	0.45
4:A:1355:VAL:O	4:A:1355:VAL:HG12	2.17	0.45
4:A:1404:GLU:HB2	4:A:1408:ILE:HG13	1.98	0.45
5:B:282:ILE:CD1	5:B:382:ILE:HD13	2.47	0.45
5:B:294:ASP:C	5:B:296:GLU:H	2.22	0.45
5:B:315:LYS:HE3	12:I:4:PHE:CD2	2.52	0.45
6:C:107:SER:O	6:C:109:SER:N	2.47	0.45
8:E:145:THR:HG21	8:E:187:TYR:CE2	2.51	0.45
9:F:73:ALA:HA	9:F:143:PHE:CE1	2.52	0.45
10:G:143:ILE:CG2	10:G:144:ARG:H	2.29	0.45
12:I:82:GLU:O	12:I:104:LEU:HG	2.16	0.45
4:A:95:PHE:O	4:A:96:ILE:C	2.59	0.45
4:A:146:MET:CA	4:A:171:GLN:HB2	2.47	0.45
4:A:249:SER:C	4:A:250:ILE:HG13	2.40	0.45
4:A:418:SER:C	4:A:420:ARG:H	2.25	0.45
4:A:1121:GLU:O	4:A:1122:PRO:C	2.59	0.45
4:A:1226:VAL:HG12	4:A:1227:ILE:N	2.32	0.45
4:A:1299:VAL:CG1	4:A:1300:LYS:H	2.28	0.45
4:A:1377:THR:O	4:A:1378:GLN:C	2.59	0.45
5:B:167:ILE:HG22	5:B:167:ILE:O	2.15	0.45
5:B:270:LYS:HA	5:B:281:PRO:HA	1.99	0.45
5:B:466:TRP:O	5:B:468:GLU:N	2.48	0.45
5:B:512:ARG:HG2	5:B:512:ARG:HH11	1.82	0.45
5:B:877:PRO:C	5:B:878:GLN:HG3	2.42	0.45
5:B:979:LYS:HG2	5:B:1095:LEU:HD13	1.99	0.45
12:I:69:PRO:HG2	12:I:85:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:43:THR:HG22	15:L:43:THR:O	2.15	0.45
4:A:3:GLY:C	4:A:4:GLN:HG3	2.42	0.45
4:A:360:GLU:O	4:A:361:LEU:C	2.57	0.45
4:A:438:ASP:CG	4:A:462:VAL:HG23	2.42	0.45
4:A:445:ASN:HA	4:A:478:TYR:CE2	2.52	0.45
4:A:683:ILE:HD13	4:A:801:GLU:CG	2.47	0.45
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.49	0.45
4:A:936:LEU:O	4:A:939:ASP:HB2	2.17	0.45
4:A:1394:THR:CG2	4:A:1398:MET:SD	3.04	0.45
5:B:436:VAL:O	5:B:436:VAL:HG12	2.17	0.45
5:B:828:ALA:O	5:B:834:ASN:ND2	2.48	0.45
6:C:179:GLU:CG	6:C:180:TYR:N	2.78	0.45
6:C:183:TRP:CZ2	6:C:207:CYS:HB3	2.51	0.45
6:C:226:ASP:O	6:C:227:THR:CB	2.61	0.45
8:E:134:THR:C	8:E:135:PHE:CD1	2.93	0.45
12:I:58:VAL:O	12:I:58:VAL:HG12	2.16	0.45
13:J:12:LYS:O	13:J:14:VAL:CG2	2.59	0.45
4:A:34:LYS:CD	4:A:34:LYS:N	2.80	0.45
4:A:853:ASP:OD1	4:A:853:ASP:C	2.60	0.45
4:A:1152:ILE:HG22	4:A:1192:LEU:O	2.17	0.45
4:A:1170:ILE:HG22	4:A:1174:PHE:HE1	1.82	0.45
4:A:1224:LEU:HD11	4:A:1240:CYS:HB2	1.99	0.45
4:A:1299:VAL:CG1	4:A:1300:LYS:N	2.78	0.45
4:A:1315:GLU:C	4:A:1317:MET:N	2.73	0.45
5:B:281:PRO:O	5:B:283:VAL:N	2.50	0.45
5:B:284:ILE:HG23	5:B:324:ILE:CD1	2.47	0.45
5:B:519:TRP:HE1	5:B:635:ARG:NH2	2.15	0.45
5:B:641:GLU:OE1	5:B:641:GLU:HA	2.15	0.45
5:B:882:THR:O	5:B:883:LEU:HB2	2.16	0.45
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.98	0.45
5:B:1096:ARG:O	5:B:1097:HIS:CG	2.70	0.45
5:B:1151:LEU:N	5:B:1151:LEU:CD1	2.80	0.45
6:C:29:MET:CE	14:K:98:LEU:HG	2.47	0.45
8:E:24:LYS:HG3	8:E:25:ASP:N	2.32	0.45
8:E:42:PHE:CZ	8:E:58:MET:HE3	2.52	0.45
8:E:133:GLU:HB3	8:E:135:PHE:HE1	1.81	0.45
10:G:7:LEU:CD1	10:G:45:ILE:HD11	2.47	0.45
14:K:56:VAL:HA	14:K:77:THR:HG22	1.98	0.45
4:A:106:VAL:HG13	4:A:112:LYS:H	1.82	0.44
4:A:774:ARG:H	4:A:774:ARG:HG2	1.49	0.44
4:A:788:SER:O	4:A:789:LYS:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:963:ILE:HD13	4:A:1049:ILE:CG1	2.46	0.44
4:A:1120:LEU:H	4:A:1120:LEU:HD13	1.82	0.44
4:A:1211:GLN:O	4:A:1212:VAL:C	2.60	0.44
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.17	0.44
5:B:558:LEU:O	5:B:561:TRP:N	2.49	0.44
5:B:564:GLU:O	5:B:565:PRO:C	2.60	0.44
5:B:695:ALA:O	5:B:698:GLU:HB3	2.17	0.44
5:B:758:PHE:C	5:B:760:ASP:N	2.75	0.44
5:B:797:TYR:HE1	5:B:854:LEU:CD2	2.30	0.44
5:B:799:PRO:CB	5:B:818:PRO:HG2	2.47	0.44
5:B:1033:LYS:NZ	5:B:1070:GLU:OE1	2.49	0.44
5:B:1147:LEU:C	5:B:1147:LEU:HD23	2.42	0.44
6:C:242:GLN:C	6:C:244:VAL:H	2.24	0.44
7:D:138:ASN:C	7:D:140:ASP:N	2.74	0.44
7:D:195:ILE:O	7:D:198:LEU:HG	2.17	0.44
8:E:22:MET:HE1	8:E:26:ARG:HH21	1.82	0.44
8:E:114:ASN:O	8:E:115:ASN:CB	2.63	0.44
9:F:128:LYS:HD3	9:F:149:GLU:O	2.17	0.44
10:G:22:MET:O	10:G:23:LYS:C	2.61	0.44
13:J:64:ASN:CB	13:J:65:PRO:HD3	2.44	0.44
4:A:23:SER:O	4:A:26:GLU:N	2.50	0.44
4:A:305:ASP:CG	4:A:326:ARG:HD2	2.42	0.44
4:A:409:SER:O	4:A:410:GLY:C	2.59	0.44
4:A:568:PRO:HG2	4:A:569:LYS:H	1.83	0.44
4:A:994:GLN:HA	4:A:997:LEU:HG	1.99	0.44
4:A:1428:VAL:HG22	5:B:1147:LEU:HD21	1.98	0.44
4:A:1433:MET:CE	10:G:63:PRO:HB2	2.47	0.44
5:B:221:ASN:C	5:B:222:ILE:HG13	2.42	0.44
5:B:596:LEU:O	5:B:600:LEU:HG	2.17	0.44
5:B:600:LEU:O	5:B:609:ILE:HD12	2.17	0.44
5:B:1177:HIS:O	5:B:1179:GLN:N	2.51	0.44
6:C:239:PRO:O	6:C:241:ASP:N	2.50	0.44
7:D:48:ILE:HG21	10:G:4:ILE:HD12	1.99	0.44
7:D:151:PHE:N	7:D:151:PHE:HD1	2.15	0.44
8:E:21:GLU:O	8:E:24:LYS:HG2	2.17	0.44
11:H:91:ASP:O	11:H:93:TYR:N	2.47	0.44
11:H:116:TYR:HE2	11:H:140:ALA:HB1	1.82	0.44
11:H:130:ARG:HB3	11:H:133:ASN:HB2	1.99	0.44
14:K:93:SER:O	14:K:97:LYS:HG3	2.17	0.44
1:T:24:DT:OP2	5:B:942:ARG:NH2	2.50	0.44
4:A:35:ILE:HA	4:A:52:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:53:LEU:CD2	4:A:54:ASN:HD22	2.30	0.44
4:A:114:LEU:HD13	4:A:171:GLN:OE1	2.17	0.44
4:A:138:ILE:HD12	4:A:222:LEU:HD23	1.98	0.44
4:A:332:LYS:C	4:A:334:GLY:H	2.25	0.44
4:A:353:ILE:HB	4:A:470:LEU:CD2	2.47	0.44
4:A:373:THR:HG21	5:B:1105:ALA:HB3	1.98	0.44
4:A:1213:GLY:O	4:A:1214:GLU:C	2.60	0.44
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.18	0.44
5:B:758:PHE:C	5:B:760:ASP:H	2.25	0.44
5:B:840:ILE:CG2	5:B:994:TYR:HD1	2.30	0.44
5:B:952:VAL:HG12	5:B:953:LEU:N	2.33	0.44
5:B:995:ARG:HH12	6:C:165:LYS:HG2	1.82	0.44
5:B:1030:LEU:HD12	5:B:1030:LEU:HA	1.83	0.44
6:C:238:ILE:HD11	6:C:246:ARG:NH1	2.32	0.44
8:E:61:GLN:HG2	8:E:62:ALA:N	2.32	0.44
9:F:123:LYS:O	9:F:124:GLU:C	2.59	0.44
14:K:103:THR:O	14:K:105:PHE:N	2.50	0.44
4:A:108:MET:O	4:A:109:HIS:HB2	2.18	0.44
4:A:472:LEU:O	4:A:475:THR:CG2	2.65	0.44
4:A:784:LEU:HB3	4:A:785:PRO:HD2	1.98	0.44
4:A:1100:ARG:NH2	4:A:1351:GLU:CG	2.76	0.44
4:A:1130:GLN:HA	4:A:1133:LEU:HD12	2.00	0.44
4:A:1162:VAL:CG1	12:I:41:PRO:HG3	2.48	0.44
5:B:797:TYR:C	5:B:798:TYR:CD2	2.95	0.44
5:B:882:THR:HG21	5:B:935:ARG:HA	2.00	0.44
5:B:999:MET:HE2	5:B:1011:ILE:CD1	2.48	0.44
5:B:1110:PRO:C	5:B:1119:VAL:HG13	2.42	0.44
6:C:18:VAL:O	6:C:19:ASP:C	2.59	0.44
8:E:168:TYR:C	8:E:169:ARG:HG3	2.43	0.44
14:K:49:GLU:OE2	14:K:97:LYS:HE3	2.16	0.44
14:K:57:LEU:N	14:K:76:GLN:O	2.50	0.44
2:N:4:DG:H1'	2:N:5:DT:H5'	1.99	0.44
4:A:412:ARG:NH2	5:B:1108:ARG:NH2	2.65	0.44
4:A:563:PRO:HG3	4:A:572:TRP:CE2	2.52	0.44
4:A:1068:ALA:HA	4:A:1367:HIS:ND1	2.32	0.44
4:A:1116:LEU:C	4:A:1116:LEU:HD12	2.43	0.44
4:A:1125:ALA:C	4:A:1127:ASP:N	2.75	0.44
4:A:1148:ILE:O	12:I:48:LEU:N	2.46	0.44
4:A:1376:THR:O	4:A:1377:THR:C	2.61	0.44
5:B:595:ARG:O	5:B:596:LEU:C	2.61	0.44
5:B:615:MET:HA	5:B:625:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:810:GLU:HA	5:B:815:ARG:NH1	2.29	0.44
5:B:846:ILE:HG23	5:B:974:PRO:CG	2.46	0.44
6:C:61:GLU:HA	6:C:64:ALA:HB3	2.00	0.44
7:D:29:LEU:HD22	10:G:82:PHE:CE2	2.53	0.44
8:E:55:ARG:NH1	8:E:113:GLN:NE2	2.66	0.44
10:G:152:SER:O	10:G:153:GLN:HB2	2.17	0.44
11:H:81:PRO:HB2	11:H:82:PRO:CD	2.44	0.44
13:J:36:LEU:HB2	13:J:47:ARG:NH1	2.33	0.44
14:K:24:ASP:OD1	14:K:26:LYS:N	2.51	0.44
14:K:68:PHE:HB3	14:K:70:ARG:NH1	2.32	0.44
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.51	0.44
4:A:1193:LEU:C	4:A:1193:LEU:HD12	2.43	0.44
4:A:1260:LEU:O	4:A:1260:LEU:CG	2.64	0.44
4:A:1450:LEU:O	4:A:1450:LEU:CG	2.65	0.44
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.99	0.44
5:B:402:GLY:HA2	5:B:695:ALA:HB3	1.99	0.44
5:B:842:ASN:HB3	5:B:1009:ASP:HA	2.00	0.44
6:C:193:TYR:C	6:C:193:TYR:HD1	2.26	0.44
7:D:153:ARG:HG2	7:D:218:GLU:HG3	1.99	0.44
8:E:138:ALA:HA	8:E:141:VAL:HG23	2.00	0.44
10:G:48:VAL:HG13	10:G:74:TYR:HD1	1.82	0.44
11:H:143:LEU:C	11:H:144:ILE:HG13	2.42	0.44
12:I:78:CYS:O	12:I:80:SER:N	2.51	0.44
13:J:28:ASP:O	13:J:29:GLU:C	2.61	0.44
2:N:1:DC:H2"	2:N:2:DA:OP2	2.16	0.44
4:A:456:MET:HB3	4:A:507:VAL:HG22	2.00	0.44
4:A:1265:ASN:O	4:A:1267:MET:N	2.51	0.44
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.82	0.44
5:B:23:ALA:HB1	5:B:24:PRO:CD	2.42	0.44
5:B:203:PHE:HB3	5:B:205:ILE:CD1	2.48	0.44
5:B:244:LEU:HD13	5:B:247:GLY:O	2.18	0.44
5:B:278:GLN:HG2	5:B:279:ASP:N	2.26	0.44
5:B:386:LEU:O	5:B:387:LEU:C	2.61	0.44
5:B:1099:VAL:C	5:B:1101:ASP:N	2.76	0.44
6:C:200:GLU:O	6:C:202:PRO:HD3	2.18	0.44
7:D:51:ASN:O	7:D:54:GLU:HB3	2.18	0.44
8:E:104:ASN:C	8:E:104:ASN:HD22	2.26	0.44
14:K:7:PHE:CD1	14:K:7:PHE:C	2.96	0.44
4:A:14:VAL:CG2	5:B:1216:LEU:HD12	2.46	0.44
4:A:56:PRO:O	4:A:57:ARG:CG	2.57	0.44
4:A:626:ASN:O	4:A:628:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:LEU:CD2	4:A:813:PHE:HA	2.45	0.44
4:A:834:THR:HG21	4:A:1077:THR:OG1	2.18	0.44
4:A:903:ASN:ND2	4:A:905:ASP:H	2.16	0.44
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.99	0.44
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.45	0.44
4:A:1191:TRP:CE3	4:A:1191:TRP:HA	2.53	0.44
4:A:1289:ARG:HD2	4:A:1303:GLU:OE2	2.18	0.44
5:B:525:ALA:O	5:B:768:THR:HA	2.17	0.44
5:B:958:GLN:C	5:B:960:GLY:H	2.26	0.44
7:D:50:LEU:HD13	7:D:55:ALA:CB	2.48	0.44
8:E:180:ARG:NH2	8:E:192:ARG:HD2	2.32	0.44
10:G:101:VAL:HG12	10:G:102:GLN:N	2.33	0.44
14:K:59:ALA:HA	14:K:74:ARG:O	2.17	0.44
14:K:78:THR:O	14:K:81:TYR:HB3	2.18	0.44
15:L:28:LYS:CB	15:L:39:SER:HA	2.47	0.44
4:A:130:ASP:HB3	4:A:133:LYS:HB2	2.00	0.44
4:A:341:MET:CE	4:A:843:LYS:HZ1	2.24	0.44
4:A:343:LYS:CE	5:B:1156:ASP:OD2	2.66	0.44
4:A:345:VAL:CG1	5:B:1130:PHE:HB2	2.48	0.44
4:A:688:LYS:C	4:A:690:VAL:N	2.74	0.44
4:A:845:LEU:HB3	4:A:848:ILE:HD12	2.00	0.44
4:A:1293:SER:OG	4:A:1295:THR:CG2	2.66	0.44
4:A:1313:LEU:HD23	4:A:1338:VAL:HB	2.00	0.44
5:B:37:PHE:HE1	5:B:41:LYS:HG3	1.78	0.44
5:B:123:THR:OG1	5:B:458:LYS:HE2	2.18	0.44
5:B:196:PRO:HG2	5:B:197:PHE:H	1.82	0.44
5:B:222:ILE:HG22	5:B:223:VAL:N	2.32	0.44
5:B:314:LEU:O	5:B:318:VAL:HG23	2.18	0.44
5:B:361:LEU:HD11	5:B:377:PHE:CE2	2.52	0.44
5:B:981:ALA:HB3	5:B:1095:LEU:HD21	1.99	0.44
6:C:62:PHE:O	6:C:66:ARG:HG3	2.18	0.44
6:C:121:VAL:O	6:C:121:VAL:HG12	2.17	0.44
6:C:241:ASP:OD1	6:C:242:GLN:N	2.48	0.44
7:D:18:VAL:O	7:D:18:VAL:HG23	2.18	0.44
7:D:130:LEU:C	7:D:132:GLN:N	2.65	0.44
8:E:55:ARG:HB2	8:E:84:ASP:OD2	2.18	0.44
9:F:103:MET:HE2	10:G:66:GLY:H	1.82	0.44
11:H:82:PRO:C	11:H:84:ALA:N	2.74	0.44
13:J:1:MET:H1	13:J:56:LEU:CA	2.31	0.44
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.83	0.44
4:A:103:CYS:C	4:A:105:CYS:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:103:CYS:C	4:A:105:CYS:H	2.25	0.43
4:A:224:PHE:HD2	4:A:229:SER:O	2.00	0.43
4:A:289:ILE:C	4:A:291:GLU:N	2.74	0.43
4:A:368:LYS:O	4:A:369:SER:C	2.61	0.43
4:A:418:SER:O	4:A:420:ARG:N	2.51	0.43
4:A:576:GLN:HG3	11:H:119:GLY:HA3	2.00	0.43
4:A:690:VAL:O	4:A:691:LEU:C	2.61	0.43
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.53	0.43
4:A:1339:LEU:HD13	8:E:147:HIS:CD2	2.52	0.43
4:A:1429:ILE:O	5:B:1197:PRO:HG3	2.18	0.43
5:B:314:LEU:O	5:B:315:LYS:C	2.60	0.43
5:B:610:ASN:C	5:B:612:GLU:N	2.76	0.43
5:B:866:TYR:O	5:B:867:GLY:C	2.61	0.43
5:B:1015:HIS:C	5:B:1017:ILE:H	2.26	0.43
5:B:1147:LEU:CD2	5:B:1151:LEU:HD22	2.48	0.43
4:A:427:GLN:HB2	4:A:430:TRP:CE2	2.53	0.43
4:A:504:LEU:HD11	9:F:91:ALA:CB	2.48	0.43
4:A:552:TRP:HE1	14:K:62:LYS:HB3	1.83	0.43
4:A:666:ILE:N	5:B:1026:LEU:HD13	2.33	0.43
4:A:996:ASN:O	4:A:998:LEU:HD12	2.17	0.43
4:A:1434:ALA:O	4:A:1436:ILE:N	2.50	0.43
4:A:1444:MET:O	9:F:133:VAL:N	2.51	0.43
5:B:840:ILE:HD13	5:B:994:TYR:HE1	1.83	0.43
5:B:1064:TYR:O	5:B:1065:GLN:C	2.61	0.43
5:B:1110:PRO:HG2	5:B:1119:VAL:HG22	2.00	0.43
6:C:208:GLU:C	6:C:210:GLU:N	2.76	0.43
8:E:207:ARG:CB	8:E:207:ARG:NH1	2.81	0.43
11:H:11:GLN:C	11:H:28:ALA:HB1	2.44	0.43
11:H:116:TYR:O	11:H:122:LEU:HA	2.17	0.43
12:I:8:ARG:HB2	12:I:9:ASP:OD1	2.18	0.43
15:L:49:LYS:O	15:L:50:ASP:HB3	2.17	0.43
4:A:270:LEU:HD12	4:A:270:LEU:O	2.18	0.43
4:A:396:PRO:HG3	4:A:416:ARG:HB3	1.99	0.43
4:A:412:ARG:HH22	5:B:1108:ARG:NH2	2.16	0.43
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.32	0.43
4:A:886:ILE:HG13	4:A:943:LEU:HD12	1.99	0.43
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.18	0.43
5:B:38:PHE:HD1	5:B:811:TYR:CD2	2.36	0.43
5:B:333:PHE:O	5:B:334:ILE:CG1	2.66	0.43
5:B:558:LEU:O	5:B:560:GLU:N	2.50	0.43
5:B:681:TRP:HA	5:B:684:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:TYR:HB2	6:C:116:LYS:HG2	2.01	0.43
7:D:52:LEU:C	7:D:54:GLU:N	2.76	0.43
7:D:134:THR:CG2	7:D:135:GLY:H	2.29	0.43
7:D:139:LYS:HE2	7:D:139:LYS:HB2	1.88	0.43
7:D:191:ALA:C	7:D:193:THR:N	2.76	0.43
8:E:81:GLU:HG2	8:E:82:PHE:N	2.33	0.43
8:E:102:GLU:O	8:E:104:ASN:N	2.51	0.43
9:F:79:ARG:NH2	9:F:150:GLU:OE1	2.39	0.43
10:G:21:ARG:HD3	10:G:21:ARG:HA	1.68	0.43
11:H:100:THR:HG22	11:H:101:ALA:H	1.81	0.43
4:A:26:GLU:O	4:A:27:VAL:C	2.61	0.43
4:A:54:ASN:HB3	4:A:247:ARG:NH1	2.31	0.43
4:A:108:MET:HB3	4:A:210:ILE:HD13	2.00	0.43
4:A:680:THR:HA	4:A:683:ILE:CD1	2.48	0.43
4:A:814:PHE:O	4:A:817:ALA:HB3	2.19	0.43
4:A:1227:ILE:CG2	4:A:1228:TRP:N	2.81	0.43
5:B:129:PHE:HE2	5:B:166:PHE:CD1	2.36	0.43
5:B:284:ILE:HD13	5:B:333:PHE:CD2	2.43	0.43
5:B:312:GLU:O	5:B:313:MET:C	2.62	0.43
5:B:597:MET:HA	5:B:597:MET:HE3	2.00	0.43
5:B:785:TYR:CD1	5:B:786:ASN:N	2.86	0.43
5:B:812:LEU:O	5:B:813:LYS:C	2.61	0.43
5:B:992:ILE:HD11	14:K:66:PRO:HB2	1.99	0.43
5:B:1204:PHE:O	5:B:1205:GLN:C	2.59	0.43
8:E:28:TYR:CD1	8:E:78:LEU:HD13	2.53	0.43
8:E:171:LYS:HD3	8:E:171:LYS:N	2.33	0.43
10:G:115:MET:HB2	10:G:116:PRO:CD	2.47	0.43
11:H:4:THR:HG22	11:H:5:LEU:N	2.33	0.43
11:H:95:TYR:HE2	11:H:97:MET:CG	2.31	0.43
14:K:65:HIS:CG	14:K:66:PRO:HD2	2.53	0.43
15:L:55:ILE:O	15:L:56:LEU:CB	2.64	0.43
1:T:12:DA:C2'	1:T:13:DC:H5'	2.49	0.43
4:A:78:PRO:HA	5:B:1201:LYS:NZ	2.33	0.43
4:A:203:SER:O	4:A:204:THR:C	2.61	0.43
4:A:277:GLU:C	4:A:279:LEU:H	2.26	0.43
4:A:384:ASN:CG	4:A:388:LEU:CD1	2.91	0.43
4:A:494:SER:O	4:A:495:GLU:C	2.60	0.43
4:A:548:ASN:OD1	14:K:60:ALA:HB1	2.18	0.43
4:A:570:PRO:C	4:A:571:LEU:HD12	2.43	0.43
4:A:738:LYS:HZ1	6:C:194:GLU:C	2.27	0.43
5:B:34:ILE:O	5:B:37:PHE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:414:ALA:O	5:B:415:GLN:C	2.61	0.43
5:B:582:VAL:HG12	5:B:587:HIS:NE2	2.33	0.43
5:B:882:THR:O	5:B:883:LEU:CB	2.67	0.43
5:B:1147:LEU:HD23	5:B:1151:LEU:HD22	2.00	0.43
6:C:20:PHE:CD1	6:C:20:PHE:C	2.96	0.43
6:C:82:TYR:O	6:C:83:SER:C	2.60	0.43
7:D:135:GLY:C	7:D:137:ASN:H	2.27	0.43
8:E:29:PHE:C	8:E:30:ILE:HG13	2.43	0.43
9:F:99:LEU:O	9:F:103:MET:HG2	2.19	0.43
1:T:12:DA:H2''	1:T:13:DC:H5'	2.00	0.43
4:A:122:MET:O	4:A:123:ARG:C	2.61	0.43
4:A:709:THR:CG2	4:A:711:ARG:HB2	2.49	0.43
4:A:853:ASP:O	4:A:854:ASN:CB	2.62	0.43
4:A:963:ILE:HD13	4:A:1049:ILE:HG12	2.01	0.43
4:A:1042:PHE:CE2	4:A:1046:LEU:HD11	2.53	0.43
4:A:1114:PRO:HG2	4:A:1115:SER:H	1.82	0.43
5:B:280:ILE:HG21	5:B:285:ILE:HG13	2.00	0.43
5:B:393:LYS:HA	5:B:393:LYS:CE	2.45	0.43
5:B:520:GLY:CA	5:B:748:ILE:HG22	2.48	0.43
15:L:61:THR:HG22	15:L:62:LYS:N	2.33	0.43
4:A:29:ALA:HB1	5:B:1184:GLY:HA3	2.01	0.43
4:A:399:HIS:NE2	4:A:462:VAL:HG11	2.33	0.43
4:A:1259:MET:C	4:A:1261:LYS:N	2.77	0.43
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.83	0.43
5:B:37:PHE:HE2	5:B:542:MET:HA	1.84	0.43
5:B:97:VAL:HG12	5:B:178:ASN:ND2	2.32	0.43
5:B:388:CYS:C	5:B:390:LEU:N	2.77	0.43
5:B:435:THR:C	5:B:437:GLU:N	2.66	0.43
5:B:1034:VAL:O	5:B:1036:ALA:N	2.51	0.43
5:B:1115:THR:HG22	5:B:1117:GLN:HG3	2.01	0.43
7:D:48:ILE:CG2	10:G:4:ILE:HB	2.39	0.43
13:J:21:TYR:C	13:J:23:ASN:N	2.75	0.43
4:A:71:GLN:C	4:A:73:GLY:N	2.74	0.43
4:A:415:LEU:HD23	4:A:415:LEU:HA	1.83	0.43
4:A:535:THR:HG21	4:A:616:VAL:CA	2.33	0.43
4:A:1102:LYS:O	4:A:1106:ASN:ND2	2.51	0.43
4:A:1435:PRO:O	4:A:1436:ILE:HG13	2.19	0.43
5:B:259:TYR:HD1	5:B:259:TYR:H	1.67	0.43
5:B:308:TRP:N	5:B:308:TRP:CD1	2.85	0.43
5:B:400:HIS:O	5:B:401:PHE:C	2.61	0.43
5:B:552:MET:C	5:B:554:ILE:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:765:PRO:O	5:B:766:ARG:C	2.62	0.43
5:B:826:ALA:HB2	5:B:1008:PRO:HB3	1.99	0.43
5:B:879:ARG:HA	5:B:879:ARG:HD3	1.81	0.43
8:E:28:TYR:CE1	8:E:78:LEU:CD1	3.02	0.43
8:E:177:ARG:O	8:E:212:ARG:CD	2.66	0.43
9:F:84:TYR:N	9:F:84:TYR:CD1	2.87	0.43
10:G:80:LYS:N	10:G:80:LYS:CD	2.78	0.43
10:G:110:VAL:HG22	10:G:161:GLY:O	2.19	0.43
11:H:10:PHE:N	11:H:10:PHE:CD1	2.87	0.43
4:A:47:ARG:HH12	4:A:254:GLU:CG	2.31	0.43
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.84	0.43
4:A:106:VAL:CG1	4:A:112:LYS:N	2.82	0.43
4:A:466:SER:HB2	5:B:1099:VAL:CG1	2.49	0.43
4:A:475:THR:CG2	4:A:476:SER:N	2.67	0.43
4:A:709:THR:HB	4:A:712:GLU:H	1.84	0.43
4:A:850:VAL:HG21	4:A:1058:VAL:HG11	2.01	0.43
4:A:1017:LEU:HD12	4:A:1017:LEU:O	2.18	0.43
5:B:95:ILE:HG13	5:B:130:VAL:CG2	2.47	0.43
5:B:125:SER:CA	5:B:171:PRO:HA	2.42	0.43
5:B:612:GLU:O	5:B:613:VAL:C	2.62	0.43
5:B:687:GLU:O	5:B:688:GLY:C	2.61	0.43
5:B:708:GLU:O	5:B:709:ASP:C	2.61	0.43
5:B:761:HIS:HB2	5:B:1024:ALA:HB2	2.00	0.43
5:B:763:GLN:O	5:B:765:PRO:N	2.52	0.43
5:B:848:ARG:NH1	13:J:8:PHE:O	2.52	0.43
5:B:872:GLU:OE2	5:B:914:LYS:HE2	2.18	0.43
5:B:1187:ASN:O	5:B:1188:LYS:CB	2.66	0.43
5:B:1196:ILE:HD12	5:B:1200:ALA:HB3	2.00	0.43
5:B:1219:ASP:OD1	5:B:1219:ASP:C	2.62	0.43
6:C:47:ASP:CA	15:L:69:ALA:CB	2.93	0.43
9:F:82:THR:HA	9:F:83:PRO:HD3	1.87	0.43
9:F:89:GLU:HB3	9:F:134:ILE:HD11	2.01	0.43
10:G:50:ASP:O	10:G:51:TYR:C	2.62	0.43
11:H:93:TYR:N	11:H:93:TYR:CD1	2.87	0.43
12:I:98:VAL:HG12	12:I:99:LEU:N	2.33	0.43
13:J:57:ILE:CA	13:J:60:PHE:HD2	2.24	0.43
4:A:12:ARG:NE	5:B:1192:TYR:HE2	2.17	0.43
4:A:1402:PHE:CD1	4:A:1403:GLU:HG3	2.54	0.43
4:A:1434:ALA:HA	4:A:1435:PRO:HD3	1.82	0.43
5:B:236:HIS:CE1	5:B:389:ALA:HA	2.54	0.43
5:B:508:LEU:O	5:B:509:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:542:MET:HB3	5:B:636:PRO:CD	2.48	0.43
5:B:654:ARG:C	5:B:656:GLY:H	2.27	0.43
5:B:918:ILE:HD12	5:B:935:ARG:HD3	2.01	0.43
6:C:65:HIS:O	6:C:69:LEU:HD13	2.19	0.43
7:D:66:ARG:O	7:D:67:ARG:C	2.61	0.43
14:K:65:HIS:CD2	14:K:65:HIS:C	2.97	0.43
15:L:46:VAL:CG1	15:L:56:LEU:HD12	2.48	0.43
4:A:61:ILE:O	4:A:63:ARG:N	2.52	0.42
4:A:62:ASP:O	4:A:63:ARG:C	2.62	0.42
4:A:106:VAL:HG13	4:A:112:LYS:C	2.43	0.42
4:A:340:LEU:HD21	5:B:1199:ALA:HB3	2.01	0.42
4:A:899:VAL:HG22	4:A:908:LEU:HD21	2.00	0.42
4:A:1006:ILE:HD11	8:E:163:GLU:HG3	2.00	0.42
4:A:1225:PHE:CE2	4:A:1227:ILE:HD11	2.53	0.42
4:A:1313:LEU:C	4:A:1315:GLU:N	2.77	0.42
5:B:56:ASP:HB2	5:B:57:TYR:HD1	1.84	0.42
5:B:100:PRO:HD2	5:B:180:TYR:HE1	1.81	0.42
5:B:449:ASN:C	5:B:451:LYS:N	2.76	0.42
5:B:522:VAL:HG12	5:B:523:CYS:N	2.34	0.42
5:B:603:LEU:HB3	5:B:609:ILE:HG13	2.01	0.42
5:B:763:GLN:C	5:B:765:PRO:HD2	2.44	0.42
5:B:840:ILE:HG21	5:B:994:TYR:HD1	1.84	0.42
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.37	0.42
11:H:127:GLY:HA3	11:H:130:ARG:HH22	1.83	0.42
15:L:46:VAL:HG13	15:L:56:LEU:HD12	1.99	0.42
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.59	0.42
4:A:497:THR:O	4:A:498:ARG:C	2.62	0.42
4:A:557:ASP:O	4:A:559:VAL:HG23	2.19	0.42
4:A:794:PRO:C	4:A:796:SER:H	2.26	0.42
4:A:830:LYS:HG2	4:A:1098:VAL:HG21	2.01	0.42
4:A:843:LYS:HD3	4:A:843:LYS:HA	1.75	0.42
4:A:964:ILE:O	4:A:967:ALA:HB3	2.19	0.42
4:A:1010:ALA:O	4:A:1013:ASP:HB2	2.19	0.42
4:A:1191:TRP:HD1	4:A:1256:GLU:HB2	1.83	0.42
4:A:1261:LYS:HA	4:A:1264:GLU:HB3	2.00	0.42
5:B:189:LEU:O	5:B:192:LEU:HB2	2.19	0.42
5:B:496:ARG:NH1	5:B:539:LEU:HB2	2.33	0.42
5:B:542:MET:CG	5:B:747:MET:HB3	2.46	0.42
5:B:549:THR:HG22	5:B:550:ASP:N	2.23	0.42
5:B:562:GLY:C	5:B:590:HIS:ND1	2.77	0.42
5:B:908:GLU:O	5:B:909:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:OE1	6:C:189:THR:HG22	2.18	0.42
5:B:1107:ALA:O	5:B:1108:ARG:O	2.36	0.42
5:B:1162:ILE:HG22	5:B:1163:CYS:N	2.33	0.42
6:C:213:PRO:O	6:C:214:ASN:CB	2.65	0.42
7:D:192:LYS:HE3	7:D:204:ASP:OD1	2.19	0.42
8:E:147:HIS:CD2	8:E:149:LEU:H	2.36	0.42
12:I:13:MET:O	12:I:14:LEU:HD23	2.19	0.42
14:K:8:GLU:O	14:K:37:LYS:HD2	2.20	0.42
4:A:70:CYS:O	4:A:71:GLN:C	2.61	0.42
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.19	0.42
4:A:391:LEU:O	4:A:394:ASN:HB2	2.20	0.42
4:A:453:MET:C	4:A:455:MET:N	2.77	0.42
4:A:806:ARG:HD3	5:B:728:ARG:HA	2.01	0.42
4:A:914:GLU:HB2	4:A:979:SER:O	2.18	0.42
4:A:932:GLU:O	4:A:935:GLN:HB3	2.20	0.42
4:A:1074:GLU:H	4:A:1075:PRO:HD2	1.82	0.42
4:A:1214:GLU:OE1	4:A:1214:GLU:HA	2.19	0.42
5:B:100:PRO:HD3	5:B:172:ILE:HD12	2.00	0.42
5:B:129:PHE:HE2	5:B:166:PHE:HD1	1.67	0.42
5:B:240:ILE:CD1	5:B:377:PHE:HE2	2.32	0.42
5:B:860:MET:HG2	5:B:861:ASP:H	1.84	0.42
6:C:138:GLU:OE1	6:C:138:GLU:N	2.48	0.42
7:D:63:LEU:O	7:D:129:LEU:HD11	2.20	0.42
4:A:266:LEU:O	4:A:267:ALA:C	2.62	0.42
4:A:452:LYS:HE3	5:B:1141:HIS:ND1	2.34	0.42
4:A:960:ILE:C	4:A:963:ILE:HG22	2.44	0.42
4:A:1072:ILE:C	4:A:1075:PRO:HD2	2.44	0.42
4:A:1107:VAL:HG12	4:A:1107:VAL:O	2.19	0.42
4:A:1265:ASN:C	4:A:1267:MET:H	2.26	0.42
5:B:822:ASN:O	13:J:48:ARG:NH1	2.52	0.42
5:B:848:ARG:HD2	13:J:7:CYS:O	2.19	0.42
6:C:66:ARG:NH2	13:J:5:VAL:CG2	2.81	0.42
6:C:263:THR:C	6:C:265:MET:N	2.77	0.42
7:D:122:GLU:HA	7:D:125:SER:OG	2.19	0.42
8:E:164:LEU:HD21	8:E:211:TYR:CG	2.54	0.42
11:H:145:ARG:O	11:H:146:ARG:HB2	2.19	0.42
12:I:56:ALA:O	12:I:57:GLY:O	2.37	0.42
12:I:74:GLU:HA	12:I:80:SER:O	2.19	0.42
13:J:63:TYR:O	13:J:64:ASN:HB2	2.18	0.42
1:T:24:DT:OP1	5:B:857:ARG:NH2	2.52	0.42
4:A:47:ARG:HH12	4:A:254:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:302:THR:CG2	4:A:303:TYR:N	2.81	0.42
4:A:344:ARG:NE	5:B:1120:GLU:HB2	2.35	0.42
4:A:618:GLU:O	4:A:619:LYS:C	2.62	0.42
4:A:796:SER:C	4:A:798:GLY:H	2.27	0.42
4:A:899:VAL:CG2	4:A:1029:ARG:HG2	2.49	0.42
4:A:909:ASP:C	4:A:911:SER:N	2.77	0.42
4:A:961:ARG:O	4:A:965:GLN:HG3	2.18	0.42
5:B:180:TYR:CD1	5:B:180:TYR:N	2.86	0.42
5:B:199:MET:SD	5:B:199:MET:N	2.76	0.42
5:B:424:LEU:HD22	5:B:453:ILE:HD11	2.00	0.42
6:C:160:LYS:O	6:C:161:LYS:O	2.37	0.42
7:D:47:LEU:CD1	10:G:3:PHE:CD2	3.02	0.42
8:E:16:PHE:HZ	8:E:20:LYS:HE2	1.74	0.42
9:F:72:LYS:O	9:F:73:ALA:CB	2.67	0.42
9:F:117:PRO:C	9:F:119:ARG:H	2.27	0.42
11:H:55:LEU:HD22	11:H:144:ILE:HG21	1.98	0.42
11:H:81:PRO:HB3	11:H:82:PRO:HD2	1.99	0.42
14:K:18:LYS:NZ	14:K:38:GLU:HG2	2.34	0.42
14:K:63:VAL:O	14:K:63:VAL:CG2	2.63	0.42
14:K:109:TRP:O	14:K:112:GLN:HB2	2.19	0.42
2:N:5:DT:H6	2:N:5:DT:H2'	1.53	0.42
4:A:84:ILE:HD11	4:A:270:LEU:HD13	2.02	0.42
4:A:120:GLU:O	4:A:121:LEU:C	2.62	0.42
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.83	0.42
4:A:534:LEU:O	4:A:534:LEU:HG	2.19	0.42
4:A:577:ILE:C	4:A:579:SER:H	2.25	0.42
4:A:664:THR:CG2	4:A:665:GLY:N	2.83	0.42
4:A:857:ARG:CZ	9:F:139:PRO:HG3	2.49	0.42
4:A:1036:ARG:HG2	4:A:1036:ARG:HH11	1.85	0.42
4:A:1129:GLU:C	4:A:1131:ALA:N	2.77	0.42
5:B:112:LEU:HD21	5:B:117:ALA:HB2	2.02	0.42
5:B:121:ASN:HD22	5:B:207:GLY:HA3	1.84	0.42
5:B:197:PHE:HZ	5:B:816:GLU:HG2	1.85	0.42
5:B:498:THR:HB	5:B:537:LYS:O	2.20	0.42
5:B:737:THR:O	5:B:738:PHE:C	2.63	0.42
5:B:776:GLN:O	5:B:1095:LEU:HA	2.19	0.42
5:B:806:THR:O	5:B:809:MET:HG3	2.19	0.42
5:B:831:SER:HB3	5:B:994:TYR:OH	2.20	0.42
5:B:1055:ILE:O	5:B:1056:SER:C	2.63	0.42
5:B:1110:PRO:O	5:B:1119:VAL:HG13	2.20	0.42
6:C:133:ILE:CD1	6:C:237:SER:CA	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:161:GLY:O	7:D:165:GLN:HG3	2.20	0.42
8:E:124:VAL:HG13	8:E:132:ILE:CD1	2.50	0.42
10:G:95:SER:C	10:G:97:HIS:H	2.27	0.42
10:G:99:PHE:CZ	10:G:143:ILE:HD13	2.54	0.42
13:J:41:LEU:N	13:J:41:LEU:HD23	2.34	0.42
15:L:34:CYS:O	15:L:36:SER:N	2.53	0.42
2:N:3:DA:H1'	2:N:4:DG:C8	2.55	0.42
4:A:204:THR:C	4:A:206:GLU:N	2.78	0.42
4:A:207:ILE:O	4:A:211:PHE:HD1	2.02	0.42
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.83	0.42
4:A:793:SER:HB2	4:A:794:PRO:HD2	2.01	0.42
4:A:872:GLY:O	4:A:1058:VAL:HG23	2.20	0.42
4:A:1197:LEU:HD11	4:A:1238:ILE:HD11	2.01	0.42
4:A:1344:GLY:O	4:A:1345:ARG:C	2.62	0.42
4:A:1409:LEU:O	4:A:1410:PHE:C	2.61	0.42
5:B:263:GLY:O	5:B:264:SER:C	2.62	0.42
6:C:235:VAL:HG21	13:J:6:ARG:NH2	2.35	0.42
6:C:236:GLY:O	6:C:237:SER:C	2.62	0.42
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.93	0.42
7:D:47:LEU:CD1	7:D:48:ILE:N	2.81	0.42
8:E:22:MET:CE	8:E:26:ARG:NH2	2.80	0.42
8:E:136:ASN:OD1	8:E:138:ALA:N	2.53	0.42
8:E:205:SER:O	8:E:206:GLY:C	2.62	0.42
14:K:43:GLY:HA2	14:K:71:PHE:CZ	2.55	0.42
4:A:33:ALA:O	4:A:83:HIS:HD2	2.02	0.42
4:A:207:ILE:O	4:A:208:LEU:C	2.63	0.42
4:A:683:ILE:HD13	4:A:801:GLU:HG3	2.02	0.42
4:A:901:LEU:HD13	4:A:919:ILE:HG23	2.02	0.42
4:A:1120:LEU:HD23	4:A:1124:HIS:O	2.19	0.42
5:B:468:GLU:HB3	5:B:469:GLN:H	1.70	0.42
5:B:469:GLN:HB2	5:B:470:LYS:H	1.52	0.42
5:B:579:ARG:HD2	5:B:586:TRP:CZ2	2.55	0.42
5:B:789:MET:HE3	5:B:965:LYS:HB3	2.00	0.42
5:B:889:THR:HG22	5:B:891:ASP:H	1.84	0.42
5:B:1115:THR:HG21	5:B:1117:GLN:CD	2.44	0.42
5:B:1143:ALA:O	5:B:1144:ALA:C	2.63	0.42
6:C:44:LEU:HD21	6:C:159:ALA:CB	2.50	0.42
6:C:104:PHE:HD2	6:C:105:GLY:H	1.67	0.42
8:E:16:PHE:O	8:E:17:ARG:C	2.62	0.42
9:F:72:LYS:O	9:F:73:ALA:HB3	2.20	0.42
10:G:22:MET:C	10:G:24:GLN:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:47:ARG:NH1	13:J:47:ARG:HG2	2.31	0.42
14:K:65:HIS:HD2	14:K:67:PHE:HB2	1.84	0.42
4:A:98:LYS:O	4:A:99:ILE:C	2.63	0.42
4:A:399:HIS:CG	4:A:400:PRO:N	2.87	0.42
4:A:434:ARG:HE	4:A:437:MET:HG3	1.85	0.42
4:A:525:GLN:HG3	5:B:836:GLU:HG2	2.02	0.42
4:A:883:LEU:CD2	4:A:1021:LEU:HB2	2.50	0.42
4:A:889:SER:C	4:A:891:ALA:N	2.75	0.42
5:B:169:ARG:HB2	5:B:454:THR:CG2	2.33	0.42
5:B:234:ILE:HG21	5:B:237:VAL:CG2	2.50	0.42
5:B:903:VAL:CG1	5:B:904:ARG:N	2.83	0.42
5:B:1216:LEU:O	5:B:1217:TYR:HD1	2.01	0.42
6:C:56:THR:HG22	6:C:58:LEU:HD23	2.01	0.42
6:C:80:LEU:HD11	6:C:95:CYS:CA	2.49	0.42
6:C:112:ASN:CB	6:C:114:TYR:CE1	3.02	0.42
6:C:248:ILE:HG13	6:C:248:ILE:H	1.65	0.42
9:F:97:ARG:HA	9:F:97:ARG:HD2	1.79	0.42
10:G:18:PHE:CA	10:G:22:MET:HE3	2.41	0.42
11:H:113:ALA:HB1	11:H:125:LEU:O	2.20	0.42
12:I:2:THR:O	12:I:2:THR:HG22	2.20	0.42
13:J:3:VAL:CG2	13:J:18:TRP:CG	3.01	0.42
4:A:91:PHE:HB3	4:A:96:ILE:HG12	2.02	0.42
4:A:407:ARG:HB3	4:A:430:TRP:NE1	2.34	0.42
4:A:433:GLU:OE1	5:B:1108:ARG:NH1	2.53	0.42
4:A:600:PRO:O	4:A:602:ASP:N	2.52	0.42
4:A:1120:LEU:O	4:A:1323:ASP:N	2.52	0.42
4:A:1334:ASP:C	4:A:1336:MET:N	2.76	0.42
4:A:1346:ALA:CB	8:E:149:LEU:HD13	2.50	0.42
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.68	0.42
5:B:956:THR:HG22	5:B:957:ASN:N	2.35	0.42
7:D:195:ILE:HG22	7:D:195:ILE:O	2.20	0.42
8:E:22:MET:HB2	8:E:187:TYR:CE1	2.55	0.42
8:E:173:SER:C	8:E:175:LEU:H	2.28	0.42
12:I:92:ARG:HB3	12:I:95:THR:OG1	2.19	0.42
3:P:3:U:H4'	4:A:323:LYS:NZ	2.19	0.41
4:A:49:LYS:HZ2	4:A:60:SER:HA	1.84	0.41
4:A:249:SER:O	4:A:250:ILE:CG1	2.60	0.41
4:A:353:ILE:HG21	4:A:487:MET:HG3	2.01	0.41
4:A:463:ILE:HB	4:A:464:PRO:HD2	2.01	0.41
4:A:590:ARG:HD2	4:A:605:MET:CB	2.50	0.41
4:A:639:PRO:HG2	4:A:640:GLN:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:942:PHE:C	4:A:942:PHE:HD2	2.27	0.41
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
4:A:1208:THR:O	4:A:1209:MET:C	2.63	0.41
4:A:1310:GLY:C	4:A:1311:VAL:HG23	2.44	0.41
4:A:1334:ASP:O	4:A:1335:ILE:C	2.63	0.41
5:B:39:ARG:NH2	5:B:665:GLU:CG	2.83	0.41
5:B:423:LYS:HZ3	5:B:470:LYS:HZ2	1.68	0.41
5:B:581:PHE:HA	5:B:585:VAL:O	2.19	0.41
5:B:603:LEU:HD22	5:B:603:LEU:HA	1.87	0.41
5:B:1198:TYR:CD2	5:B:1198:TYR:C	2.98	0.41
6:C:187:LYS:HG3	6:C:219:PHE:CE1	2.54	0.41
7:D:16:LYS:O	7:D:16:LYS:HG2	2.20	0.41
7:D:64:VAL:C	7:D:66:ARG:N	2.78	0.41
9:F:79:ARG:HG3	9:F:144:GLU:OE1	2.19	0.41
12:I:50:THR:HG22	12:I:51:ASN:N	2.35	0.41
14:K:6:ARG:HD3	14:K:6:ARG:HA	1.94	0.41
14:K:68:PHE:N	14:K:68:PHE:CD2	2.85	0.41
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.61	0.41
4:A:606:LEU:O	4:A:613:ILE:HB	2.20	0.41
4:A:715:GLU:O	4:A:717:ASN:N	2.53	0.41
4:A:873:MET:HE3	4:A:957:PRO:HG3	2.01	0.41
4:A:886:ILE:CD1	4:A:943:LEU:HB3	2.42	0.41
4:A:1265:ASN:O	4:A:1266:THR:C	2.63	0.41
5:B:286:PHE:O	5:B:289:LEU:HB2	2.20	0.41
5:B:331:LEU:HD12	5:B:331:LEU:N	2.35	0.41
5:B:412:LEU:HB3	5:B:466:TRP:HZ2	1.85	0.41
5:B:807:ARG:HG2	5:B:1045:SER:HG	1.83	0.41
6:C:111:THR:C	6:C:112:ASN:HD22	2.28	0.41
6:C:216:GLY:O	6:C:217:ASP:C	2.63	0.41
8:E:91:LYS:C	8:E:93:MET:H	2.27	0.41
8:E:192:ARG:HG3	8:E:192:ARG:NH1	2.34	0.41
9:F:147:SER:OG	9:F:150:GLU:HG3	2.20	0.41
4:A:106:VAL:HA	4:A:114:LEU:HD21	2.03	0.41
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.85	0.41
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.35	0.41
4:A:858:ASN:ND2	4:A:860:LEU:N	2.59	0.41
4:A:867:ILE:CG2	4:A:872:GLY:N	2.84	0.41
4:A:943:LEU:C	4:A:945:GLU:H	2.28	0.41
4:A:996:ASN:HA	4:A:998:LEU:HD12	2.02	0.41
4:A:1138:ILE:CG2	4:A:1316:VAL:HG13	2.51	0.41
4:A:1409:LEU:HD23	4:A:1409:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:298:LEU:N	5:B:298:LEU:CD2	2.83	0.41
5:B:557:PHE:C	5:B:557:PHE:HD2	2.26	0.41
5:B:1119:VAL:HG23	5:B:1126:GLY:HA2	2.02	0.41
5:B:1169:MET:CE	5:B:1204:PHE:HB2	2.50	0.41
6:C:58:LEU:CD2	6:C:58:LEU:N	2.83	0.41
6:C:104:PHE:HD2	6:C:105:GLY:N	2.19	0.41
8:E:62:ALA:HB3	8:E:78:LEU:HD22	2.01	0.41
8:E:117:THR:O	8:E:120:ALA:HB3	2.20	0.41
8:E:153:HIS:C	8:E:154:ILE:HG13	2.46	0.41
10:G:79:PHE:CE2	10:G:105:PRO:HG2	2.53	0.41
10:G:96:GLN:HB3	10:G:121:PHE:CE2	2.55	0.41
10:G:111:THR:HB	10:G:114:LEU:HB2	2.01	0.41
11:H:42:ILE:CG2	11:H:43:ASN:N	2.82	0.41
15:L:28:LYS:HB2	15:L:39:SER:HB2	2.02	0.41
15:L:40:LEU:HD23	15:L:40:LEU:HA	1.91	0.41
4:A:6:TYR:CD1	4:A:7:SER:N	2.88	0.41
4:A:414:ASP:OD1	4:A:414:ASP:C	2.63	0.41
4:A:567:LYS:CD	11:H:95:TYR:HA	2.50	0.41
4:A:711:ARG:HH11	12:I:95:THR:HB	1.85	0.41
4:A:775:ILE:HG21	4:A:783:THR:HG23	2.02	0.41
4:A:986:ILE:O	4:A:990:VAL:HG23	2.19	0.41
4:A:996:ASN:HB3	4:A:1050:GLU:OE2	2.20	0.41
4:A:1042:PHE:C	4:A:1044:TRP:N	2.78	0.41
4:A:1157:ASP:C	4:A:1159:ARG:H	2.28	0.41
5:B:172:ILE:HG22	5:B:173:MET:H	1.84	0.41
5:B:405:ARG:NH2	5:B:632:ARG:HD3	2.35	0.41
5:B:604:ARG:O	5:B:607:GLY:N	2.54	0.41
5:B:801:LYS:O	13:J:52:THR:CG2	2.60	0.41
5:B:824:ILE:HG12	13:J:48:ARG:NH1	2.36	0.41
6:C:145:CYS:HA	13:J:2:ILE:CD1	2.43	0.41
6:C:243:VAL:O	6:C:243:VAL:HG12	2.20	0.41
7:D:51:ASN:C	7:D:52:LEU:O	2.62	0.41
8:E:128:PRO:HA	8:E:129:PRO:C	2.45	0.41
9:F:88:TYR:CD1	9:F:88:TYR:N	2.88	0.41
15:L:65:VAL:O	15:L:65:VAL:HG23	2.21	0.41
4:A:54:ASN:HA	4:A:58:LEU:HD12	2.03	0.41
4:A:472:LEU:O	4:A:475:THR:CB	2.69	0.41
4:A:683:ILE:O	4:A:686:ALA:N	2.53	0.41
4:A:920:LEU:C	4:A:920:LEU:CD2	2.94	0.41
4:A:1362:TYR:HD1	4:A:1363:VAL:N	2.18	0.41
5:B:20:ASP:C	5:B:22:SER:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:211:VAL:HG23	5:B:483:LEU:HB2	2.02	0.41
5:B:218:SER:O	5:B:219:ALA:O	2.38	0.41
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.85	0.41
5:B:591:ARG:O	5:B:592:ASN:C	2.62	0.41
5:B:605:ARG:NH1	5:B:639:ILE:HD13	2.35	0.41
5:B:618:ASP:OD1	5:B:621:GLU:HB3	2.20	0.41
5:B:726:ALA:O	5:B:727:LYS:O	2.39	0.41
5:B:865:LYS:NZ	5:B:869:SER:HA	2.35	0.41
6:C:17:ASN:N	6:C:240:VAL:HG11	2.35	0.41
6:C:100:THR:CG2	6:C:101:LEU:N	2.83	0.41
6:C:131:HIS:HA	6:C:132:PRO:HD3	1.93	0.41
6:C:175:ALA:HB2	13:J:10:CYS:HB2	2.03	0.41
6:C:229:TYR:N	6:C:229:TYR:CD1	2.87	0.41
8:E:24:LYS:HB2	8:E:24:LYS:HE3	1.77	0.41
10:G:106:MET:HE2	10:G:106:MET:HB3	1.97	0.41
10:G:126:ASN:HD22	10:G:126:ASN:HA	1.54	0.41
10:G:145:VAL:CG1	10:G:146:LYS:H	2.32	0.41
14:K:31:VAL:O	14:K:74:ARG:HA	2.21	0.41
15:L:55:ILE:HG12	15:L:55:ILE:H	1.41	0.41
4:A:42:ASP:HB3	4:A:45:GLN:CA	2.51	0.41
4:A:224:PHE:CD2	4:A:231:PRO:HG3	2.56	0.41
4:A:270:LEU:HD12	4:A:270:LEU:C	2.45	0.41
4:A:329:LEU:O	4:A:330:LYS:C	2.63	0.41
4:A:438:ASP:OD1	4:A:462:VAL:HG23	2.21	0.41
4:A:971:PHE:CD1	4:A:971:PHE:N	2.88	0.41
4:A:973:ILE:HD11	4:A:1038:THR:HG23	2.03	0.41
4:A:1138:ILE:HG21	4:A:1316:VAL:HG13	2.03	0.41
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.19	0.41
5:B:616:ILE:HG13	5:B:697:GLU:HA	2.02	0.41
5:B:770:GLN:HG2	5:B:983:ARG:O	2.20	0.41
5:B:843:GLN:N	5:B:994:TYR:O	2.37	0.41
5:B:862:GLN:HG2	5:B:963:PHE:CD1	2.42	0.41
6:C:254:LYS:HE2	6:C:254:LYS:HB3	1.89	0.41
10:G:1:MET:HE1	10:G:80:LYS:H	1.85	0.41
10:G:14:HIS:HD2	10:G:16:SER:CB	2.33	0.41
1:T:15:DT:H73	16:T:67:CPT:N1	2.35	0.41
1:T:19:DC:H2''	1:T:20:DC:H5'	2.02	0.41
4:A:52:GLY:O	4:A:56:PRO:HG2	2.21	0.41
4:A:53:LEU:CD2	4:A:54:ASN:N	2.64	0.41
4:A:243:PRO:CB	4:A:244:PRO:HD2	2.50	0.41
4:A:302:THR:HG22	4:A:303:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:404:TYR:CD2	4:A:414:ASP:HA	2.56	0.41
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.95	0.41
4:A:1365:TYR:O	4:A:1367:HIS:N	2.54	0.41
5:B:313:MET:O	5:B:316:PRO:HG2	2.20	0.41
5:B:466:TRP:CE3	5:B:466:TRP:HA	2.54	0.41
5:B:1034:VAL:C	5:B:1036:ALA:N	2.78	0.41
6:C:167:HIS:HD2	6:C:168:ALA:H	1.69	0.41
6:C:239:PRO:C	6:C:241:ASP:N	2.78	0.41
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.47	0.41
10:G:1:MET:HE1	10:G:80:LYS:C	2.46	0.41
4:A:224:PHE:CD2	4:A:231:PRO:HD3	2.56	0.41
4:A:316:GLN:HB2	4:A:322:VAL:HG23	2.02	0.41
4:A:361:LEU:CD1	4:A:474:VAL:HB	2.51	0.41
4:A:860:LEU:CB	4:A:862:ASN:OD1	2.69	0.41
4:A:1142:THR:O	4:A:1143:LEU:C	2.63	0.41
4:A:1273:LEU:N	4:A:1273:LEU:CD1	2.83	0.41
4:A:1364:ASN:O	4:A:1366:ARG:HG3	2.21	0.41
4:A:1405:THR:HB	4:A:1406:VAL:H	1.58	0.41
4:A:1409:LEU:O	4:A:1412:ALA:HB3	2.20	0.41
5:B:172:ILE:CG2	5:B:173:MET:H	2.34	0.41
5:B:1079:LYS:N	6:C:27:LEU:HD21	2.36	0.41
6:C:179:GLU:CG	6:C:180:TYR:H	2.28	0.41
7:D:173:HIS:NE2	7:D:201:LYS:NZ	2.69	0.41
10:G:1:MET:O	10:G:1:MET:HE2	2.20	0.41
14:K:40:HIS:O	14:K:41:THR:C	2.63	0.41
14:K:55:LYS:CB	14:K:81:TYR:CE1	3.04	0.41
4:A:42:ASP:HB3	4:A:45:GLN:N	2.33	0.41
4:A:43:GLU:O	4:A:44:THR:CB	2.68	0.41
4:A:58:LEU:HD13	4:A:243:PRO:HA	2.02	0.41
4:A:71:GLN:O	4:A:73:GLY:N	2.50	0.41
4:A:512:VAL:O	4:A:512:VAL:HG12	2.21	0.41
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.50	0.41
4:A:665:GLY:O	4:A:666:ILE:C	2.64	0.41
4:A:714:PHE:CG	12:I:97:MET:HE1	2.56	0.41
4:A:730:GLY:C	4:A:732:LEU:H	2.29	0.41
4:A:818:MET:HA	5:B:514:LEU:HB3	2.02	0.41
4:A:838:GLN:O	4:A:842:VAL:HG23	2.21	0.41
4:A:872:GLY:C	4:A:1058:VAL:HG23	2.46	0.41
4:A:935:GLN:O	4:A:938:LYS:N	2.54	0.41
4:A:1072:ILE:O	4:A:1075:PRO:HG2	2.21	0.41
4:A:1348:LEU:HG	4:A:1372:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:26:THR:O	5:B:29:ASP:HB2	2.21	0.41
5:B:27:ALA:O	5:B:30:SER:OG	2.38	0.41
5:B:48:LEU:O	5:B:49:ASP:C	2.63	0.41
5:B:255:GLN:HB2	5:B:272:THR:HB	2.01	0.41
5:B:334:ILE:HG22	5:B:334:ILE:O	2.21	0.41
5:B:431:TYR:CD2	5:B:447:ALA:HB2	2.56	0.41
5:B:526:GLU:CG	5:B:538:ASN:HD22	2.31	0.41
5:B:729:ILE:O	5:B:729:ILE:HG22	2.21	0.41
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.42	0.41
5:B:979:LYS:HG2	5:B:1095:LEU:CD1	2.50	0.41
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.35	0.41
6:C:69:LEU:HD12	6:C:69:LEU:H	1.85	0.41
7:D:53:SER:H	7:D:148:LEU:CD2	2.34	0.41
7:D:192:LYS:HZ2	7:D:192:LYS:HB3	1.85	0.41
8:E:124:VAL:N	8:E:125:PRO:HD2	2.35	0.41
10:G:154:VAL:HG12	10:G:155:SER:N	2.36	0.41
11:H:118:PHE:O	11:H:120:GLY:N	2.53	0.41
11:H:143:LEU:HD12	11:H:143:LEU:N	2.36	0.41
12:I:62:ILE:O	12:I:62:ILE:CG1	2.66	0.41
12:I:85:PHE:HD1	12:I:99:LEU:HD13	1.83	0.41
13:J:56:LEU:O	13:J:57:ILE:C	2.64	0.41
14:K:6:ARG:C	14:K:8:GLU:N	2.78	0.41
14:K:68:PHE:HB3	14:K:70:ARG:HH11	1.84	0.41
4:A:116:ASP:C	4:A:118:HIS:H	2.28	0.41
4:A:388:LEU:HD22	4:A:432:VAL:HB	2.02	0.41
4:A:412:ARG:NH2	5:B:1108:ARG:NH1	2.69	0.41
4:A:666:ILE:HD11	5:B:1086:PHE:HE1	1.86	0.41
4:A:671:ALA:O	4:A:672:ASP:C	2.64	0.41
4:A:860:LEU:HB3	4:A:862:ASN:OD1	2.21	0.41
4:A:925:LEU:C	4:A:927:VAL:N	2.77	0.41
4:A:1119:TYR:O	4:A:1120:LEU:O	2.39	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.89	0.41
5:B:212:LEU:HD13	5:B:409:ALA:HA	2.03	0.41
5:B:329:THR:O	5:B:332:ASP:HB3	2.20	0.41
5:B:465:ASN:ND2	5:B:477:ALA:HB2	2.35	0.41
5:B:615:MET:O	5:B:697:GLU:HG3	2.20	0.41
5:B:777:ALA:HA	5:B:1095:LEU:HA	2.02	0.41
5:B:806:THR:HG21	5:B:808:ALA:HB3	2.02	0.41
5:B:977:GLY:HA3	5:B:1099:VAL:CG2	2.50	0.41
8:E:55:ARG:O	8:E:57:MET:N	2.53	0.41
12:I:54:GLU:OE2	12:I:118:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:11:DT:H1'	1:T:12:DA:H5'	2.02	0.40
4:A:472:LEU:CD1	5:B:835:GLN:CD	2.93	0.40
4:A:522:GLY:HA2	4:A:630:ILE:CD1	2.51	0.40
4:A:901:LEU:HD22	4:A:919:ILE:HG22	2.03	0.40
4:A:939:ASP:O	4:A:940:ARG:C	2.63	0.40
4:A:1242:VAL:O	4:A:1243:VAL:HB	2.21	0.40
5:B:174:LEU:HD22	5:B:202:TYR:CE1	2.56	0.40
5:B:174:LEU:HD21	5:B:204:ILE:HD11	2.03	0.40
5:B:258:LEU:O	5:B:258:LEU:CG	2.67	0.40
5:B:1001:PHE:HD2	6:C:34:ARG:NH2	2.17	0.40
6:C:80:LEU:CD1	6:C:95:CYS:HA	2.51	0.40
6:C:167:HIS:CE1	15:L:70:ARG:HA	2.57	0.40
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.56	0.40
6:C:217:ASP:HA	6:C:218:PRO:HD3	1.89	0.40
7:D:158:GLU:O	7:D:161:GLY:N	2.51	0.40
11:H:5:LEU:N	11:H:60:ALA:HB2	2.37	0.40
11:H:118:PHE:C	11:H:120:GLY:N	2.79	0.40
11:H:127:GLY:O	11:H:128:ASN:CB	2.69	0.40
13:J:59:LYS:H	13:J:59:LYS:HG2	1.72	0.40
2:N:3:DA:C1'	2:N:4:DG:H5'	2.52	0.40
4:A:42:ASP:HB3	4:A:45:GLN:HA	2.03	0.40
4:A:64:ASN:O	4:A:65:LEU:C	2.64	0.40
4:A:486:GLU:O	4:A:487:MET:HG2	2.21	0.40
4:A:596:THR:O	4:A:597:LEU:C	2.64	0.40
4:A:781:ASP:O	4:A:782:ARG:HB3	2.21	0.40
4:A:1237:ILE:HG22	4:A:1238:ILE:N	2.36	0.40
4:A:1317:MET:HE1	4:A:1338:VAL:HG11	2.02	0.40
4:A:1369:ALA:O	4:A:1370:LEU:C	2.61	0.40
5:B:129:PHE:CE2	5:B:166:PHE:HD1	2.39	0.40
5:B:758:PHE:O	5:B:760:ASP:N	2.54	0.40
6:C:54:ASN:HB2	6:C:153:LEU:CD1	2.52	0.40
6:C:146:LYS:C	6:C:147:LEU:CD2	2.92	0.40
7:D:63:LEU:HD22	7:D:63:LEU:HA	1.66	0.40
8:E:191:LYS:O	8:E:193:GLY:N	2.55	0.40
10:G:17:PHE:C	10:G:19:GLY:H	2.29	0.40
10:G:79:PHE:CE2	10:G:105:PRO:CG	3.03	0.40
14:K:82:ASP:OD1	14:K:82:ASP:C	2.64	0.40
15:L:25:ALA:O	15:L:26:THR:CB	2.69	0.40
2:N:5:DT:H1'	2:N:6:DA:H5'	2.03	0.40
4:A:7:SER:CB	5:B:1193:GLN:NE2	2.83	0.40
4:A:18:GLN:H	5:B:1215:ARG:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:219:PHE:CD2	4:A:231:PRO:HD2	2.56	0.40
4:A:711:ARG:O	4:A:714:PHE:N	2.51	0.40
4:A:842:VAL:O	4:A:843:LYS:C	2.63	0.40
4:A:960:ILE:O	4:A:961:ARG:C	2.64	0.40
4:A:964:ILE:O	4:A:967:ALA:N	2.55	0.40
4:A:1215:ARG:HH11	4:A:1215:ARG:HG2	1.87	0.40
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.52	0.40
5:B:27:ALA:O	5:B:28:GLU:C	2.64	0.40
5:B:33:VAL:O	5:B:36:ALA:HB3	2.22	0.40
5:B:57:TYR:O	5:B:58:THR:C	2.63	0.40
5:B:69:LEU:CD1	5:B:432:MET:HE1	2.48	0.40
5:B:205:ILE:O	5:B:206:ASN:C	2.63	0.40
5:B:616:ILE:CG1	5:B:697:GLU:HA	2.51	0.40
5:B:858:SER:HA	5:B:966:VAL:O	2.22	0.40
6:C:52:GLU:HB3	6:C:154:LYS:HB2	2.03	0.40
6:C:59:ALA:O	6:C:62:PHE:CB	2.69	0.40
7:D:29:LEU:N	7:D:29:LEU:HD23	2.35	0.40
7:D:51:ASN:O	7:D:52:LEU:C	2.62	0.40
9:F:77:ASP:O	9:F:79:ARG:N	2.54	0.40
10:G:61:ILE:C	10:G:62:LEU:O	2.64	0.40
11:H:9:ILE:HA	11:H:55:LEU:O	2.21	0.40
13:J:27:GLU:C	13:J:29:GLU:N	2.78	0.40
4:A:325:ILE:HG21	5:B:1210:MET:HE2	2.01	0.40
4:A:535:THR:CG2	4:A:575:LYS:HE2	2.50	0.40
4:A:693:VAL:HA	4:A:696:GLU:HB3	2.03	0.40
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.56	0.40
5:B:118:ARG:HG2	5:B:204:ILE:HD13	2.03	0.40
5:B:205:ILE:N	5:B:205:ILE:CD1	2.84	0.40
5:B:564:GLU:HA	5:B:565:PRO:HD2	1.93	0.40
5:B:766:ARG:HA	5:B:766:ARG:HD3	1.91	0.40
5:B:796:LEU:HD12	5:B:797:TYR:N	2.37	0.40
5:B:797:TYR:HE1	5:B:854:LEU:HD21	1.86	0.40
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.74	0.40
6:C:29:MET:HE2	14:K:98:LEU:CG	2.50	0.40
6:C:67:LEU:HD11	6:C:155:LEU:HD13	2.02	0.40
7:D:159:THR:O	7:D:163:VAL:HG23	2.21	0.40
9:F:154:ASP:HB3	9:F:155:LEU:H	1.67	0.40
10:G:119:LEU:HD13	10:G:132:SER:HB2	2.03	0.40
12:I:34:TYR:HE2	12:I:36:GLU:HB3	1.86	0.40
13:J:52:THR:O	13:J:52:THR:HG22	2.20	0.40
4:A:57:ARG:O	4:A:68:GLN:NE2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:431:LYS:HE3	4:A:431:LYS:HB2	1.95	0.40
4:A:463:ILE:HD13	4:A:469:ARG:HG3	2.00	0.40
4:A:534:LEU:CD1	4:A:541:ILE:HD11	2.51	0.40
4:A:551:TYR:CE2	14:K:62:LYS:HE2	2.57	0.40
4:A:605:MET:HE3	4:A:614:PHE:O	2.21	0.40
4:A:709:THR:HG22	4:A:711:ARG:N	2.18	0.40
4:A:783:THR:HG21	4:A:815:PHE:CE2	2.56	0.40
4:A:804:TYR:OH	5:B:763:GLN:HA	2.21	0.40
4:A:878:ILE:HG23	4:A:956:LEU:N	2.36	0.40
4:A:986:ILE:HG22	4:A:987:VAL:N	2.37	0.40
4:A:1215:ARG:HG2	4:A:1215:ARG:NH1	2.37	0.40
4:A:1313:LEU:HD23	4:A:1338:VAL:CB	2.52	0.40
5:B:126:SER:HB3	5:B:172:ILE:CD1	2.51	0.40
5:B:203:PHE:CD1	5:B:203:PHE:N	2.89	0.40
5:B:308:TRP:HA	5:B:311:LEU:HD12	2.03	0.40
5:B:889:THR:CG2	5:B:891:ASP:OD2	2.69	0.40
5:B:1035:ALA:HB1	5:B:1040:ASN:O	2.21	0.40
5:B:1110:PRO:HG2	5:B:1119:VAL:CG2	2.51	0.40
5:B:1163:CYS:HB3	5:B:1166:CYS:O	2.22	0.40
5:B:1169:MET:HE2	5:B:1204:PHE:HB2	2.04	0.40
6:C:62:PHE:O	6:C:65:HIS:HB3	2.22	0.40
6:C:89:GLU:O	6:C:90:ASP:HB3	2.21	0.40
6:C:165:LYS:O	14:K:6:ARG:NH1	2.53	0.40
8:E:63:ASN:HA	8:E:64:PRO:HD3	1.78	0.40
8:E:102:GLU:C	8:E:104:ASN:H	2.29	0.40
8:E:120:ALA:O	8:E:122:LYS:N	2.55	0.40
12:I:13:MET:HG3	12:I:14:LEU:N	2.37	0.40
13:J:36:LEU:HD12	13:J:47:ARG:HH12	1.82	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	
4	A	1406/1733 (81%)	988 (70%)	277 (20%)	141 (10%)	0	7
5	B	1090/1224 (89%)	754 (69%)	217 (20%)	119 (11%)	0	5
6	C	264/318 (83%)	181 (69%)	50 (19%)	33 (12%)	0	4
7	D	173/221 (78%)	125 (72%)	28 (16%)	20 (12%)	0	4
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1	10
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	14
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	2	18
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0	2
12	I	117/122 (96%)	84 (72%)	23 (20%)	10 (8%)	0	9
13	J	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0	1
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	1	16
15	L	44/70 (63%)	17 (39%)	14 (32%)	13 (30%)	0	0
All	All	3861/4565 (85%)	2711 (70%)	746 (19%)	404 (10%)	0	6

All (404) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	42	ASP
4	A	44	THR
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	62	ASP
4	A	66	LYS
4	A	67	CYS
4	A	73	GLY
4	A	74	MET
4	A	93	VAL
4	A	154	SER
4	A	223	GLY
4	A	250	ILE
4	A	253	ASN
4	A	255	SER
4	A	286	HIS
4	A	311	GLN
4	A	312	PRO
4	A	318	SER
4	A	322	VAL

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Mol	Chain	Res	Type
4	A	332	LYS
4	A	335	ARG
4	A	336	ILE
4	A	385	ILE
4	A	423	ASP
4	A	536	LEU
4	A	567	LYS
4	A	597	LEU
4	A	626	ASN
4	A	780	VAL
4	A	789	LYS
4	A	968	GLN
4	A	1002	GLY
4	A	1036	ARG
4	A	1115	SER
4	A	1120	LEU
4	A	1122	PRO
4	A	1223	ASP
4	A	1314	SER
4	A	1365	TYR
4	A	1366	ARG
4	A	1378	GLN
4	A	1405	THR
5	B	21	GLU
5	B	45	SER
5	B	108	VAL
5	B	206	ASN
5	B	219	ALA
5	B	229	ALA
5	B	258	LEU
5	B	259	TYR
5	B	266	ALA
5	B	334	ILE
5	B	367	LEU
5	B	401	PHE
5	B	474	SER
5	B	509	ALA
5	B	643	ASP
5	B	709	ASP
5	B	727	LYS
5	B	731	VAL
5	B	751	VAL

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Mol	Chain	Res	Type
5	B	764	SER
5	B	943	SER
5	B	951	GLN
5	B	958	GLN
5	B	1046	PRO
5	B	1069	PHE
5	B	1097	HIS
5	B	1100	ASP
5	B	1108	ARG
5	B	1156	ASP
5	B	1157	ALA
5	B	1171	VAL
5	B	1175	LEU
5	B	1178	ASN
5	B	1181	GLU
5	B	1182	CYS
5	B	1183	LYS
5	B	1188	LYS
6	C	87	PHE
6	C	141	GLY
6	C	149	LYS
6	C	161	LYS
6	C	173	ALA
6	C	184	ASN
6	C	209	TYR
6	C	214	ASN
6	C	215	GLU
7	D	5	THR
7	D	8	PHE
7	D	19	GLU
7	D	20	GLU
7	D	21	GLU
7	D	52	LEU
7	D	131	GLU
7	D	192	LYS
7	D	199	ASN
8	E	44	ALA
8	E	130	ALA
8	E	192	ARG
8	E	206	GLY
10	G	62	LEU
10	G	63	PRO

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Mol	Chain	Res	Type
10	G	118	ASP
10	G	139	ILE
11	H	108	SER
11	H	128	ASN
12	I	3	THR
12	I	9	ASP
12	I	47	GLU
13	J	2	ILE
13	J	6	ARG
13	J	17	LYS
13	J	29	GLU
13	J	32	GLU
13	J	55	ASP
13	J	64	ASN
14	K	7	PHE
15	L	35	SER
15	L	50	ASP
15	L	53	HIS
15	L	60	ARG
4	A	58	LEU
4	A	59	GLY
4	A	69	THR
4	A	76	GLU
4	A	113	LEU
4	A	117	GLU
4	A	205	GLU
4	A	226	GLU
4	A	263	THR
4	A	283	GLY
4	A	410	GLY
4	A	465	TYR
4	A	517	ASN
4	A	543	LEU
4	A	601	LYS
4	A	609	ASP
4	A	619	LYS
4	A	661	GLY
4	A	666	ILE
4	A	716	ASP
4	A	731	ARG
4	A	775	ILE
4	A	847	ASP

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Mol	Chain	Res	Type
4	A	875	ALA
4	A	986	ILE
4	A	1124	HIS
4	A	1212	VAL
4	A	1221	LYS
4	A	1255	GLU
5	B	58	THR
5	B	67	SER
5	B	68	THR
5	B	260	GLY
5	B	282	ILE
5	B	328	GLU
5	B	369	GLY
5	B	394	ASP
5	B	450	ALA
5	B	467	GLY
5	B	470	LYS
5	B	477	ALA
5	B	591	ARG
5	B	605	ARG
5	B	613	VAL
5	B	712	PRO
5	B	792	MET
5	B	867	GLY
5	B	884	ARG
5	B	907	GLY
5	B	1003	ALA
5	B	1041	GLU
5	B	1103	ILE
5	B	1126	GLY
5	B	1131	GLY
5	B	1155	SER
5	B	1167	GLY
5	B	1186	ASP
6	C	78	GLU
6	C	84	ARG
6	C	108	GLU
6	C	110	THR
6	C	156	THR
6	C	175	ALA
6	C	216	GLY
6	C	231	ASN

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Mol	Chain	Res	Type
7	D	9	GLN
7	D	53	SER
7	D	177	VAL
8	E	73	PRO
8	E	74	ASP
8	E	106	GLN
8	E	121	MET
8	E	174	GLN
9	F	73	ALA
9	F	81	THR
9	F	154	ASP
10	G	167	TYR
11	H	59	ILE
11	H	62	SER
11	H	81	PRO
11	H	82	PRO
11	H	84	ALA
11	H	90	ALA
11	H	140	ALA
12	I	11	ASN
12	I	57	GLY
12	I	79	HIS
12	I	91	ARG
12	I	106	CYS
13	J	28	ASP
14	K	15	GLY
14	K	104	ASN
15	L	43	THR
15	L	54	ARG
4	A	4	GLN
4	A	232	GLU
4	A	298	PHE
4	A	321	PRO
4	A	331	GLY
4	A	399	HIS
4	A	418	SER
4	A	846	GLU
4	A	854	ASN
4	A	871	ASP
4	A	1016	THR
4	A	1324	PRO
4	A	1335	ILE

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Mol	Chain	Res	Type
4	A	1377	THR
4	A	1393	ASN
4	A	1402	PHE
5	B	46	GLN
5	B	184	ALA
5	B	193	LYS
5	B	257	LYS
5	B	460	ALA
5	B	559	SER
5	B	641	GLU
5	B	708	GLU
5	B	711	GLU
5	B	738	PHE
5	B	746	SER
5	B	754	SER
5	B	878	GLN
5	B	879	ARG
5	B	881	ASN
5	B	942	ARG
5	B	1016	ALA
5	B	1035	ALA
5	B	1143	ALA
6	C	90	ASP
6	C	153	LEU
6	C	212	PRO
6	C	213	PRO
6	C	240	VAL
7	D	6	SER
7	D	218	GLU
8	E	43	LYS
8	E	45	LYS
8	E	59	SER
8	E	103	LYS
8	E	115	ASN
9	F	112	GLU
10	G	35	GLU
11	H	32	THR
11	H	109	LYS
12	I	107	SER
13	J	27	GLU
14	K	111	LEU
15	L	44	ASP

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Mol	Chain	Res	Type
15	L	55	ILE
15	L	59	ALA
4	A	45	GLN
4	A	70	CYS
4	A	128	ILE
4	A	169	ASN
4	A	219	PHE
4	A	400	PRO
4	A	424	ILE
4	A	592	ASP
4	A	852	TYR
4	A	916	GLY
4	A	958	VAL
4	A	1126	ALA
4	A	1229	SER
4	A	1281	ARG
4	A	1302	PRO
4	A	1438	THR
5	B	65	GLU
5	B	171	PRO
5	B	333	PHE
5	B	365	THR
5	B	409	ALA
5	B	478	GLY
5	B	480	SER
5	B	869	SER
5	B	909	ASP
5	B	1017	ILE
6	C	60	ASP
6	C	132	PRO
6	C	167	HIS
6	C	208	GLU
6	C	217	ASP
7	D	13	ARG
8	E	76	GLY
10	G	154	VAL
11	H	17	PRO
11	H	60	ALA
11	H	77	ARG
11	H	92	ASP
11	H	139	ASN
12	I	95	THR

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Mol	Chain	Res	Type
13	J	24	LEU
13	J	33	GLY
14	K	29	ASN
15	L	64	LEU
4	A	61	ILE
4	A	84	ILE
4	A	245	PRO
4	A	544	ASP
4	A	591	PHE
4	A	599	SER
4	A	782	ARG
4	A	910	PRO
4	A	920	LEU
4	A	1114	PRO
4	A	1116	LEU
4	A	1128	GLN
4	A	1165	GLU
4	A	1242	VAL
4	A	1297	GLU
4	A	1300	LYS
5	B	24	PRO
5	B	28	GLU
5	B	114	PRO
5	B	115	GLN
5	B	262	GLU
5	B	295	GLY
5	B	309	GLN
5	B	346	GLU
5	B	362	PRO
5	B	421	PHE
5	B	436	VAL
5	B	551	PRO
5	B	565	PRO
5	B	978	ASP
5	B	1045	SER
6	C	142	VAL
6	C	148	ARG
7	D	15	LEU
7	D	31	GLN
7	D	174	PRO
8	E	104	ASN
9	F	104	ASN

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Mol	Chain	Res	Type
11	H	52	GLN
14	K	4	PRO
15	L	40	LEU
4	A	5	GLN
4	A	111	GLY
4	A	419	LYS
4	A	492	PRO
4	A	598	LEU
4	A	753	GLY
4	A	1071	SER
5	B	283	VAL
5	B	611	PRO
5	B	688	GLY
5	B	1011	ILE
6	C	195	GLN
7	D	16	LYS
11	H	12	VAL
11	H	83	GLN
15	L	26	THR
15	L	56	LEU
4	A	568	PRO
4	A	600	PRO
4	A	627	GLY
4	A	1341	ILE
5	B	575	PRO
7	D	202	ILE
10	G	20	PRO
4	A	244	PRO
4	A	1435	PRO
5	B	818	PRO
6	C	51	VAL
6	C	139	GLY
13	J	14	VAL
4	A	196	GLU
4	A	284	ALA
4	A	1031	VAL
4	A	1164	PRO
5	B	511	PRO
5	B	1214	PRO
6	C	6	PRO
8	E	38	PRO
4	A	357	PRO

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Mol	Chain	Res	Type
4	A	765	VAL
5	B	658	ILE
5	B	901	PRO
11	H	44	VAL

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	
4	A	1239/1520 (82%)	1123 (91%)	116 (9%)	8	30
5	B	962/1061 (91%)	883 (92%)	79 (8%)	10	35
6	C	234/274 (85%)	210 (90%)	24 (10%)	7	27
7	D	159/200 (80%)	130 (82%)	29 (18%)	2	12
8	E	196/197 (100%)	188 (96%)	8 (4%)	27	51
9	F	74/137 (54%)	64 (86%)	10 (14%)	4	19
10	G	152/152 (100%)	140 (92%)	12 (8%)	11	36
11	H	117/128 (91%)	113 (97%)	4 (3%)	32	55
12	I	113/116 (97%)	104 (92%)	9 (8%)	11	36
13	J	60/65 (92%)	56 (93%)	4 (7%)	15	41
14	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
15	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3445/4009 (86%)	3138 (91%)	307 (9%)	9	32

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	18	GLN
4	A	34	LYS
4	A	37	PHE
4	A	38	PRO
4	A	41	MET

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Mol	Chain	Res	Type
4	A	62	ASP
4	A	68	GLN
4	A	93	VAL
4	A	108	MET
4	A	215	SER
4	A	221	SER
4	A	236	LEU
4	A	270	LEU
4	A	289	ILE
4	A	302	THR
4	A	308	ILE
4	A	312	PRO
4	A	320	ARG
4	A	321	PRO
4	A	322	VAL
4	A	326	ARG
4	A	335	ARG
4	A	345	VAL
4	A	350	ARG
4	A	354	SER
4	A	381	THR
4	A	385	ILE
4	A	396	PRO
4	A	406	ILE
4	A	407	ARG
4	A	408	ASP
4	A	412	ARG
4	A	418	SER
4	A	425	GLN
4	A	431	LYS
4	A	442	VAL
4	A	443	LEU
4	A	445	ASN
4	A	449	SER
4	A	450	LEU
4	A	451	HIS
4	A	460	VAL
4	A	461	LYS
4	A	462	VAL
4	A	466	SER
4	A	470	LEU
4	A	487	MET

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Mol	Chain	Res	Type
4	A	493	GLN
4	A	503	GLN
4	A	512	VAL
4	A	515	GLN
4	A	560	ILE
4	A	562	THR
4	A	590	ARG
4	A	629	LEU
4	A	666	ILE
4	A	670	ILE
4	A	692	ASP
4	A	711	ARG
4	A	768	GLN
4	A	774	ARG
4	A	786	HIS
4	A	821	ARG
4	A	830	LYS
4	A	834	THR
4	A	845	LEU
4	A	858	ASN
4	A	886	ILE
4	A	907	THR
4	A	919	ILE
4	A	929	LEU
4	A	969	GLN
4	A	988	LEU
4	A	992	ASP
4	A	997	LEU
4	A	1001	ARG
4	A	1017	LEU
4	A	1029	ARG
4	A	1035	TYR
4	A	1037	LEU
4	A	1050	GLU
4	A	1067	LEU
4	A	1110	ASN
4	A	1111	MET
4	A	1116	LEU
4	A	1120	LEU
4	A	1122	PRO
4	A	1127	ASP
4	A	1138	ILE

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Mol	Chain	Res	Type
4	A	1146	VAL
4	A	1152	ILE
4	A	1170	ILE
4	A	1173	HIS
4	A	1187	GLN
4	A	1206	ASP
4	A	1240	CYS
4	A	1264	GLU
4	A	1271	ILE
4	A	1291	VAL
4	A	1295	THR
4	A	1329	THR
4	A	1332	PHE
4	A	1333	ILE
4	A	1359	ASP
4	A	1372	VAL
4	A	1386	ARG
4	A	1389	PHE
4	A	1405	THR
4	A	1408	ILE
4	A	1415	SER
4	A	1428	VAL
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
5	B	30	SER
5	B	46	GLN
5	B	57	TYR
5	B	63	ILE
5	B	104	GLU
5	B	175	ARG
5	B	188	ASP
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	223	VAL
5	B	250	PHE
5	B	268	THR
5	B	283	VAL
5	B	298	LEU
5	B	365	THR

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Mol	Chain	Res	Type
5	B	371	GLU
5	B	393	LYS
5	B	399	ASP
5	B	408	LEU
5	B	427	ASP
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP
5	B	485	ARG
5	B	496	ARG
5	B	498	THR
5	B	502	ILE
5	B	513	GLN
5	B	516	ASN
5	B	555	ILE
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	616	ILE
5	B	628	THR
5	B	644	GLU
5	B	649	LYS
5	B	682	SER
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	748	ILE
5	B	751	VAL
5	B	755	ILE
5	B	787	VAL
5	B	830	TYR
5	B	835	GLN
5	B	839	MET
5	B	878	GLN
5	B	894	ASP
5	B	901	PRO
5	B	909	ASP
5	B	939	THR
5	B	957	ASN
5	B	999	MET

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Mol	Chain	Res	Type
5	B	1002	THR
5	B	1006	ILE
5	B	1018	PRO
5	B	1022	THR
5	B	1047	PHE
5	B	1084	GLN
5	B	1085	ILE
5	B	1095	LEU
5	B	1099	VAL
5	B	1103	ILE
5	B	1108	ARG
5	B	1112	GLN
5	B	1122	ARG
5	B	1138	MET
5	B	1159	ARG
5	B	1165	ILE
5	B	1170	THR
5	B	1183	LYS
5	B	1202	LEU
5	B	1212	ILE
5	B	1216	LEU
6	C	22	LEU
6	C	35	ARG
6	C	54	ASN
6	C	56	THR
6	C	57	VAL
6	C	58	LEU
6	C	74	SER
6	C	77	ILE
6	C	89	GLU
6	C	93	ASP
6	C	106	GLU
6	C	108	GLU
6	C	128	ASN
6	C	129	ILE
6	C	140	ASN
6	C	147	LEU
6	C	163	ILE
6	C	166	GLU
6	C	209	TYR
6	C	214	ASN
6	C	233	GLU

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Mol	Chain	Res	Type
6	C	240	VAL
6	C	251	LEU
6	C	266	ASP
7	D	5	THR
7	D	8	PHE
7	D	11	ARG
7	D	13	ARG
7	D	15	LEU
7	D	16	LYS
7	D	17	LYS
7	D	19	GLU
7	D	47	LEU
7	D	50	LEU
7	D	63	LEU
7	D	70	PHE
7	D	126	ILE
7	D	137	ASN
7	D	139	LYS
7	D	148	LEU
7	D	149	THR
7	D	151	PHE
7	D	152	SER
7	D	170	THR
7	D	174	PRO
7	D	182	SER
7	D	187	THR
7	D	192	LYS
7	D	193	THR
7	D	202	ILE
7	D	206	GLU
7	D	216	ASN
7	D	221	TYR
8	E	40	GLU
8	E	60	PHE
8	E	74	ASP
8	E	78	LEU
8	E	114	ASN
8	E	132	ILE
8	E	153	HIS
8	E	184	VAL
9	F	79	ARG
9	F	81	THR

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Mol	Chain	Res	Type
9	F	90	ARG
9	F	99	LEU
9	F	111	LEU
9	F	119	ARG
9	F	122	MET
9	F	143	PHE
9	F	148	VAL
9	F	153	VAL
10	G	1	MET
10	G	13	LEU
10	G	21	ARG
10	G	45	ILE
10	G	74	TYR
10	G	78	VAL
10	G	79	PHE
10	G	80	LYS
10	G	87	VAL
10	G	88	ASP
10	G	126	ASN
10	G	171	ILE
11	H	26	ILE
11	H	102	TYR
11	H	130	ARG
11	H	134	ASN
12	I	4	PHE
12	I	9	ASP
12	I	15	TYR
12	I	75	CYS
12	I	84	VAL
12	I	85	PHE
12	I	86	PHE
12	I	100	PHE
12	I	101	PHE
13	J	2	ILE
13	J	16	ASP
13	J	44	TYR
13	J	46	CYS
14	K	1	MET
14	K	10	PHE
14	K	25	THR
14	K	41	THR
14	K	47	ARG

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Mol	Chain	Res	Type
14	K	50	LEU
14	K	61	TYR
14	K	78	THR
14	K	114	LEU
15	L	27	LEU
15	L	54	ARG
15	L	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	54	ASN
4	A	68	GLN
4	A	92	HIS
4	A	225	ASN
4	A	253	ASN
4	A	299	HIS
4	A	339	ASN
4	A	435	HIS
4	A	447	GLN
4	A	451	HIS
4	A	493	GLN
4	A	503	GLN
4	A	515	GLN
4	A	517	ASN
4	A	611	GLN
4	A	631	HIS
4	A	654	ASN
4	A	736	ASN
4	A	741	ASN
4	A	742	ASN
4	A	757	ASN
4	A	768	GLN
4	A	786	HIS
4	A	858	ASN
4	A	903	ASN
4	A	926	GLN
4	A	994	GLN
4	A	1070	GLN
4	A	1106	ASN
4	A	1128	GLN

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Mol	Chain	Res	Type
4	A	1130	GLN
4	A	1140	HIS
4	A	1173	HIS
4	A	1222	ASN
4	A	1265	ASN
4	A	1364	ASN
4	A	1432	GLN
5	B	103	ASN
5	B	110	HIS
5	B	121	ASN
5	B	178	ASN
5	B	215	GLN
5	B	236	HIS
5	B	350	GLN
5	B	363	HIS
5	B	366	GLN
5	B	465	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	538	ASN
5	B	706	GLN
5	B	734	HIS
5	B	744	HIS
5	B	762	ASN
5	B	763	GLN
5	B	767	ASN
5	B	786	ASN
5	B	794	ASN
5	B	821	GLN
5	B	842	ASN
5	B	843	GLN
5	B	951	GLN
5	B	957	ASN
5	B	975	GLN
5	B	1015	HIS
5	B	1062	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1084	GLN
5	B	1117	GLN

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Mol	Chain	Res	Type
5	B	1179	GLN
5	B	1193	GLN
5	B	1211	ASN
6	C	17	ASN
6	C	65	HIS
6	C	73	GLN
6	C	79	GLN
6	C	112	ASN
6	C	123	ASN
6	C	140	ASN
6	C	167	HIS
6	C	252	GLN
7	D	9	GLN
7	D	39	ASN
7	D	40	HIS
7	D	132	GLN
7	D	137	ASN
7	D	157	GLN
8	E	8	ASN
8	E	32	GLN
8	E	101	GLN
8	E	104	ASN
8	E	113	GLN
8	E	114	ASN
8	E	143	ASN
8	E	146	HIS
8	E	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	96	GLN
10	G	97	HIS
10	G	122	ASN
10	G	126	ASN
11	H	131	ASN
11	H	137	GLN
12	I	12	ASN
12	I	60	GLN
12	I	89	GLN
12	I	90	GLN
13	J	64	ASN
14	K	44	ASN
14	K	65	HIS

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Mol	Chain	Res	Type
14	K	76	GLN
14	K	89	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CPT	T	67	1	0,2,4	-	-	-		

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	67	CPT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	17/17 (100%)	0.88	1 (5%) 28 23	110, 139, 169, 175	0
2	N	7/7 (100%)	1.14	1 (14%) 6 9	148, 156, 169, 171	0
3	P	10/10 (100%)	0.80	1 (10%) 12 15	118, 128, 165, 172	0
4	A	1416/1733 (81%)	0.00	28 (1%) 65 44	44, 103, 161, 199	0
5	B	1108/1224 (90%)	0.21	45 (4%) 41 30	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.05	1 (0%) 88 74	64, 100, 144, 162	0
7	D	177/221 (80%)	0.33	11 (6%) 26 22	70, 120, 177, 190	0
8	E	214/215 (99%)	0.25	2 (0%) 81 60	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.28	1 (1%) 76 54	53, 81, 115, 132	0
10	G	171/171 (100%)	0.07	1 (0%) 85 68	82, 103, 141, 150	0
11	H	133/146 (91%)	0.64	10 (7%) 20 18	119, 149, 180, 188	0
12	I	119/122 (97%)	0.49	5 (4%) 40 29	94, 150, 183, 199	0
13	J	65/70 (92%)	0.01	1 (1%) 72 50	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.22	1 (0%) 81 60	64, 101, 130, 149	0
15	L	46/70 (65%)	0.60	4 (8%) 16 16	96, 154, 172, 178	0
All	All	3947/4599 (85%)	0.13	113 (2%) 53 37	44, 111, 175, 199	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	7.7
4	A	1081	LEU	4.6
7	D	25	ALA	4.5
11	H	63	LEU	4.3
5	B	883	LEU	4.2
5	B	879	ARG	4.2
9	F	72	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
4	A	3	GLY	4.1
5	B	882	THR	4.1
5	B	335	GLY	4.1
7	D	24	ALA	4.1
3	P	1	U	4.0
7	D	13	ARG	4.0
5	B	250	PHE	4.0
5	B	963	PHE	3.9
5	B	730	ARG	3.9
4	A	56	PRO	3.9
5	B	731	VAL	3.9
5	B	732	SER	3.7
4	A	1175	SER	3.7
15	L	25	ALA	3.6
14	K	114	LEU	3.6
7	D	8	PHE	3.5
13	J	65	PRO	3.3
4	A	251	SER	3.3
4	A	1173	HIS	3.3
5	B	70	ILE	3.2
5	B	508	LEU	3.2
5	B	734	HIS	3.2
5	B	134	LYS	3.2
5	B	934	LYS	3.2
11	H	119	GLY	3.1
4	A	69	THR	3.1
5	B	471	LYS	3.0
4	A	252	PHE	3.0
15	L	26	THR	3.0
4	A	2	VAL	3.0
5	B	507	LYS	2.9
5	B	446	LEU	2.9
11	H	139	ASN	2.9
11	H	140	ALA	2.9
11	H	76	THR	2.8
10	G	21	ARG	2.8
6	C	3	GLU	2.8
2	N	1	DC	2.7
4	A	51	GLY	2.7
5	B	349	ILE	2.7
4	A	1257	ASP	2.7
5	B	715	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	904	THR	2.6
7	D	4	SER	2.6
12	I	57	GLY	2.6
5	B	723	VAL	2.6
5	B	724	ASP	2.6
4	A	1254	ALA	2.6
4	A	292	ALA	2.5
11	H	136	LYS	2.5
4	A	830	LYS	2.4
5	B	862	GLN	2.4
12	I	120	GLN	2.4
11	H	135	LEU	2.4
5	B	620	ARG	2.4
4	A	40	THR	2.4
5	B	887	HIS	2.4
5	B	709	ASP	2.4
4	A	1172	LEU	2.4
5	B	710	LEU	2.4
7	D	18	VAL	2.4
7	D	118	THR	2.4
5	B	1222	ARG	2.4
5	B	266	ALA	2.4
5	B	610	ASN	2.4
5	B	933	SER	2.4
5	B	641	GLU	2.4
7	D	17	LYS	2.4
4	A	1187	GLN	2.3
5	B	832	GLY	2.3
15	L	53	HIS	2.3
8	E	86	PRO	2.3
5	B	864	LYS	2.3
12	I	64	SER	2.3
7	D	14	ARG	2.3
4	A	1243	VAL	2.3
5	B	470	LYS	2.2
5	B	1224	PHE	2.2
4	A	65	LEU	2.2
4	A	1080	THR	2.2
1	T	11	DT	2.2
5	B	884	ARG	2.2
15	L	27	LEU	2.2
5	B	251	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
11	H	90	ALA	2.2
4	A	74	MET	2.2
7	D	155	ARG	2.1
5	B	561	TRP	2.1
5	B	877	PRO	2.1
8	E	107	THR	2.1
5	B	502	ILE	2.1
5	B	510	LYS	2.1
12	I	93	LYS	2.1
4	A	59	GLY	2.1
4	A	34	LYS	2.1
7	D	35	LEU	2.1
5	B	725	PRO	2.1
5	B	241	ARG	2.1
12	I	4	PHE	2.1
11	H	95	TYR	2.0
5	B	345	LYS	2.0
4	A	171	GLN	2.0
5	B	964	VAL	2.0
4	A	253	ASN	2.0
4	A	226	GLU	2.0
11	H	120	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	CPT	T	67	3/5	0.95	0.30	131,131,131,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	ZN	I	204	1/1	0.95	0.13	196,196,196,196	0
18	MG	A	1736	1/1	0.98	0.10	58,58,58,58	0
17	ZN	L	105	1/1	0.99	0.05	127,127,127,127	0
17	ZN	A	1734	1/1	0.99	0.05	108,108,108,108	0
17	ZN	I	203	1/1	1.00	0.07	113,113,113,113	0
17	ZN	A	1735	1/1	1.00	0.03	65,65,65,65	0
17	ZN	J	101	1/1	1.00	0.03	68,68,68,68	0
17	ZN	B	1307	1/1	1.00	0.04	71,71,71,71	0
17	ZN	C	319	1/1	1.00	0.06	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.