



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 11:59 AM EST

PDB ID : 2R7Z
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

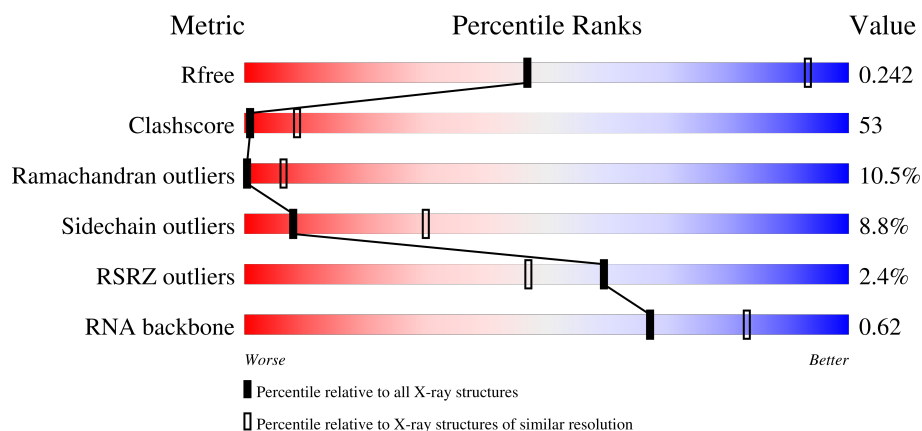
1 Overall quality at a glance

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}	164625	1025 (3.98-3.62)
Clashscore	180529	1005 (3.96-3.64)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)
RNA backbone	3690	1131 (4.60-3.00)

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	<div> <div>6%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>
2	N	7	<div> <div>14%</div> <div>71%</div> <div>29%</div> </div>
3	P	10	<div> <div>10%</div> <div>20%</div> <div>70%</div> <div>10%</div> </div>
4	A	1733	<div> <div>%</div> <div>26%</div> <div>45%</div> <div>10%</div> <div>18%</div> </div>

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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			

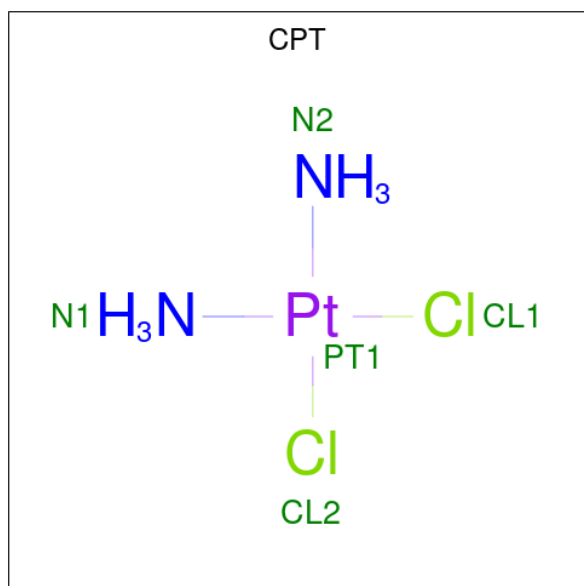
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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 (three-letter code: 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 (three-letter code: 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

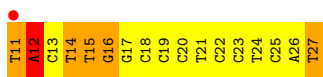
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

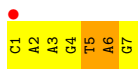
3 Residue-property plots [i](#)

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',



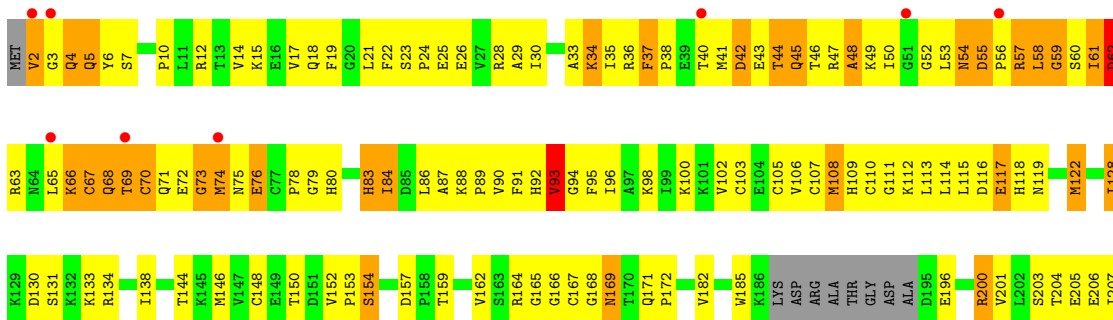
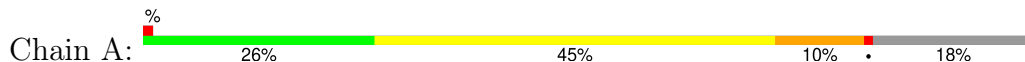
- Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'



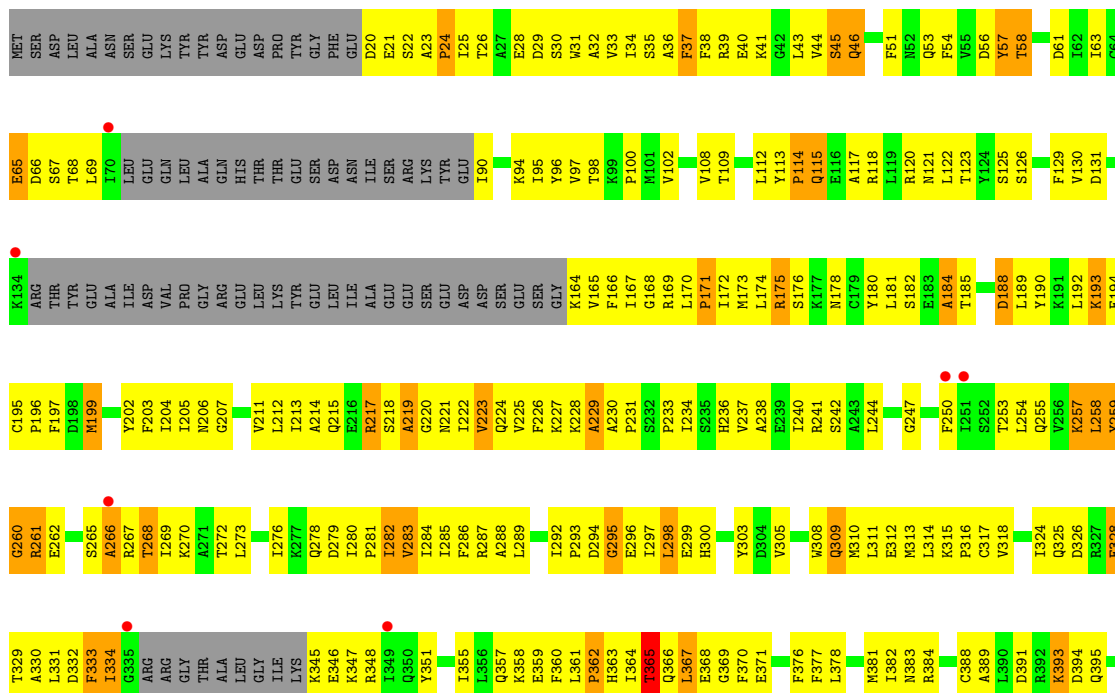
- Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

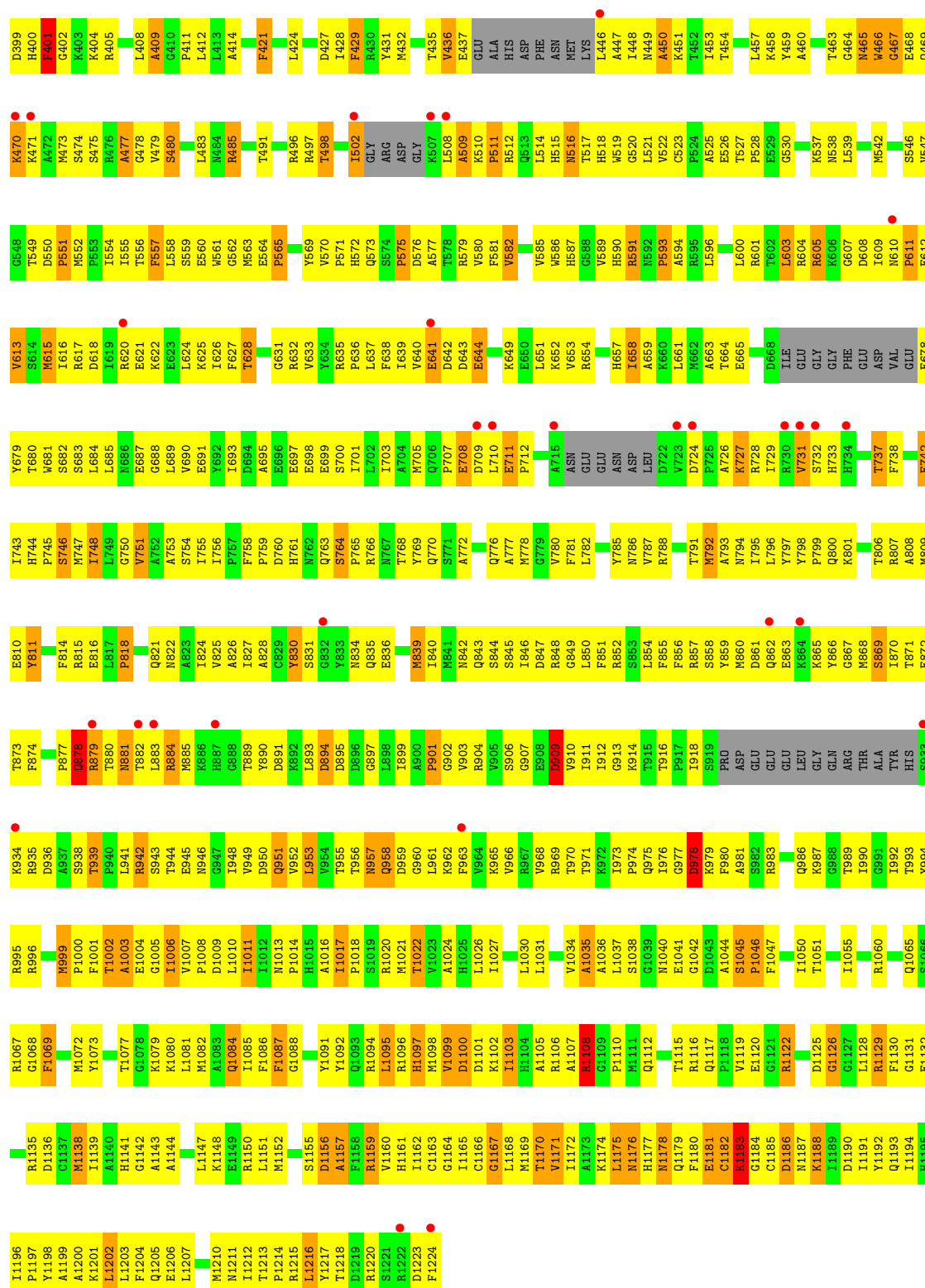


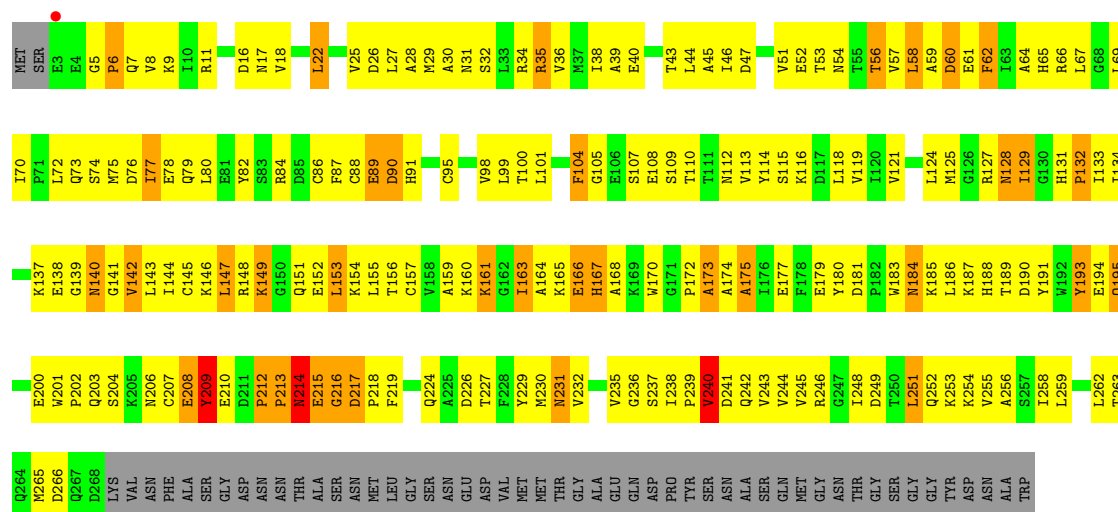
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



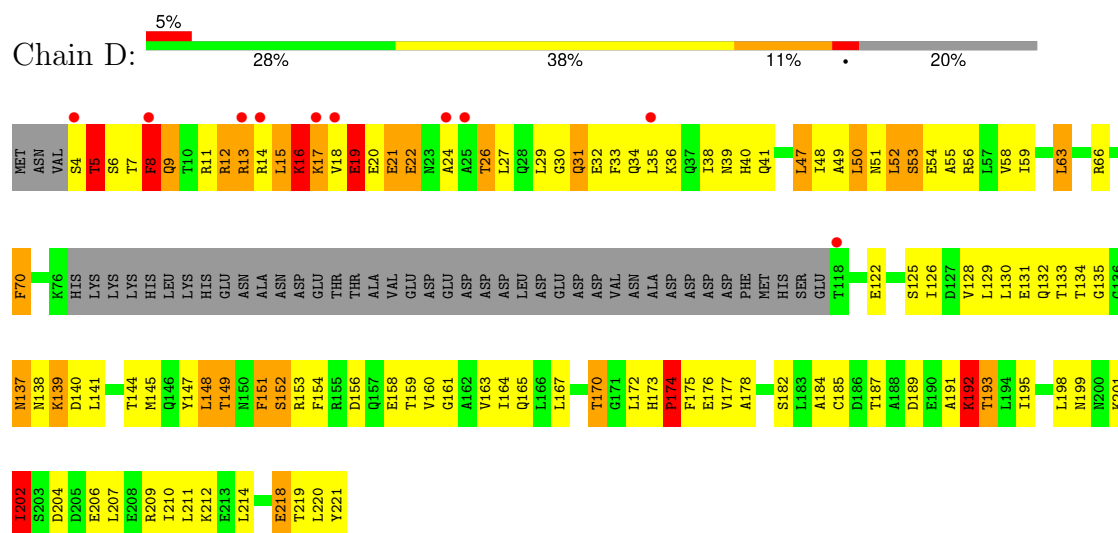
T1161	K1092	SER	R1025	G887	I825	S751	M676	L607	R537	L470	S409	L340	E277	L208
V1162	K1093		R1029	G888	D826	K752	I679	D609	I541	I471	G410	K341	T278	R209
P1163	K1094		R1035	S889	T827	K753	T680	D609	E542	L472	R412	K342	L279	T210
D1164	V1030		V1031	D890	A928	S754	E681	I613	E543	T474	L413	K343	E280	F211
E1165	V1031		V1032		A929		T682	I614	D544	T475	D414	K344	N281	
D1166	V1032		V1033	R896	K830	M757	I683	G615	O545	S476	L415	D346	C283	I214
E1167	P1098		P1099	R897	T831		E684	G616	O546	S477	R416	F347	C284	S215
E1168	P1099		P1100	R898	A932	M761	E685	V617	O547	T478	Y417	F348	P285	D218
L1169	P1100		P1101	R899	A933	S762	A686	E618	O548	S479	S418	K349	P286	F219
K1170	L1036		L1037	D900	E933	K763	E687	K619	N549	A480	R419	A349	H287	T220
Q1171	L1037		L1038	D901	T834	A763	D692	K620	N550	A481	R420	R350	H288	S221
E1172	T1038		T1039	L902	G835	G764	O693	K621	O551	F482		T351	L289	L222
H1173	H972		H973	N903	X836	G765	D694	T622	O552			V352	L289	L223
F1174	H972		H973	T904	I837	G766	T694	V622	O553			I353	E290	G223
S1175	L1105		L1106	D905	K838	Q767	K695	G623	O554	D485	D423	G623	E291	F224
L1176	N1106		N1107	H906	R839	Q768	E696	S624	O555	E486	Q425	G624	E292	N225
LEU	N1107		N1108	T907	R840	I775	O697	S625	O556	N487	Q426	D356	E293	E226
ASP	M1110		M1111	L908	R841	R774	Q698	N626	O557	N488	Q427	D357		F228
GLU	V1044		V1045	L909	V842	I775	N700	G627	O558	L489	Y428	E360	Q297	S229
GLU	L1046		L1047	P910	K843		L701	G628	O559	H490	G429	L361	F298	R230
ALA	P1113		P1114	S911	A844	F779	L702	L629	O560	V491	G430	K372	H299	R231
GLU	M1114		M1115	D985	L845	V780	L702	L630	O561	P492	K431	K373	V300	P240
GLN	S1115		S1116	L913	E846	D781		H631	O562	Q493	V432	T373	A301	E232
GLN	L1116		L1117	L914	D847	R782	T709	V632	O563	S494	E433	V366	Y302	P242
PER	T1117		T1118	S915	I848	K783	L710	V633	O564	F495	R434	P367	Y303	P243
ASP	V1118		V1119	G916	M849	L784	R711	G642	O565	E496	H435	K368	K304	P244
Q1187	L1120		L1121	S917	V850	R785	E712	R635	O566	T497	T436	S369	D305	P245
Q1188	H991		H992	E918	H851	H786	S713	R635	O567	R498	Y437	K372	N306	L239
S1189	P1059		P1060	L919	Y852	F787	E714	P639	O568	A499	D438	K373	D307	P240
P1190	L1062		L1063	D922	D853	S788	E715	Q640	O569	E500	N439	T373	I308	V241
W1191	G1061		G1062	G921	N854	K789	D716	V641	O570		D440	L374	A309	P242
L1192	E995		E996	D922	T855		D717	G642	O571	Q603	P441	T375	G310	P243
L1193	A1125		A1126	Q926	T856	S793	V718	F646	O572	L504	V442	Y376	Q311	P244
L1194	V1065		V1066	R957	R857	F794	V719	G647	O573	L504	F443	F377	P312	P245
L1195	L1067		L1068	L929	N858	E795	R720	G648	O574	V507	F444		Q313	P246
L1196	V1067		V1068	E832	S859	S796	F721	N648	O575		N445	T381	A314	R247
L1197	L1067		L1068	R933	G861	K797	L722	T649	O576		R446	P382	L315	P248
L1198	E1068		E1069	Y933	G862	G798	N723	Q650	O577	V512	Q447	Y383	Q316	S249
L1201	K1069		K1070	K934	V863	F799	E724	K651	O578	S513	F448	N384	K317	T250
L1202	S1071		S1072	Q935	I864	E801	A725	N654	O579	P514	S449	T385	S318	S251
L1203	L1071		L1072	L936	Q865	N802	D727	F655	O580	O515	L450	D386	Q319	F252
L1204	E1073		E1074	V937	F866	S903	K728	F655	O581	S516	H451	R387	R320	N253
L1205	K1073		K1074	K938	I867	Y804	A729	L658	O582	N517	K452	L388	P321	E254
L1206	P1075		P1076	D939	Y868	L805	G730	H659	O583	K518	N453		S255	S256
L1207	L1076		L1077	R940	G869	R806	R731	H660	O584	P519	S454	L391	S324	E259
L1208	T1077		T1078	K941	E870	G807	L732	G661	O585	C520	N455	V392	S324	D260
L1209	Q1078		Q1079	F942	D871	L808	N736	F662	O586	G522	A457	R393	I326	L266
L1210	R1012		R1013	L943	G872	T809	P810	S663	O587	V523	H458	G395	R326	D261
L1211	D1013		D1014	V946	M873	Q810	L737	T664	O588	V524	R459	P396	A327	L262
L1212	V1015		V1016	F947	D874	Q811	K738	G665	O589	Q525	V460		R328	T283
L1213	L1017		L1018	P947	A875	E812	D739	T666	O590	D526	K461	R399	G331	F284
L1214	PHE		PHE	N953	I878	F813	N741	G667	O591	T527	V462	P400	K332	K265
L1215	HIS		HIS	W954		F814	N741	G667	O592	L528	G401	R393	E333	L266
L1216	PHE		PHE	P955		F815	N742	F667	O593	P600	P464	R394	G334	A267
L1217	ALA		ALA	L956	S882	H816	V743	A671	O594	K601	Y465	G395	R335	D268
L1218	GLY		GLY	L957	L883	A817	K744	D672	O595	D602	S466		I336	L289
L1219	VAL		VAL	P957	D884	M818	Q745	G673	O596	M605	T467	R407	R337	L270
L1220	ALA		ALA	N959	I886	R821	V747	T675	O597	L606	R469		N339	L276



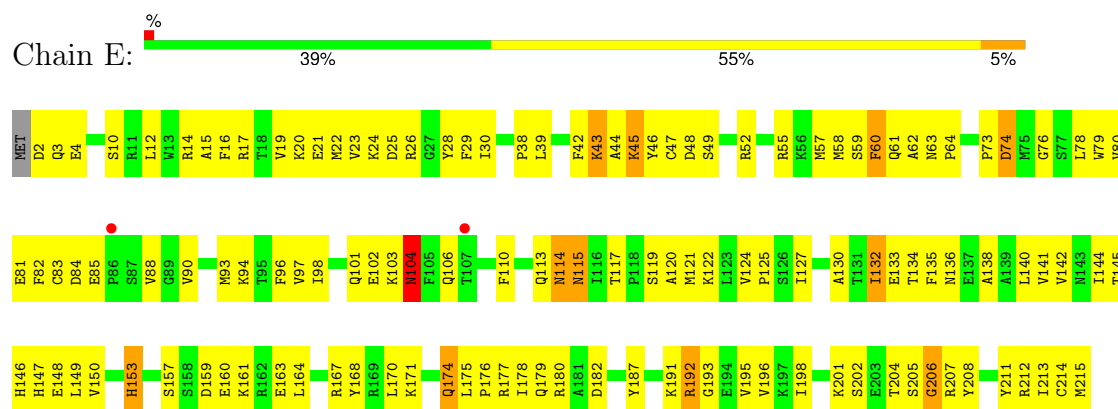




• Molecule 7: DNA-directed RNA polymerase II subunit RPB4

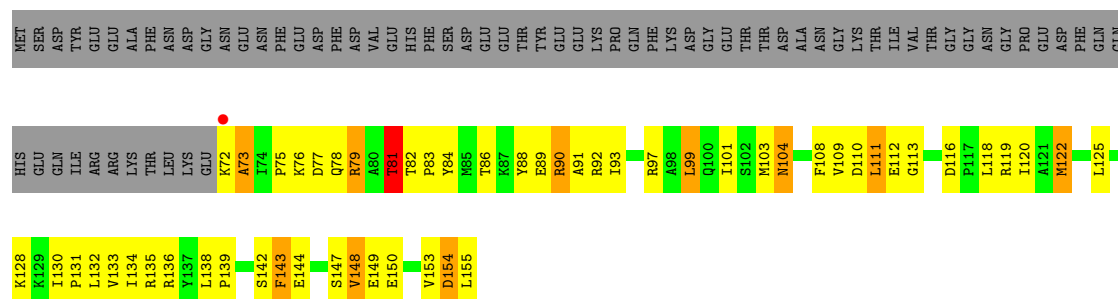


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

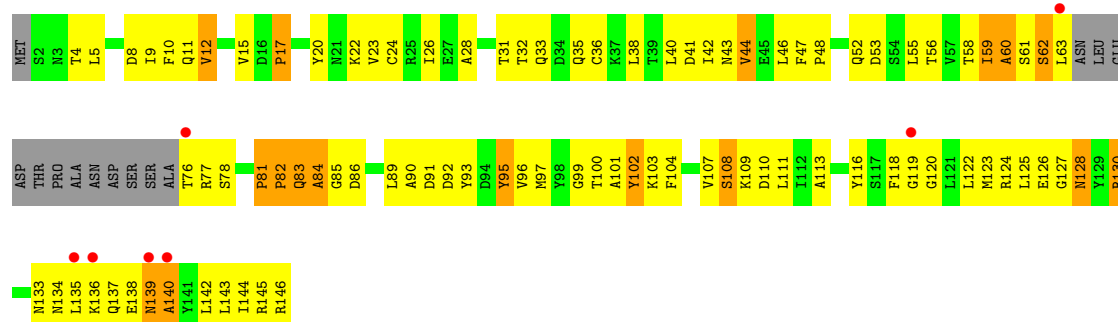




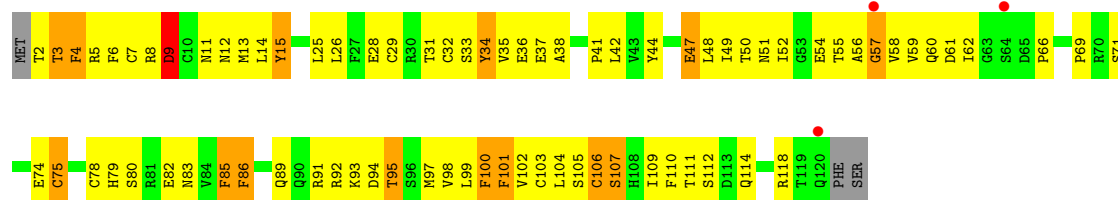
- Molecule 10: DNA-directed RNA polymerase II subunit RPB7



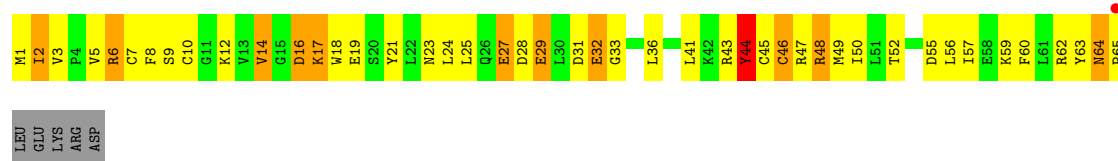
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3



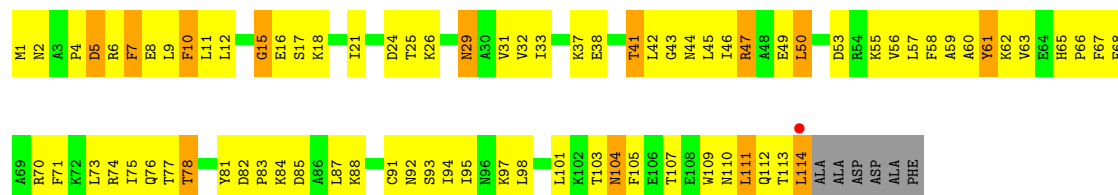
- Molecule 12: DNA-directed RNA polymerase II subunit RPB9



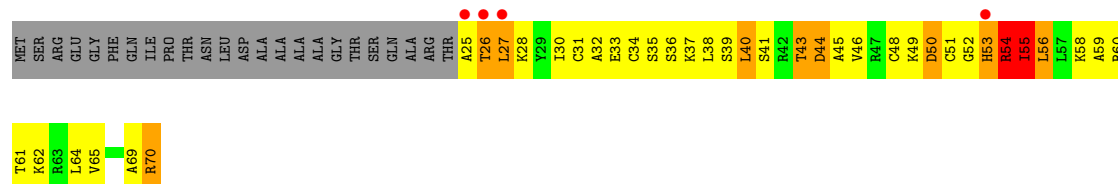
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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 [i](#)

5.1 Standard geometry [i](#)

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	1.41	5/373 (1.3%)	1.79	11/572 (1.9%)
2	N	1.38	0/161	1.10	0/247
3	P	0.95	0/242	0.98	0/377
4	A	0.43	0/11339	0.72	4/15334 (0.0%)
5	B	0.42	0/8981	0.68	0/12108
6	C	0.44	0/2133	0.72	0/2891
7	D	0.42	0/1437	0.69	1/1925 (0.1%)
8	E	0.41	0/1788	0.65	0/2406
9	F	0.49	0/691	0.77	0/933
10	G	0.45	0/1368	0.72	0/1844
11	H	0.38	0/1086	0.65	0/1470
12	I	0.36	0/989	0.65	0/1331
13	J	0.47	0/541	0.74	0/727
14	K	0.45	0/937	0.68	0/1265
15	L	0.47	0/366	0.71	0/485
All	All	0.46	5/32432 (0.0%)	0.73	16/43915 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	16	DG	N3-C4	8.85	1.41	1.35
1	T	17	DG	N3-C4	7.68	1.40	1.35
1	T	17	DG	C2-N3	6.93	1.38	1.32
1	T	16	DG	N1-C2	5.71	1.42	1.37
1	T	14	DT	O3'-P	5.20	1.67	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	17	DG	O4'-C1'-N9	11.85	116.29	108.00
1	T	16	DG	O4'-C1'-N9	9.50	114.65	108.00
1	T	17	DG	N3-C2-N2	7.61	125.22	119.90
4	A	567	LYS	C-N-CD	6.05	141.11	128.40
1	T	16	DG	N1-C2-N3	-5.93	120.34	123.90
1	T	15	DT	C4'-C3'-C2'	5.50	108.05	103.10
1	T	17	DG	O4'-C4'-C3'	5.42	109.25	106.00
1	T	12	DA	O4'-C1'-N9	5.42	111.79	108.00
4	A	425	GLN	N-CA-C	-5.42	96.38	111.00
4	A	466	SER	N-CA-C	5.31	125.33	111.00
1	T	16	DG	C4'-C3'-C2'	-5.09	98.52	103.10
7	D	26	THR	N-CA-C	-5.06	97.33	111.00
1	T	27	DT	C4'-C3'-C2'	5.04	107.63	103.10
4	A	311	GLN	N-CA-C	5.01	124.53	111.00
1	T	17	DG	N1-C2-N3	-5.00	120.90	123.90
1	T	16	DG	C8-N9-C1'	5.00	133.50	127.00

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	1294	0
5	B	8810	0	8847	1025	0
6	C	2095	0	2052	253	0
7	D	1427	0	1451	136	0
8	E	1752	0	1776	149	0
9	F	679	0	701	79	0
10	G	1340	0	1357	152	0
11	H	1068	0	1040	131	0
12	I	971	0	930	102	0
13	J	532	0	543	106	0
14	K	919	0	929	115	0
15	L	364	0	388	57	0
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	3347	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 53.

All (3347) 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
1:T:22:DC:H2"	1:T:23:DC:H5"	1.16	1.08
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.37	1.06
5:B:792:MET:HE2	5:B:857:ARG:HH12	1.16	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:E:22:MET:HE3	8:E:26:ARG:HH21	1.18	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
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.22	1.00
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
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:563:MET:HE3	5:B:580:VAL:HB	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
8:E:22:MET:HE3	8:E:26:ARG:NH2	1.91	0.85
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
10:G:138:THR:HG22	10:G:139:ILE:N	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:55:ASP:C	4:A:57:ARG:H	1.81	0.83
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.61	0.83
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
6:C:43:THR:HG22	6:C:44:LEU:N	1.93	0.82
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:353:ILE:HG21	4:A:487:MET:HE3	1.61	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
5:B:792:MET:HE2	5:B:857:ARG:NH1	1.94	0.81
5:B:821:GLN:HE22	5:B:851:PHE:HA	1.45	0.81
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.63	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:A:475:THR:HG23	4:A:476:SER:N	1.96	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:F:111:LEU:C	9:F:113:GLY:H	1.86	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
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
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
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: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
10:G:18:PHE:HA	10:G:22:MET:HE3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	1.86	0.76
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
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
13:J:8:PHE:H	13:J:49:MET:HE3	1.50	0.75
4:A:866:PHE:C	4:A:867:ILE:HD12	2.07	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
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
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:981:LEU:CD2	4:A:1039:LYS:HA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:A:19:PHE:O	4:A:1416:ALA:HA	1.86	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
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
4:A:55:ASP:CG	4:A:55:ASP:O	2.22	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
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
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
5:B:542:MET:HE2	5:B:743:ILE:HG13	1.72	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:LEU:O	4:A:122:MET:HE3	1.92	0.70
11:H:83:GLN:C	11:H:85:GLY:H	1.92	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
13:J:1:MET:H1	13:J:57:ILE:H	1.37	0.70
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.73	0.70
4:A:541:ILE:HD13	4:A:549:MET:CE	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	11:H:46:LEU:HB2	2.07	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
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
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
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
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.57	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
11:H:89:LEU:C	11:H:91:ASP:H	1.96	0.69
4:A:311:GLN:O	4:A:312:PRO:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:770:GLN:CD	5:B:983:ARG:HA	2.13	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:341:MET:HE1	4:A:843:LYS:NZ	2.07	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
5:B:435:THR:C	5:B:437:GLU:H	1.97	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:35:GLU:OE2	10:G:48:VAL:HG23	1.94	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
5:B:589:VAL:HG12	5:B:590:HIS:N	2.03	0.68
7:D:130:LEU:C	7:D:132:GLN:H	1.97	0.68
12:I:34:TYR:CD2	12:I:35:VAL:N	2.62	0.68
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.75	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
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
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
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:50:ILE:C	4:A:52:GLY:H	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:353:ILE:HD13	4:A:487:MET:HE2	1.77	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:756:ILE:O	5:B:759:PRO:HD3	1.96	0.66
5:B:778:MET:HE2	5:B:1094:ARG:HG2	1.77	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:GLN:C	4:A:70:CYS:H	1.99	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
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
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:746:MET:HE3	5:B:1018:PRO:HG2	1.79	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:416:ARG:C	4:A:417:TYR:HD2	2.00	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
13:J:1:MET:H1	13:J:57:ILE:N	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.79	0.64
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.10	0.64
5:B:1138:MET:HA	5:B:1138:MET:HE3	1.80	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
13:J:1:MET:H1	13:J:56:LEU:N	1.96	0.64
13:J:23:ASN:C	13:J:25:LEU:H	2.01	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
7:D:170:THR:HB	7:D:172:LEU:H	1.62	0.64
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.19	0.63
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.34	0.63
10:G:18:PHE:HA	10:G:22:MET:HE2	1.81	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
4:A:117:GLU:H	4:A:117:GLU:CD	2.01	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
6:C:146:LYS:C	6:C:147:LEU:HD23	2.20	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
1:T:23:DC:H2''	1:T:24:DT:C5'	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:A:541:ILE:HG21	4:A:549:MET:HE3	1.81	0.62
4:A:590:ARG:O	4:A:591:PHE:HB2	2.00	0.62
4:A:1323:ASP:C	4:A:1325:THR:H	2.03	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
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:429:PHE:HA	5:B:432:MET:HE3	1.82	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
10:G:51:TYR:C	10:G:51:TYR:CD2	2.72	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:91:VAL:HA	10:G:101:VAL:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:91:ASP:C	11:H:93:TYR:H	2.04	0.62
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
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: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:117:GLN:C	10:G:119:LEU:H	2.03	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:1164:GLY:HA3	5:B:1190:ASP:OD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:T:11:DT:O2	2:N:7:DG:N2	2.33	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
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:872:GLU:CD	5:B:914:LYS:HE2	2.21	0.60
5:B:948:ILE:HG22	5:B:949:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:145:VAL:CG1	10:G:146:LYS:N	2.64	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
5:B:1097:HIS:H	5:B:1098:MET:HE2	1.66	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
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:384:ASN:CG	4:A:388:LEU:HD12	2.22	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
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
8:E:48:ASP:CG	8:E:49:SER:H	2.05	0.60
5:B:570:VAL:CG2	5:B:573:GLN:HB3	2.31	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
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:903:ASN:HD22	4:A:903:ASN:C	2.04	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
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:858:ASN:C	4:A:858:ASN:HD22	2.04	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
8:E:14:ARG:NH2	8:E:141:VAL:HG12	2.13	0.59
9:F:111:LEU:C	9:F:113:GLY:N	2.53	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
6:C:98:VAL:C	6:C:99:LEU:HD23	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:L:55:ILE:O	15:L:56:LEU:HB2	2.02	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
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.27	0.59
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:1114:PRO:HB2	4:A:1311:VAL:HG23	1.84	0.59
9:F:130:ILE:O	9:F:148:VAL:CG2	2.51	0.59
10:G:1:MET:SD	10:G:1:MET:C	2.81	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
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:341:MET:CE	4:A:843:LYS:HZ3	2.16	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:503:GLN:NE2	9:F:90:ARG:HH21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:918:ILE:HG21	5:B:935:ARG:NH1	2.17	0.59
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.23	0.58
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: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
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: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: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:254:LEU:HD23	5:B:381:MET:HE1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:ASN:O	6:C:34:ARG:HB3	2.04	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
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: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
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: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:92:HIS:CD2	4:A:304:MET:HE3	2.39	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:980:PHE:CA	5:B:1095:LEU:HD11	2.34	0.58
4:A:55:ASP:C	4:A:57:ARG:N	2.52	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
6:C:107:SER:C	6:C:109:SER:H	2.07	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:494:SER:O	4:A:497:THR:N	2.37	0.57
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:27:LEU:HB3	15:L:37:LYS:HD3	1.86	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
7:D:54:GLU:O	7:D:58:VAL:HG23	2.03	0.57
3:P:3:U:H4'	4:A:323:LYS:NZ	2.19	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
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
5:B:217:ARG:HD2	5:B:217:ARG:C	2.24	0.57
9:F:118:LEU:HD12	9:F:118:LEU:O	2.05	0.57
4:A:138:ILE:HD13	4:A:222:LEU:HD23	1.86	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
11:H:142:LEU:C	11:H:143:LEU:HD12	2.25	0.57
4:A:34:LYS:CG	4:A:36:ARG:HH21	2.18	0.57
4:A:844:ALA:O	4:A:845:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.03	0.57
5:B:557:PHE:C	5:B:557:PHE:CD2	2.77	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:71:GLN:C	4:A:73:GLY:H	2.08	0.57
4:A:477:PRO:HG2	4:A:521:MET:HG2	1.87	0.57
4:A:600:PRO:C	4:A:602:ASP:H	2.05	0.57
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.35	0.57
5:B:794:ASN:C	5:B:795:ILE:HD12	2.25	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
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
5:B:847:ASP:C	5:B:849:GLY:H	2.07	0.57
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.35	0.57
8:E:134:THR:C	8:E:135:PHE:HD1	2.08	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
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
10:G:1:MET:SD	10:G:1:MET:O	2.63	0.57
4:A:44:THR:O	4:A:45:GLN:HB2	2.04	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
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:115:LEU:HB2	4:A:122:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.41	0.56
4:A:168:GLY:O	4:A:169:ASN:C	2.44	0.56
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.35	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
5:B:1102:LYS:O	5:B:1103:ILE:C	2.44	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:3:GLN:HG3	8:E:4:GLU:N	2.20	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: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
5:B:1072:MET:HE1	5:B:1085:ILE:HB	1.87	0.56
6:C:40:GLU:HA	6:C:163:ILE:HG21	1.87	0.56
7:D:7:THR:HG21	7:D:32:GLU:CD	2.25	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:384:ASN:O	4:A:385:ILE:C	2.43	0.56
4:A:860:LEU:CD1	4:A:1393:ASN:HB2	2.31	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:254:LYS:O	6:C:258:ILE:HD13	2.05	0.56
7:D:40:HIS:CB	10:G:73:LYS:HZ3	2.05	0.56
9:F:143:PHE:C	9:F:143:PHE:HD1	2.09	0.56
11:H:23:VAL:HG13	11:H:42:ILE:O	2.05	0.56
3:P:3:U:H4'	4:A:323:LYS:HZ3	1.71	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: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: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
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: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
5:B:516:ASN:N	5:B:516:ASN:ND2	2.47	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:605:MET:HE3	4:A:614:PHE:O	2.06	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
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
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
13:J:1:MET:H1	13:J:56:LEU:CA	2.20	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
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
5:B:1065:GLN:HE21	5:B:1067:ARG:HG2	1.72	0.55
8:E:78:LEU:HD23	8:E:78:LEU:C	2.27	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: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:332:ASP:O	5:B:334:ILE:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
8:E:42:PHE:HZ	8:E:58:MET:HE3	1.72	0.55
10:G:1:MET:HE3	10:G:80:LYS:O	2.06	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
5:B:215:GLN:HA	5:B:215:GLN:NE2	2.21	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
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
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: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:806:THR:CG2	5:B:808:ALA:HB3	2.37	0.55
7:D:176:GLU:C	7:D:178:ALA:H	2.10	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:981:LEU:HD23	4:A:1039:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:A:69:THR:C	4:A:71:GLN:N	2.61	0.54
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.34	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
5:B:1038:SER:C	5:B:1040:ASN:H	2.10	0.54
7:D:40:HIS:CB	10:G:73:LYS:HZ2	2.18	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:1435:PRO:HA	4:A:1439:GLY:O	2.06	0.54
5:B:39:ARG:HH21	5:B:665:GLU:CD	2.11	0.54
5:B:309:GLN:CD	12:I:52:ILE:HD11	2.28	0.54
5:B:825:VAL:HG12	5:B:826:ALA:N	2.21	0.54
4:A:265:LYS:NZ	4:A:322:VAL:HG13	2.23	0.54
4:A:401:GLY:C	4:A:435:HIS:CD2	2.81	0.54
4:A:829:VAL:C	4:A:831:THR:H	2.10	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:774:ARG:O	4:A:775:ILE:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:85:GLU:HB2	8:E:88:VAL:HG22	1.89	0.54
9:F:143:PHE:C	9:F:143:PHE:CD1	2.78	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: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: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:172:PRO:HG3	4:A:185:TRP:CZ2	2.43	0.53
4:A:401:GLY:C	4:A:435:HIS:HD2	2.10	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
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
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:27:GLU:C	13:J:29:GLU:H	2.12	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
7:D:52:LEU:C	7:D:54:GLU:H	2.11	0.53
10:G:88:ASP:OD2	10:G:88:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:A:130:ASP:O	4:A:131:SER:C	2.47	0.53
4:A:504:LEU:HD12	4:A:504:LEU:N	2.24	0.53
5:B:449:ASN:C	5:B:451:LYS:H	2.12	0.53
5:B:1176:ASN:C	5:B:1178:ASN:H	2.10	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
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
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:416:ARG:C	4:A:417:TYR:CD2	2.81	0.53
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.91	0.53
4:A:541:ILE:HD13	4:A:549:MET:HE3	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
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:42:ASP:C	4:A:44:THR:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:GLN:C	11:H:85:GLY:N	2.60	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: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
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
12:I:2:THR:O	12:I:3:THR:C	2.46	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
4:A:1076:ALA:HA	4:A:1079:MET:CE	2.38	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
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:50:ILE:C	4:A:52:GLY:N	2.60	0.52
4:A:157:ASP:C	4:A:159:THR:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
10:G:143:ILE:HG23	10:G:169:GLY:O	2.09	0.52
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.39	0.52
4:A:1329:THR:HG21	4:A:1331:SER:HB3	1.92	0.52
4:A:1364:ASN:O	4:A:1365:TYR:C	2.47	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: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
11:H:12:VAL:HA	11:H:28:ALA:HB2	1.92	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
9:F:77:ASP:C	9:F:79:ARG:H	2.12	0.52
11:H:126:GLU:C	11:H:130:ARG:HH22	2.13	0.52
1:T:16:DG:N2	2:N:2:DA:C2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:CD2	4:A:299:HIS:N	2.78	0.52
4:A:853:ASP:OD2	4:A:855:THR:CG2	2.58	0.52
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.82	0.52
4:A:1445:ILE:HD12	4:A:1445:ILE:N	2.07	0.52
5:B:25:ILE:HD11	5:B:653:VAL:C	2.29	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
11:H:40:LEU:HD22	11:H:123:MET:CE	2.40	0.52
13:J:1:MET:H3	13:J:56:LEU:H	1.57	0.52
14:K:61:TYR:C	14:K:61:TYR:CD2	2.80	0.52
4:A:254:GLU:O	4:A:256:GLN:N	2.41	0.52
6:C:263:THR:C	6:C:265:MET:H	2.12	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
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: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
7:D:191:ALA:C	7:D:193:THR:H	2.12	0.52
11:H:107:VAL:O	11:H:108:SER:O	2.28	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
4:A:1259:MET:C	4:A:1261:LYS:H	2.12	0.52
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.92	0.52
11:H:89:LEU:C	11:H:91:ASP:N	2.63	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
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: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
5:B:20:ASP:C	5:B:22:SER:H	2.14	0.51
5:B:189:LEU:O	5:B:192:LEU:N	2.39	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
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:137:ASN:C	7:D:137:ASN:HD22	2.13	0.51
15:L:28:LYS:HB2	15:L:39:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:903:ASN:ND2	4:A:903:ASN:C	2.63	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
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
6:C:29:MET:HE1	14:K:98:LEU:HG	1.93	0.51
7:D:21:GLU:HB2	7:D:22:GLU:OE1	2.11	0.51
15:L:46:VAL:O	15:L:46:VAL:HG12	2.10	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
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: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: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:640:VAL:O	5:B:641:GLU:C	2.49	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
9:F:116:ASP:HB3	9:F:119:ARG:HB2	1.93	0.51
13:J:48:ARG:HE	13:J:49:MET:HE2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.46	0.51
5:B:1099:VAL:C	5:B:1101:ASP:H	2.14	0.51
7:D:47:LEU:HD12	7:D:48:ILE:N	2.25	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:577:ILE:C	4:A:579:SER:N	2.62	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
4:A:1265:ASN:C	4:A:1267:MET:N	2.64	0.51
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.14	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
4:A:317:LYS:O	4:A:318:SER:HB3	2.11	0.51
4:A:1125:ALA:C	4:A:1127:ASP:H	2.14	0.51
4:A:1444:MET:CE	9:F:135:ARG:HB2	2.41	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:903:VAL:HG12	5:B:904:ARG:N	2.26	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:852:TYR:CD1	9:F:136:ARG:HB3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:44:VAL:O	5:B:45:SER:C	2.49	0.50
5:B:234:ILE:HD12	5:B:234:ILE:N	2.26	0.50
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
7:D:34:GLN:C	7:D:36:LYS:H	2.14	0.50
4:A:7:SER:HB3	5:B:1193:GLN:HE21	1.76	0.50
4:A:69:THR:C	4:A:71:GLN:H	2.15	0.50
4:A:89:PRO:O	4:A:204:THR:HG21	2.10	0.50
4:A:92:HIS:HD2	4:A:304:MET:HE3	1.75	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
13:J:43:ARG:HG2	13:J:46:CYS:SG	2.52	0.50
4:A:537:ARG:NH1	11:H:120:GLY:O	2.43	0.50
4:A:907:THR:HG23	4:A:908:LEU:N	2.26	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
7:D:153:ARG:C	7:D:154:PHE:CD1	2.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.93	0.50
4:A:942:PHE:C	4:A:942:PHE:CD2	2.85	0.50
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:797:TYR:C	5:B:798:TYR:HD2	2.15	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:600:PRO:HG2	4:A:601:LYS:H	1.75	0.50
4:A:873:MET:C	4:A:1058:VAL:HG23	2.31	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: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
6:C:187:LYS:C	6:C:189:THR:H	2.15	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: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
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:598:LEU:O	4:A:599:SER:C	2.49	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
10:G:17:PHE:N	10:G:17:PHE:CD2	2.78	0.50
12:I:59:VAL:C	12:I:61:ASP:H	2.15	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: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:1111:MET:CE	4:A:1330:ASN:OD1	2.60	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:1106:ARG:HD3	5:B:1126:GLY:O	2.12	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:824:ILE:CG2	5:B:1087:PHE:CE2	2.93	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
14:K:53:ASP:C	14:K:55:LYS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:LYS:NZ	4:A:61:ILE:CG1	2.71	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
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: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: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
5:B:1183:LYS:C	5:B:1185:CYS:H	2.16	0.49
6:C:73:GLN:HE21	6:C:75:MET:H	1.59	0.49
8:E:12:LEU:HD21	8:E:58:MET:SD	2.53	0.49
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.46	0.49
4:A:840:ARG:O	4:A:841:LEU:C	2.51	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
8:E:168:TYR:HB3	8:E:170:LEU:HG	1.94	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: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:779:PHE:O	4:A:780:VAL:C	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:58:THR:HB	11:H:143:LEU:HB2	1.95	0.49
14:K:47:ARG:C	14:K:47:ARG:HD2	2.32	0.49
4:A:2:VAL:HG21	5:B:1157:ALA:O	2.11	0.49
4:A:262:LEU:C	4:A:264:PHE:N	2.66	0.49
4:A:316:GLN:O	4:A:317:LYS:C	2.51	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
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:590:ARG:NH2	4:A:620:LYS:HB2	2.22	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: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: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
7:D:27:LEU:HD13	7:D:173:HIS:HD2	1.78	0.49
7:D:130:LEU:C	7:D:132:GLN:N	2.65	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:63:ARG:HA	4:A:74:MET:HE2	1.94	0.49
4:A:417:TYR:O	4:A:418:SER:C	2.50	0.49
5:B:364:ILE:HG12	5:B:585:VAL:CG1	2.36	0.49
5:B:843:GLN:O	5:B:844:SER:C	2.51	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
14:K:110:ASN:C	14:K:112:GLN:H	2.16	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:909:ASP:C	4:A:911:SER:H	2.16	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:654:ARG:H	5:B:657:HIS:HD2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:H:40:LEU:HD22	11:H:123:MET:HE3	1.94	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
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
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:894:ASP:HB2	15:L:58:LYS:HZ3	1.78	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
10:G:117:GLN:C	10:G:119:LEU:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:25:TYR:CE2	10:G:29:LYS:HD2	2.48	0.48
11:H:62:SER:O	11:H:63:LEU:C	2.52	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
1:T:26:DA:H2''	1:T:27:DT:O5'	2.11	0.48
4:A:470:LEU:HD22	4:A:487:MET:HE3	1.94	0.48
4:A:921:GLY:O	4:A:922:ASP:C	2.51	0.48
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.42	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
11:H:128:ASN:CG	11:H:128:ASN:O	2.51	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: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
6:C:215:GLU:O	6:C:216:GLY:C	2.51	0.48
11:H:139:ASN:O	11:H:140:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:34:TYR:CD2	12:I:34:TYR:C	2.87	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: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
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
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
13:J:8:PHE:N	13:J:49:MET:HE3	2.24	0.48
4:A:116:ASP:O	4:A:118:HIS:N	2.47	0.48
4:A:289:ILE:C	4:A:291:GLU:H	2.17	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: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
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:1076:ALA:HA	4:A:1079:MET:HE3	1.95	0.48
4:A:1389:PHE:CD1	4:A:1390:ASN:N	2.82	0.48
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1162:VAL:O	4:A:1162:VAL:HG12	2.14	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:683:SER:O	5:B:687:GLU:HB2	2.14	0.48
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
15:L:52:GLY:O	15:L:53:HIS:C	2.51	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: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:92:HIS:O	4:A:93:VAL:C	2.52	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:6:ARG:C	14:K:8:GLU:H	2.16	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: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
10:G:66:GLY:O	10:G:67:SER:C	2.52	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:811:GLN:O	4:A:812:GLU:C	2.53	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: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
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
12:I:4:PHE:CD1	12:I:4:PHE:C	2.88	0.47
12:I:105:SER:O	12:I:106:CYS:HB3	2.14	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:626:ASN:C	4:A:628:GLY:H	2.16	0.47
4:A:996:ASN:C	4:A:998:LEU:HD12	2.35	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
6:C:52:GLU:CD	6:C:154:LYS:HD2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:34:GLN:C	7:D:36:LYS:N	2.67	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
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
13:J:7:CYS:HA	13:J:49:MET:HE3	1.97	0.47
13:J:23:ASN:C	13:J:25:LEU:N	2.66	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
4:A:1436:ILE:O	4:A:1437:GLY:C	2.51	0.47
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.44	0.47
5:B:167:ILE:HG22	5:B:167:ILE:O	2.15	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:623:GLY:C	4:A:625:SER:H	2.17	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
4:A:873:MET:C	4:A:1058:VAL:CG2	2.83	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:847:ASP:C	5:B:849:GLY:N	2.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
5:B:435:THR:C	5:B:437:GLU:N	2.66	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
4:A:1205:LYS:O	4:A:1206:ASP:C	2.54	0.47
4:A:1315:GLU:C	4:A:1317:MET:H	2.18	0.47
5:B:29:ASP:CG	5:B:658:ILE:HD13	2.35	0.47
5:B:360:PHE:C	5:B:360:PHE:CD2	2.88	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
7:D:24:ALA:C	7:D:26:THR:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:CB	5:B:1103:ILE:HD12	2.44	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
5:B:1201:LYS:HE2	5:B:1205:GLN:CD	2.35	0.47
8:E:94:LYS:HG3	8:E:98:ILE:HD11	1.97	0.47
8:E:157:SER:C	8:E:159:ASP:N	2.68	0.47
11:H:11:GLN:HA	11:H:53:ASP:O	2.15	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: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:1138:MET:HA	5:B:1138:MET:CE	2.45	0.46
6:C:77:ILE:C	6:C:79:GLN:H	2.18	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:596:THR:C	4:A:598:LEU:N	2.69	0.46
4:A:1029:ARG:HH11	4:A:1029:ARG:HG3	1.80	0.46
4:A:1280:GLU:O	4:A:1281:ARG:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:957:ASN:O	5:B:958:GLN:C	2.53	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
1:T:11:DT:C2'	1:T:12:DA:H5'	2.46	0.46
4:A:332:LYS:H	4:A:337:ARG:HB3	1.79	0.46
4:A:349:ALA:C	5:B:1128:LEU:HD11	2.35	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
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
5:B:1142:GLY:C	5:B:1144:ALA:H	2.18	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
8:E:29:PHE:O	8:E:30:ILE:HG13	2.15	0.46
13:J:48:ARG:HD2	13:J:48:ARG:C	2.35	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
5:B:580:VAL:HG13	5:B:624:LEU:HB3	1.97	0.46
5:B:593:PRO:O	5:B:594:ALA:C	2.53	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
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
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
4:A:65:LEU:O	4:A:66:LYS:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.98	0.46
5:B:641:GLU:HA	5:B:641:GLU:OE1	2.15	0.46
5:B:871:THR:HG22	5:B:872:GLU:N	2.30	0.46
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: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
7:D:156:ASP:C	7:D:158:GLU:H	2.19	0.46
8:E:93:MET:SD	8:E:97:VAL:HG23	2.55	0.46
11:H:4:THR:O	11:H:5:LEU:HD23	2.16	0.46
4:A:218:ASP:O	4:A:219:PHE:C	2.53	0.46
4:A:265:LYS:HE2	4:A:322:VAL:HG11	1.98	0.46
4:A:1437:GLY:CA	9:F:88:TYR:CD2	2.99	0.46
5:B:39:ARG:NH2	5:B:665:GLU:CD	2.69	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:738:LYS:C	4:A:740:LEU:H	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:E:55:ARG:C	8:E:57:MET:N	2.69	0.46
4:A:61:ILE:CG2	4:A:62:ASP:H	2.22	0.46
4:A:351:THR:HB	5:B:1103:ILE:HD11	1.97	0.46
4:A:909:ASP:O	4:A:911:SER:N	2.49	0.46
5:B:227:LYS:HB2	5:B:395:GLN:OE1	2.16	0.46
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.98	0.46
5:B:893:LEU:HD22	5:B:897:GLY:C	2.36	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
11:H:138:GLU:O	11:H:139:ASN:C	2.53	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: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:346:ASP:CG	5:B:1108:ARG:HA	2.36	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
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:975:GLN:HG2	5:B:976:ILE:N	2.31	0.46
7:D:138:ASN:OD1	7:D:141:LEU:HB2	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:474:VAL:C	4:A:477:PRO:HD2	2.35	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:745:PRO:C	5:B:747:MET:N	2.69	0.45
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.95	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
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
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.45	0.45
5:B:750:GLY:O	5:B:751:VAL:C	2.54	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
8:E:55:ARG:C	8:E:57:MET:H	2.19	0.45
10:G:30:LEU:HD22	10:G:72:VAL:HG11	1.97	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: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
4:A:1323:ASP:C	4:A:1325:THR:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.16	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: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:29:LEU:O	7:D:30:GLY:C	2.52	0.45
8:E:22:MET:CE	8:E:26:ARG:HE	2.30	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
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.38	0.45
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: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
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:341:MET:CE	4:A:843:LYS:HZ1	2.30	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:311:LEU:O	5:B:312:GLU:C	2.55	0.45
5:B:315:LYS:HE3	12:I:4:PHE:CD2	2.52	0.45
5:B:1096:ARG:HA	5:B:1098:MET:HE2	1.99	0.45
6:C:107:SER:O	6:C:109:SER:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:K:53:ASP:C	14:K:55:LYS:N	2.70	0.45
4:A:28:ARG:O	4:A:29:ALA:C	2.55	0.45
4:A:146:MET:CA	4:A:171:GLN:HB2	2.47	0.45
4:A:320:ARG:HH21	4:A:323:LYS:HZ1	1.65	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
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:979:LYS:HG2	5:B:1095:LEU:HD13	1.99	0.45
5:B:1038:SER:C	5:B:1040:ASN:N	2.70	0.45
12:I:69:PRO:HG2	12:I:85:PHE:CE2	2.52	0.45
15:L:36:SER:O	15:L:37:LYS:C	2.55	0.45
15:L:43:THR:HG22	15:L:43:THR:O	2.15	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
6:C:259:LEU:HD21	14:K:92:ASN:CG	2.38	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
14:K:17:SER:O	14:K:18:LYS:C	2.54	0.45
4:A:34:LYS:CD	4:A:34:LYS:N	2.80	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
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:882:THR:O	5:B:883:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:C:31:ASN:O	6:C:32:SER:C	2.55	0.45
8:E:24:LYS:HG3	8:E:25:ASP:N	2.32	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
11:H:82:PRO:C	11:H:84:ALA:H	2.15	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:231:PRO:C	4:A:233:TRP:H	2.20	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
4:A:920:LEU:HD23	4:A:920:LEU:C	2.37	0.44
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
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:563:MET:HE2	5:B:587:HIS:C	2.37	0.44
5:B:695:ALA:O	5:B:698:GLU:HB3	2.17	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
6:C:27:LEU:O	6:C:28:ALA:C	2.56	0.44
7:D:195:ILE:O	7:D:198:LEU:HG	2.17	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:152:SER:O	10:G:153:GLN:HB2	2.17	0.44
11:H:91:ASP:C	11:H:93:TYR:N	2.70	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:157:ASP:C	4:A:159:THR:N	2.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.18	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:26:ASP:O	6:C:27:LEU:C	2.56	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
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:648:ASN:O	4:A:649:ILE:C	2.55	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:882:THR:HG21	5:B:935:ARG:HA	2.00	0.44
6:C:193:TYR:C	6:C:193:TYR:CD1	2.90	0.44
6:C:208:GLU:C	6:C:210:GLU:H	2.21	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:262:LEU:C	4:A:264:PHE:H	2.21	0.44
4:A:341:MET:CE	5:B:1135:ARG:NH1	2.80	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:1148:ILE:O	12:I:48:LEU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1277:GLU:C	4:A:1279:ILE:H	2.20	0.44
5:B:519:TRP:CD1	5:B:519:TRP:C	2.91	0.44
5:B:615:MET:HA	5:B:625:LYS:O	2.18	0.44
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:48:ASP:CG	8:E:49:SER:N	2.71	0.44
8:E:55:ARG:NH1	8:E:113:GLN:NE2	2.66	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: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
5:B:1216:LEU:C	5:B:1217:TYR:HD1	2.21	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
12:I:78:CYS:O	12:I:80:SER:N	2.51	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:615:MET:C	5:B:616:ILE:HD12	2.36	0.44
5:B:661:LEU:C	5:B:663:ALA:H	2.20	0.44
5:B:745:PRO:C	5:B:747:MET:H	2.21	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
7:D:156:ASP:C	7:D:158:GLU:N	2.71	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:844:ALA:C	4:A:845:LEU:HD23	2.38	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
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:23:SER:O	4:A:24:PRO:C	2.53	0.44
4:A:130:ASP:HB3	4:A:133:LYS:HB2	2.00	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: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:552:MET:C	5:B:554:ILE:H	2.22	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
8:E:55:ARG:HB2	8:E:84:ASP:OD2	2.18	0.44
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.83	0.44
4:A:224:PHE:HD2	4:A:229:SER:O	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1429:ILE:O	5:B:1197:PRO:HG3	2.18	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:768:GLN:NE2	4:A:816:HIS:HD1	2.16	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:1072:MET:HE3	5:B:1085:ILE:HD13	1.99	0.43
5:B:1110:PRO:HG2	5:B:1119:VAL:HG22	2.00	0.43
8:E:207:ARG:CB	8:E:207:ARG:NH1	2.81	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
14:K:87:LEU:O	14:K:88:LYS:C	2.56	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:427:GLN:O	4:A:428:TYR:C	2.56	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:166:PHE:C	5:B:167:ILE:HG13	2.39	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
5:B:806:THR:C	5:B:808:ALA:N	2.69	0.43
6:C:114:TYR:HB2	6:C:116:LYS:HG2	2.01	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:115:LEU:HB2	4:A:122:MET:CE	2.49	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:785:TYR:CD1	5:B:786:ASN:N	2.86	0.43
5:B:992:ILE:HD11	14:K:66:PRO:HB2	1.99	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:548:ASN:OD1	14:K:60:ALA:HB1	2.18	0.43
4:A:1209:MET:HE1	4:A:1236:LEU:HB3	2.00	0.43
5:B:34:ILE:O	5:B:37:PHE:N	2.52	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
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:68:GLN:C	4:A:70:CYS:N	2.68	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
4:A:1206:ASP:C	4:A:1274:ARG:NH1	2.71	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
5:B:785:TYR:CD1	5:B:785:TYR:C	2.91	0.43
13:J:31:ASP:O	13:J:32:GLU:C	2.57	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:1394:THR:HG22	4:A:1395:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:A:116:ASP:C	4:A:118:HIS:N	2.70	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:596:THR:C	4:A:598:LEU:H	2.22	0.43
4:A:600:PRO:C	4:A:602:ASP:N	2.72	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: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
6:C:107:SER:C	6:C:109:SER:N	2.72	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:89:PRO:C	4:A:204:THR:HG21	2.39	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: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:814:PHE:C	5:B:816:GLU:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:22:LEU:HD13	6:C:230:MET:HE1	2.00	0.43
6:C:47:ASP:CA	15:L:69:ALA:CB	2.93	0.43
7:D:4:SER:C	7:D:5:THR:OG1	2.56	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
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:1:MET:H1	13:J:56:LEU:HB2	1.83	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
5:B:542:MET:HB3	5:B:636:PRO:CD	2.48	0.43
5:B:918:ILE:HD12	5:B:935:ARG:HD3	2.01	0.43
6:C:16:ASP:C	6:C:17:ASN:ND2	2.71	0.43
6:C:65:HIS:O	6:C:69:LEU:HD13	2.19	0.43
9:F:77:ASP:C	9:F:79:ARG:N	2.72	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: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
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: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:840:ILE:HG21	5:B:994:TYR:HD1	1.84	0.42
5:B:1081:LEU:O	5:B:1082:MET:C	2.57	0.42
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.37	0.42
8:E:60:PHE:C	8:E:60:PHE:CD2	2.91	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:557:ASP:O	4:A:559:VAL:HG23	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:1111:MET:HE2	4:A:1330:ASN:OD1	2.19	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
5:B:1202:LEU:HD22	5:B:1206:GLU:CD	2.40	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:452:LYS:HE3	5:B:1141:HIS:ND1	2.34	0.42
4:A:573:SER:O	4:A:574:GLY:C	2.57	0.42
4:A:1107:VAL:HG12	4:A:1107:VAL:O	2.19	0.42
5:B:37:PHE:CD1	5:B:37:PHE:C	2.92	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
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
10:G:79:PHE:HZ	10:G:106:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:899:VAL:CG2	4:A:1029:ARG:HG2	2.49	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
5:B:742:GLU:O	5:B:743:ILE:C	2.58	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
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: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:574:GLY:O	4:A:575:LYS:C	2.58	0.42
4:A:577:ILE:O	4:A:578:LEU:C	2.55	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:1444:MET:HB2	4:A:1444:MET:HE3	1.86	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:763:GLN:O	5:B:764:SER:C	2.58	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: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:99:PHE:CZ	10:G:143:ILE:HD13	2.54	0.42
12:I:4:PHE:C	12:I:4:PHE:HD1	2.22	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:207:ILE:O	4:A:211:PHE:HD1	2.02	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
5:B:661:LEU:C	5:B:663:ALA:N	2.73	0.42
6:C:235:VAL:HG21	13:J:6:ARG:NH2	2.35	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:136:ASN:OD1	8:E:138:ALA:N	2.53	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:341:MET:HE1	5:B:1135:ARG:NH1	2.34	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
4:A:1364:ASN:C	4:A:1364:ASN:ND2	2.73	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:563:MET:HE2	5:B:587:HIS:O	2.19	0.42
5:B:579:ARG:HD2	5:B:586:TRP:CZ2	2.55	0.42
5:B:889:THR:HG22	5:B:891:ASP:H	1.84	0.42
6:C:44:LEU:HD21	6:C:159:ALA:CB	2.50	0.42
6:C:80:LEU:HD11	6:C:95:CYS:C	2.40	0.42
6:C:104:PHE:HD2	6:C:105:GLY:H	1.67	0.42
9:F:72:LYS:O	9:F:73:ALA:HB3	2.20	0.42
12:I:13:MET:HE2	12:I:14:LEU:H	1.84	0.42
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
14:K:83:PRO:O	14:K:84:LYS:C	2.58	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:1007:ILE:C	4:A:1009:ASN:H	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1173:HIS:C	4:A:1174:PHE:CD1	2.93	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
11:H:33:GLN:C	11:H:35:GLN:H	2.22	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:418:SER:C	4:A:420:ARG:N	2.72	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: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
12:I:59:VAL:C	12:I:61:ASP:N	2.73	0.42
12:I:92:ARG:HB3	12:I:95:THR:OG1	2.19	0.42
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
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
4:A:1385:THR:C	4:A:1387:HIS:N	2.72	0.41
5:B:39:ARG:NH2	5:B:665:GLU:CG	2.83	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:1177:HIS:C	5:B:1179:GLN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:730:GLY:C	4:A:732:LEU:N	2.73	0.41
4:A:886:ILE:CD1	4:A:943:LEU:HB3	2.42	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:558:LEU:C	5:B:560:GLU:N	2.74	0.41
5:B:807:ARG:HG2	5:B:1045:SER:HG	1.83	0.41
5:B:1202:LEU:O	5:B:1203:LEU:C	2.57	0.41
6:C:236:GLY:C	6:C:238:ILE:N	2.71	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:208:LEU:HD23	4:A:208:LEU:C	2.40	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: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:1283:VAL:CG1	4:A:1284:MET:N	2.77	0.41
4:A:1409:LEU:HD23	4:A:1409:LEU:HA	1.92	0.41
5:B:298:LEU:N	5:B:298:LEU:CD2	2.83	0.41
5:B:542:MET:HE1	5:B:743:ILE:HG21	2.01	0.41
5:B:1097:HIS:H	5:B:1098:MET:CE	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:516:SER:O	4:A:517:ASN:C	2.58	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:1007:ILE:C	4:A:1009:ASN:N	2.73	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
5:B:1147:LEU:O	5:B:1148:LYS:C	2.57	0.41
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.41	0.41
6:C:145:CYS:HA	13:J:2:ILE:CD1	2.43	0.41
6:C:242:GLN:C	6:C:244:VAL:H	2.24	0.41
6:C:243:VAL:O	6:C:243:VAL:HG12	2.20	0.41
9:F:88:TYR:CD1	9:F:88:TYR:N	2.88	0.41
10:G:26:LEU:O	10:G:27:LYS:C	2.59	0.41
15:L:65:VAL:O	15:L:65:VAL:HG23	2.21	0.41
4:A:53:LEU:O	4:A:54:ASN:C	2.59	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:1362:TYR:HD1	4:A:1363:VAL:N	2.18	0.41
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: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
5:B:1084:GLN:CD	5:B:1084:GLN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:24:LYS:HB2	8:E:24:LYS:HE3	1.77	0.41
10:G:15:PRO:O	10:G:16:SER:C	2.59	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
11:H:100:THR:HG1	11:H:138:GLU:HG3	1.84	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: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:34:ILE:O	5:B:35:SER:C	2.59	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:242:GLN:C	6:C:244:VAL:N	2.72	0.41
6:C:254:LYS:HE2	6:C:254:LYS:HB3	1.89	0.41
10:G:14:HIS:HD2	10:G:16:SER:CB	2.33	0.41
14:K:5:ASP:O	14:K:6:ARG:C	2.58	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:298:PHE:O	4:A:299:HIS:C	2.59	0.41
4:A:302:THR:HG22	4:A:303:TYR:N	2.35	0.41
4:A:404:TYR:CD2	4:A:414:ASP:HA	2.56	0.41
4:A:845:LEU:O	4:A:846:GLU:C	2.59	0.41
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.95	0.41
4:A:1315:GLU:C	4:A:1317:MET:N	2.73	0.41
4:A:1365:TYR:O	4:A:1367:HIS:N	2.54	0.41
4:A:1385:THR:C	4:A:1387:HIS:H	2.23	0.41
5:B:313:MET:O	5:B:316:PRO:HG2	2.20	0.41
5:B:383:ASN:O	5:B:384:ARG:C	2.58	0.41
5:B:466:TRP:CE3	5:B:466:TRP:HA	2.54	0.41
6:C:167:HIS:HD2	6:C:168:ALA:H	1.69	0.41
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:163:GLU:O	8:E:164:LEU:C	2.58	0.41
15:L:43:THR:C	15:L:45:ALA:H	2.22	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:360:GLU:O	4:A:361:LEU:C	2.57	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: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
4:A:1423:GLY:O	4:A:1424:VAL:C	2.59	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:138:ASN:C	7:D:140:ASP:N	2.74	0.41
7:D:173:HIS:NE2	7:D:201:LYS:NZ	2.69	0.41
10:G:1:MET:HG2	10:G:85:GLU:CD	2.41	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:252:PHE:HB2	4:A:256:GLN:CD	2.40	0.41
4:A:322:VAL:O	4:A:322:VAL:HG12	2.21	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: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: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
5:B:26:THR:O	5:B:29:ASP:HB2	2.21	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:830:TYR:O	5:B:831:SER:C	2.59	0.41
5:B:979:LYS:HG2	5:B:1095:LEU:CD1	2.50	0.41
5:B:1002:THR:O	5:B:1003:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:GLU:C	8:E:104:ASN:N	2.71	0.41
8:E:124:VAL:N	8:E:125:PRO:HD2	2.35	0.41
8:E:157:SER:C	8:E:159:ASP:H	2.23	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
14:K:68:PHE:HB3	14:K:70:ARG:HH11	1.84	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:860:LEU:HB3	4:A:862:ASN:OD1	2.21	0.41
4:A:971:PHE:O	4:A:972:HIS:C	2.59	0.41
4:A:1119:TYR:O	4:A:1120:LEU:O	2.39	0.41
4:A:1347:ALA:O	4:A:1348:LEU:C	2.59	0.41
4:A:1443:VAL:C	4:A:1444:MET:HG3	2.40	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:878:GLN:O	5:B:879:ARG:C	2.58	0.41
5:B:895:ASP:C	5:B:897:GLY:H	2.24	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
10:G:22:MET:C	10:G:24:GLN:N	2.74	0.41
10:G:99:PHE:CD1	10:G:99:PHE:C	2.95	0.41
12:I:54:GLU:OE2	12:I:118:ARG:CZ	2.69	0.41
1:T:11:DT:H1'	1:T:12:DA:H5'	2.02	0.40
4:A:335:ARG:O	4:A:336:ILE:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:877:PRO:C	5:B:878:GLN:HG3	2.42	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: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
14:K:46:ILE:O	14:K:46:ILE:HG22	2.21	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:486:GLU:O	4:A:487:MET:HG2	2.21	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
5:B:129:PHE:CE2	5:B:166:PHE:HD1	2.39	0.40
5:B:552:MET:C	5:B:554:ILE:N	2.74	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
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:79:PHE:CE2	10:G:105:PRO:CG	3.03	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
4:A:219:PHE:CD2	4:A:231:PRO:HD2	2.56	0.40
4:A:325:ILE:HG22	5:B:1210:MET:HE1	2.02	0.40
4:A:711:ARG:O	4:A:714:PHE:N	2.51	0.40
4:A:935:GLN:O	4:A:936:LEU:C	2.59	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:1317:MET:HE1	4:A:1338:VAL:HG11	2.02	0.40
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.52	0.40
5:B:33:VAL:O	5:B:36:ALA:HB3	2.22	0.40
5:B:610:ASN:C	5:B:612:GLU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:C:204:SER:C	6:C:206:ASN:N	2.73	0.40
7:D:29:LEU:N	7:D:29:LEU:HD23	2.35	0.40
9:F:77:ASP:O	9:F:79:ARG:N	2.54	0.40
11:H:9:ILE:HA	11:H:55:LEU:O	2.21	0.40
13:J:1:MET:H2	13:J:57:ILE:H	1.65	0.40
4:A:289:ILE:C	4:A:291:GLU:N	2.74	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:853:ASP:OD1	4:A:853:ASP:C	2.60	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:294:ASP:C	5:B:296:GLU:H	2.22	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:839:MET:CE	5:B:1010:LEU:HD21	2.42	0.40
5:B:895:ASP:C	5:B:897:GLY:N	2.74	0.40
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.74	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
4:A:95:PHE:O	4:A:96:ILE:C	2.59	0.40
4:A:103:CYS:C	4:A:105:CYS:N	2.75	0.40
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: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:1121:GLU:O	4:A:1122:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:1377:THR:O	4:A:1378:GLN:C	2.59	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
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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	6
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	5
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1	11
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	15
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0	3
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	2
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	1	17
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	1124 (91%)	115 (9%)	7	27
5	B	962/1061 (91%)	887 (92%)	75 (8%)	10	34
6	C	234/274 (85%)	211 (90%)	23 (10%)	6	25
7	D	159/200 (80%)	129 (81%)	30 (19%)	1	8
8	E	196/197 (100%)	190 (97%)	6 (3%)	35	56
9	F	74/137 (54%)	65 (88%)	9 (12%)	4	19
10	G	152/152 (100%)	139 (91%)	13 (9%)	8	31
11	H	117/128 (91%)	112 (96%)	5 (4%)	25	49
12	I	113/116 (97%)	104 (92%)	9 (8%)	10	33
13	J	60/65 (92%)	56 (93%)	4 (7%)	13	38
14	K	99/102 (97%)	89 (90%)	10 (10%)	6	24
15	L	40/57 (70%)	36 (90%)	4 (10%)	6	24
All	All	3445/4009 (86%)	3142 (91%)	303 (9%)	8	30

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	34	LYS
4	A	37	PHE
4	A	38	PRO
4	A	62	ASP
4	A	68	GLN
4	A	83	HIS
4	A	93	VAL
4	A	100	LYS
4	A	108	MET
4	A	122	MET
4	A	200	ARG
4	A	215	SER
4	A	221	SER

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Mol	Chain	Res	Type
4	A	270	LEU
4	A	302	THR
4	A	312	PRO
4	A	320	ARG
4	A	321	PRO
4	A	326	ARG
4	A	335	ARG
4	A	345	VAL
4	A	354	SER
4	A	381	THR
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	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	462	VAL
4	A	469	ARG
4	A	470	LEU
4	A	487	MET
4	A	493	GLN
4	A	503	GLN
4	A	512	VAL
4	A	515	GLN
4	A	518	LYS
4	A	560	ILE
4	A	562	THR
4	A	584	ASN
4	A	590	ARG
4	A	618	GLU
4	A	626	ASN
4	A	635	ARG
4	A	659	HIS
4	A	666	ILE
4	A	670	ILE

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Mol	Chain	Res	Type
4	A	692	ASP
4	A	711	ARG
4	A	727	ASP
4	A	739	ASP
4	A	768	GLN
4	A	774	ARG
4	A	779	PHE
4	A	821	ARG
4	A	834	THR
4	A	858	ASN
4	A	871	ASP
4	A	873	MET
4	A	903	ASN
4	A	907	THR
4	A	929	LEU
4	A	939	ASP
4	A	940	ARG
4	A	942	PHE
4	A	969	GLN
4	A	992	ASP
4	A	1001	ARG
4	A	1017	LEU
4	A	1029	ARG
4	A	1035	TYR
4	A	1037	LEU
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
4	A	1146	VAL
4	A	1152	ILE
4	A	1155	ASP
4	A	1173	HIS
4	A	1187	GLN
4	A	1206	ASP
4	A	1240	CYS
4	A	1264	GLU
4	A	1271	ILE

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Mol	Chain	Res	Type
4	A	1291	VAL
4	A	1295	THR
4	A	1298	TYR
4	A	1329	THR
4	A	1332	PHE
4	A	1333	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1372	VAL
4	A	1386	ARG
4	A	1389	PHE
4	A	1405	THR
4	A	1415	SER
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
5	B	30	SER
5	B	37	PHE
5	B	46	GLN
5	B	57	TYR
5	B	61	ASP
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	261	ARG
5	B	268	THR
5	B	298	LEU
5	B	365	THR
5	B	371	GLU
5	B	393	LYS
5	B	399	ASP
5	B	401	PHE
5	B	427	ASP
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP

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Mol	Chain	Res	Type
5	B	485	ARG
5	B	498	THR
5	B	502	ILE
5	B	516	ASN
5	B	557	PHE
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	628	THR
5	B	644	GLU
5	B	682	SER
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	748	ILE
5	B	755	ILE
5	B	787	VAL
5	B	811	TYR
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	953	LEU
5	B	957	ASN
5	B	978	ASP
5	B	999	MET
5	B	1002	THR
5	B	1006	ILE
5	B	1022	THR
5	B	1047	PHE
5	B	1084	GLN
5	B	1087	PHE
5	B	1095	LEU
5	B	1099	VAL
5	B	1108	ARG
5	B	1112	GLN
5	B	1122	ARG

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Mol	Chain	Res	Type
5	B	1129	ARG
5	B	1138	MET
5	B	1159	ARG
5	B	1170	THR
5	B	1176	ASN
5	B	1183	LYS
5	B	1202	LEU
5	B	1216	LEU
6	C	22	LEU
6	C	35	ARG
6	C	56	THR
6	C	58	LEU
6	C	60	ASP
6	C	62	PHE
6	C	74	SER
6	C	77	ILE
6	C	89	GLU
6	C	91	HIS
6	C	104	PHE
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	193	TYR
6	C	209	TYR
6	C	214	ASN
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	12	ARG
7	D	13	ARG
7	D	15	LEU
7	D	16	LYS
7	D	17	LYS
7	D	19	GLU
7	D	22	GLU
7	D	47	LEU

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Mol	Chain	Res	Type
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	221	TYR
8	E	60	PHE
8	E	74	ASP
8	E	104	ASN
8	E	114	ASN
8	E	132	ILE
8	E	153	HIS
9	F	79	ARG
9	F	81	THR
9	F	90	ARG
9	F	99	LEU
9	F	111	LEU
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	52	ASP
10	G	74	TYR
10	G	78	VAL
10	G	79	PHE

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Mol	Chain	Res	Type
10	G	80	LYS
10	G	87	VAL
10	G	88	ASP
10	G	126	ASN
10	G	171	ILE
11	H	86	ASP
11	H	95	TYR
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	34	TYR
12	I	75	CYS
12	I	85	PHE
12	I	86	PHE
12	I	100	PHE
12	I	101	PHE
13	J	16	ASP
13	J	44	TYR
13	J	46	CYS
13	J	48	ARG
14	K	1	MET
14	K	5	ASP
14	K	10	PHE
14	K	25	THR
14	K	41	THR
14	K	47	ARG
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
15	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	54	ASN

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Mol	Chain	Res	Type
4	A	92	HIS
4	A	225	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	517	ASN
4	A	631	HIS
4	A	654	ASN
4	A	736	ASN
4	A	741	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	965	GLN
4	A	994	GLN
4	A	1106	ASN
4	A	1130	GLN
4	A	1140	HIS
4	A	1173	HIS
4	A	1364	ASN
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	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	538	ASN
5	B	734	HIS

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Mol	Chain	Res	Type
5	B	744	HIS
5	B	763	GLN
5	B	821	GLN
5	B	842	ASN
5	B	957	ASN
5	B	1015	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1117	GLN
5	B	1161	HIS
5	B	1179	GLN
5	B	1193	GLN
5	B	1211	ASN
6	C	17	ASN
6	C	24	ASN
6	C	73	GLN
6	C	79	GLN
6	C	112	ASN
6	C	123	ASN
6	C	167	HIS
6	C	252	GLN
7	D	9	GLN
7	D	39	ASN
7	D	40	HIS
7	D	74	GLN
7	D	137	ASN
7	D	143	ASN
7	D	179	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	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	97	HIS
10	G	122	ASN
10	G	126	ASN
11	H	131	ASN

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

5.3.3 RNA ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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%)	0.72	1 (5%) 29 27	110, 139, 169, 175	0
2	N	7/7 (100%)	0.99	1 (14%) 7 11	148, 156, 169, 171	0
3	P	10/10 (100%)	0.56	1 (10%) 14 16	118, 128, 165, 172	0
4	A	1416/1733 (81%)	-0.16	23 (1%) 70 54	44, 103, 161, 199	0
5	B	1108/1224 (90%)	0.05	37 (3%) 49 40	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.21	1 (0%) 89 78	64, 100, 144, 162	0
7	D	177/221 (80%)	0.17	10 (5%) 31 28	70, 120, 177, 190	0
8	E	214/215 (99%)	0.09	2 (0%) 81 67	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.45	1 (1%) 76 60	53, 81, 115, 132	0
10	G	171/171 (100%)	-0.09	1 (0%) 85 73	82, 103, 141, 150	0
11	H	133/146 (91%)	0.48	7 (5%) 33 29	119, 149, 180, 188	0
12	I	119/122 (97%)	0.34	3 (2%) 58 46	94, 150, 183, 199	0
13	J	65/70 (92%)	-0.15	1 (1%) 71 56	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.38	1 (0%) 81 67	64, 101, 130, 149	0
15	L	46/70 (65%)	0.44	4 (8%) 17 18	96, 154, 172, 178	0
All	All	3947/4599 (85%)	-0.04	94 (2%) 59 47	44, 111, 175, 199	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	7.8
4	A	1081	LEU	4.6
11	H	63	LEU	4.4
7	D	25	ALA	4.3
5	B	883	LEU	4.2
5	B	882	THR	4.2
5	B	732	SER	4.1

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Mol	Chain	Res	Type	RSRZ
9	F	72	LYS	4.0
4	A	1175	SER	4.0
4	A	3	GLY	4.0
5	B	879	ARG	3.9
5	B	335	GLY	3.9
7	D	24	ALA	3.8
5	B	250	PHE	3.8
5	B	963	PHE	3.8
4	A	56	PRO	3.7
7	D	13	ARG	3.7
5	B	731	VAL	3.6
4	A	251	SER	3.6
5	B	730	ARG	3.6
14	K	114	LEU	3.6
3	P	1	U	3.5
15	L	25	ALA	3.4
7	D	8	PHE	3.3
5	B	508	LEU	3.2
5	B	70	ILE	3.2
13	J	65	PRO	3.2
4	A	69	THR	3.1
5	B	134	LYS	3.0
5	B	934	LYS	3.0
4	A	1173	HIS	3.0
15	L	26	THR	3.0
5	B	734	HIS	2.9
11	H	119	GLY	2.9
5	B	471	LYS	2.9
4	A	252	PHE	2.9
5	B	446	LEU	2.9
11	H	76	THR	2.8
11	H	139	ASN	2.8
7	D	4	SER	2.8
5	B	507	LYS	2.8
4	A	2	VAL	2.7
11	H	140	ALA	2.7
5	B	349	ILE	2.6
4	A	904	THR	2.6
6	C	3	GLU	2.5
10	G	21	ARG	2.5
4	A	51	GLY	2.5
5	B	933	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	1	DC	2.5
4	A	1257	ASP	2.5
5	B	715	ALA	2.4
12	I	57	GLY	2.4
12	I	64	SER	2.4
4	A	40	THR	2.4
4	A	1254	ALA	2.4
5	B	724	ASP	2.4
5	B	862	GLN	2.4
12	I	120	GLN	2.4
11	H	135	LEU	2.4
5	B	723	VAL	2.4
7	D	118	THR	2.3
4	A	1172	LEU	2.3
5	B	710	LEU	2.3
11	H	136	LYS	2.3
4	A	830	LYS	2.3
5	B	610	ASN	2.3
4	A	292	ALA	2.3
4	A	1187	GLN	2.3
7	D	17	LYS	2.2
5	B	709	ASP	2.2
5	B	266	ALA	2.2
4	A	1080	THR	2.2
5	B	620	ARG	2.2
7	D	18	VAL	2.2
4	A	65	LEU	2.2
5	B	641	GLU	2.1
5	B	832	GLY	2.1
5	B	887	HIS	2.1
15	L	27	LEU	2.1
8	E	86	PRO	2.1
5	B	864	LYS	2.1
5	B	1222	ARG	2.1
5	B	251	ILE	2.1
1	T	11	DT	2.1
5	B	470	LYS	2.1
8	E	107	THR	2.1
5	B	1224	PHE	2.1
15	L	53	HIS	2.0
4	A	74	MET	2.0
4	A	1243	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
7	D	14	ARG	2.0
5	B	502	ILE	2.0
7	D	35	LEU	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 monosaccharides 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
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.