



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 01:01 PM EDT

PDB ID : 4XLQ  
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter  
Authors : Bae, B.; Darst, S.A.  
Deposited on : unknown  
Resolution : 4.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

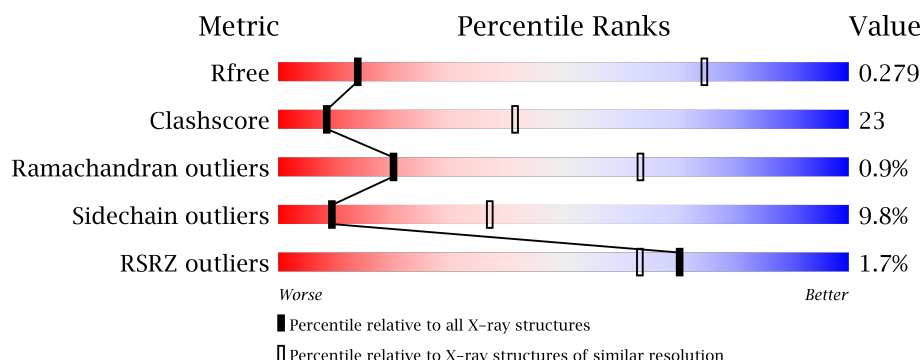
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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))
$R_{free}$	100719	1005 (5.52-3.66)
Clashscore	112137	1052 (5.50-3.70)
Ramachandran outliers	110173	1041 (5.52-3.66)
Sidechain outliers	110143	1021 (5.50-3.66)
RSRZ outliers	101464	1014 (5.52-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>0.2%</div> <div>40%</div> <div>28%</div> <div>0.2%</div> <div>28%</div> </div>
1	B	314	<div> <div>33%</div> <div>34%</div> <div>5%</div> <div>28%</div> </div>
1	G	314	<div> <div>5%</div> <div>36%</div> <div>31%</div> <div>5%</div> <div>28%</div> </div>
1	H	314	<div> <div>0.2%</div> <div>35%</div> <div>32%</div> <div>5%</div> <div>28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>45%</div> <div>48%</div> <div>6%</div> <div>0.2%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	30	
6	R	30	
7	P	26	
7	S	26	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			510	245	91	149	25			
7	S	26	Total	C	N	O	P	0	0	0
			527	255	93	154	25			

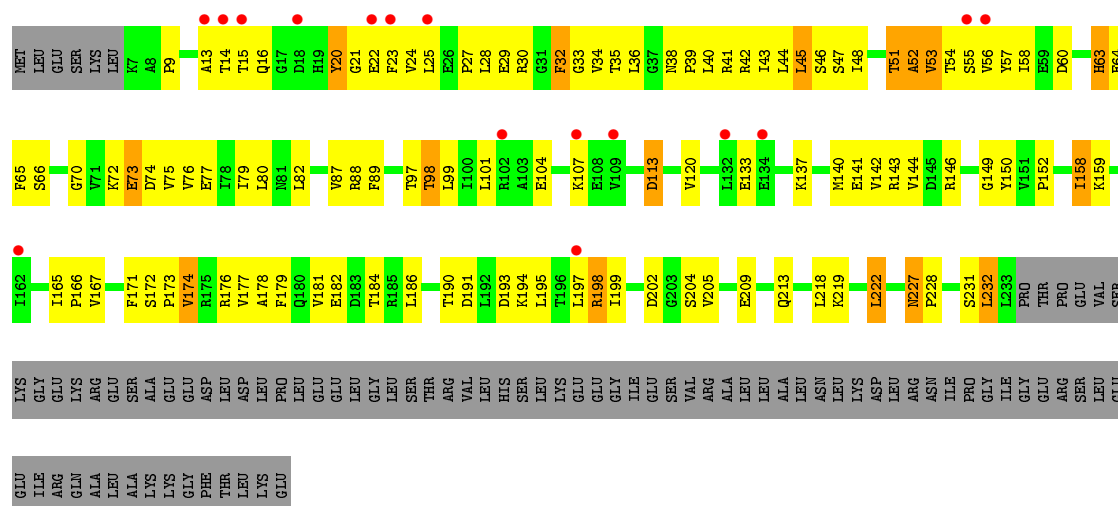
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

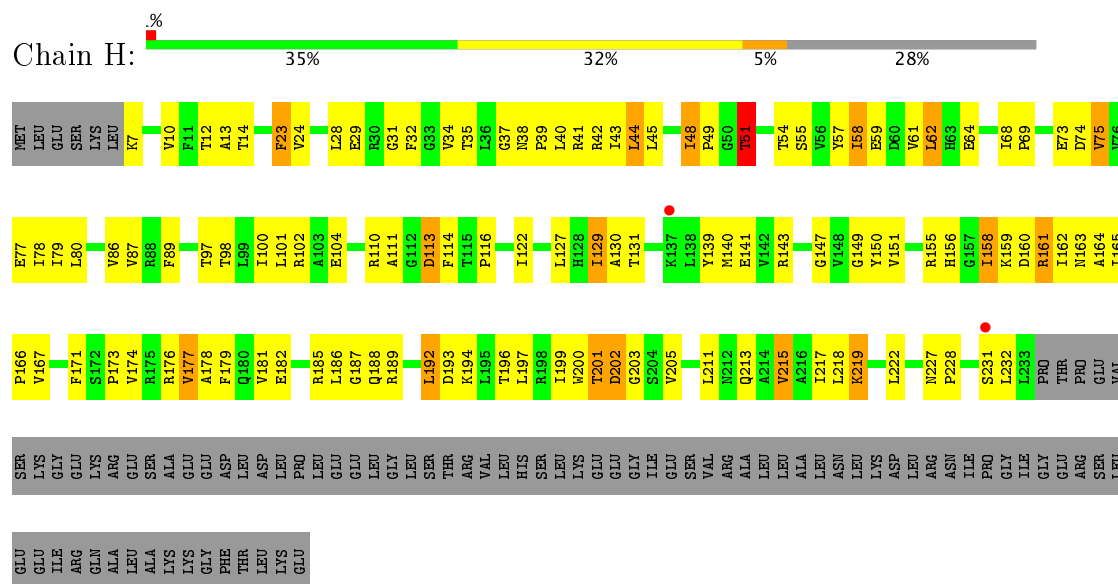
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

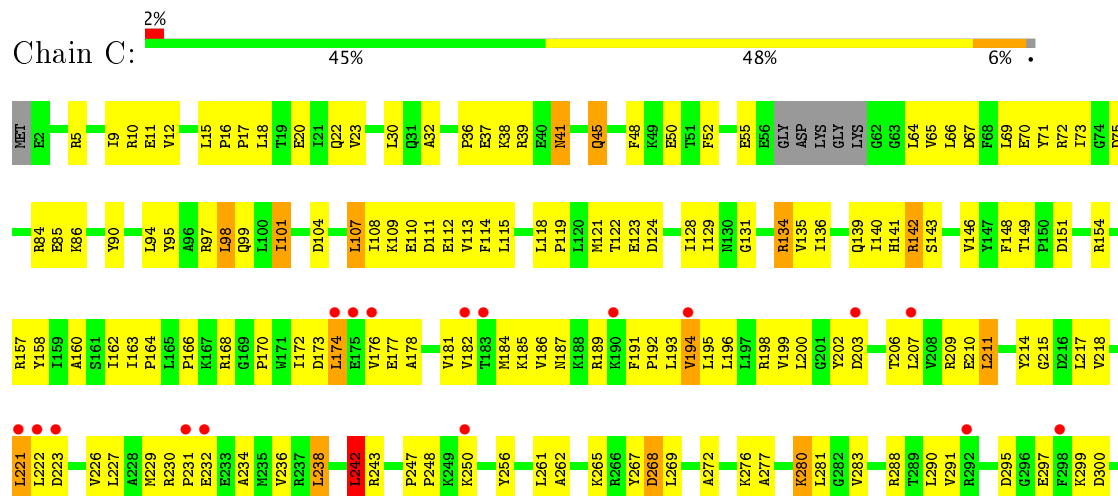




• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



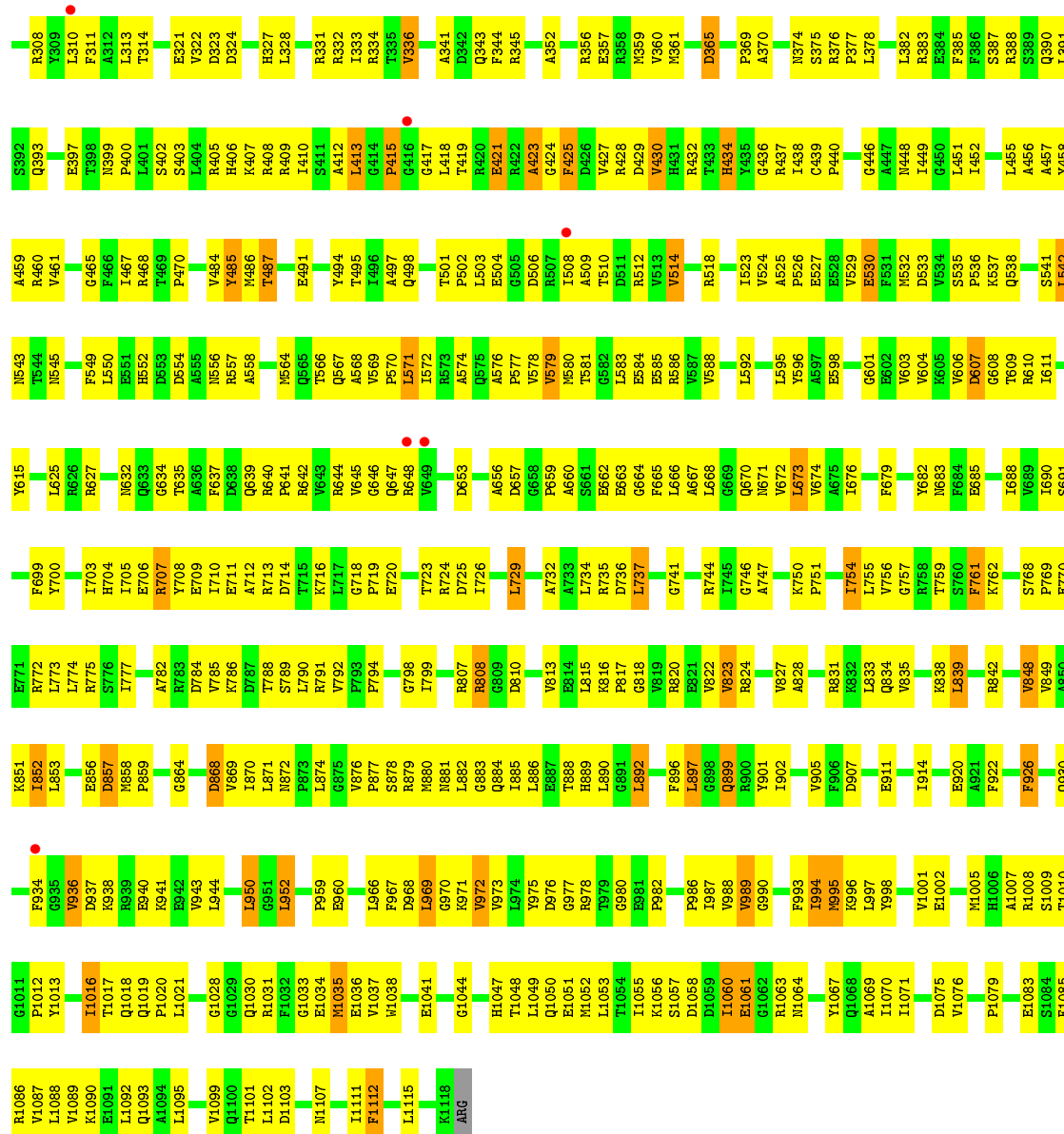
F303	S389	A456	F538	A597	L673	G746	V823	G891	P986	K1056
L304	Q390	A457	V529	E598	V674	A747	R824	L892	P987	S1057
P305	L391	A458	E530	E598	A675			F896	V988	I1060
T306	S392	A459	F531	G601	L676	K750	V827	L897	V989	E1061
L307	Q393	A460	M532	E602		P751	A828	F898	G990	G1062
R308	L309	V461	M533	E603	F679		Q829	G899	F993	R1063
V309	E397		M534	V604		L754	V830	R900	P994	M1064
L310	T398	L464	S535	R605	V682	L755	R831	A901	I994	Y1067
F311	N399	G465	P536	V606	R683	L756	R832	Y901	M995	Q1068
A312	P400	F466	K537	D807	F684	R757	L833	I902	K996	Y1069
L313	L401	L467	Q538	G608	E685	R758	Q834	P905	L997	A1070
T314	S402	R468	T509	T509		T759	V835	F906	Y998	I1071
V317	S403	T469	S541	R610	L688	T760		P907	V1001	D1075
F318	L404	P470	L542	I611	V689	F761	R838	D907	E1002	V1076
	R405		M543	A612	L690	K762	L839	E911	M1005	P1079
E321	R406	V474	T544	V613	S691	E770	R842	I914	H1006	E1083
V322	K407	V478	N545	R614	X696	E771	R846	E920	A1007	S1084
D323	R408		L546	V615		R772	G847	A921	R1008	F1085
D324	R409	V484	I547	L625	F699	L773	V848	F922	S1009	Q1086
	S411	Y485	F548	R626	Y700	L774	V849	F926	G1011	V1087
H327	A412	Y486	L550	R627		R775	V851	F934	I1012	L1088
L328	L413	T487	E551		I703	S776	R852	G935	P1013	E1089
	G414	E491	H552	Q632	H704	I777	L853	F936	I1016	E1091
R331	P415		R557	Q633	I705	A782	L854	G937	T1017	L1092
R332	G416	Y494	A558	G634	E706	R783	V855	V936	Q1018	Q1093
L333	G417	T495	G561	T535		R784	R857	G938	G1019	A1094
R334	L418	T496	G561	G635		R785	R858	G939	E1020	
T335	T419	A497	G561	D638	I710	K786	R859	E940	L1021	
V336	R420	R497	M564	Q639	E711	D787	P859	E941	G1028	V1099
	E421	Q498	Q564	R640	A712	T788		L950	Q1029	Q1100
L339	R422	A499	Q565	R640	R713	S789	G864	G951	Q1030	T1101
	A423	R500	T566	R641	R714	L790	T865	L952	R1031	L1102
D342	G424	T501	Q567	R642	D714	R791	P866	G952	F1032	D1103
Q343	F425	P502	A568	V643	T715	V792	R867	G953	G1033	N1107
	D426	L503	V569	R644	K716	P793	V867	L954	E1034	I1111
K359	V427	E504	P570	V645	L717	P794	D868	P959	M1035	I1112
V360	R428	G505	L571	G646	G718	P794	D869	E960	E1036	L1115
K361	D429	D506	I572	Q647	F719	G795	V869	L966	V1037	L1116
	V430	R507	R573	R648	E720	E796	R870	F967	M1038	K1118
D365	H431	A508	A574	D653	R721	G797	R871	P968	E1041	ARG
	R432	T508	Q575		I722	G798	R872	D969	A1042	
P369	T433	T510	A576	D653	T723	I799	L873	L966	Y1043	
A370	R434	D513	P577	D656	R724	L806	L874	F967	G1044	
	Y435	R512	V578	D657	I726	L807	G875	D968	H1047	
N374	G436	R513	V579	G658		R807	V876	L969	T1048	
S375	R437	V514	M580	P659		R808	R877	L970	L1049	
R376	I438	A515	T581	A660	L729	G809	S878	G970	Q1050	
P377	C439	R516	G582	S661		D810	R879	K971	R1051	
L378	P440	R517	L583	E662	A732		R880	V972	E1052	
E379		R518	E584	E663		V813	R881	V973	M1053	
A380	G446	G519	E585	E664	A733	E814	L882	L974	L1054	
A381	A447	E520	R586	F665	L734	L815	Q883	Y975	T1055	
L382	N448	P521	V587	L666	R735	K816	Q884	L976		
R383	I449	P522	V588	A667	D736	P817	R885	D976		
F384	G450	V522	V588	L668	L737	R818	L886	G977		
F385	L451	T523	L592	G669		V819	E887	T979		
F386	L452	A525	L595	Q670	G741	R820	R888	G980		
S387	P526	P526	L595	R671	R744	E821	R889	E981		
R388	L455	E527	Y596	V672	L745	V822	L890	P982		

• Molecule 2: DNA-directed RNA polymerase subunit beta

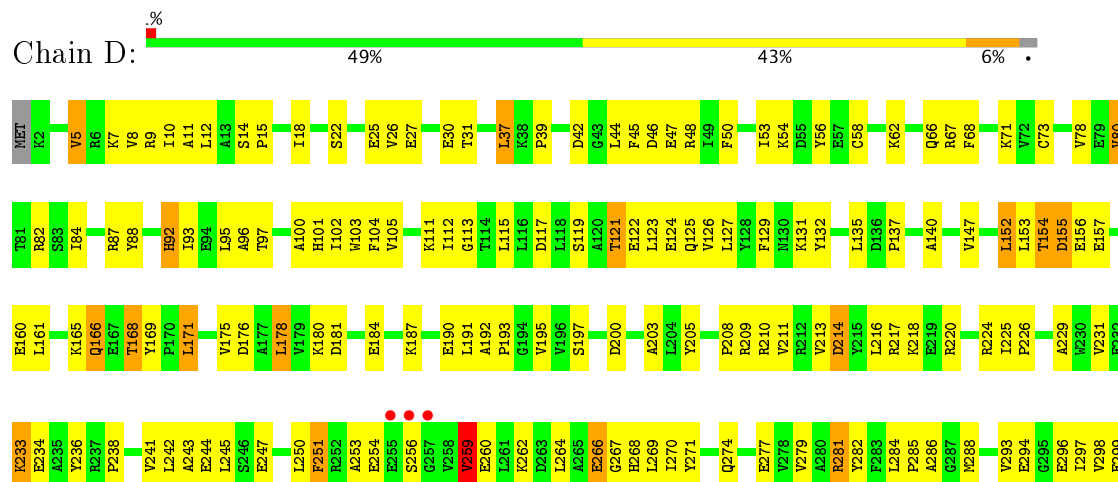


MET	K96	A160	K96							
E2	T89	S161	T89							
R5	Y90	I162	Y90							
F6	Q91	I163	Q91							
	A92		A92							
I9	P93	K167	P93							
R10	L94	R168	L94							
E11	Y95	G169	Y95							
V12	A96	P170	A96							
	R97	W171	R97							
L15	L98	L172	L98							
P16	Q99	D173	Q99							
P17	L100	E174	L100							
L18	I101	L242	I101							
T19	E102	L243	E102							
E20	I21	E177	I21							
I21	D104	A178	D104							
Q22	L107		Q22							
V23	I108		V23							
	E109									
L30	E110		L30							
Q31	D111		Q31							
A32	E112		A32							
	V113									
P36	F114		P36							
E37	L115		E37							
K38	G116		K38							
R39	H117		R39							
E40	L118		E40							
M41	P119		M41							
	L120									
Q45	M121		Q45							
	T122									
F48	E123		F48							
K49	D124		K49							
E50			E50							
T51	I128		T51							
F52	I129		F52							
E55	R134		E55							
E56	V135		E56							
GLY	I136		GLY							
ASP			ASP							
LYS	Q139		LYS							
	I140									
GLY	R141		GLY							
G62	H142		G62							
G63										
L64	R146		L64							
V65	Y147		V65							
L66	F148		L66							
	T149									
L69	P150		L69							
E70	D151		E70							
Y71			Y71							
R72	Q219		R72							
I73	G220		I73							
G74	L221		G74							
	L222									

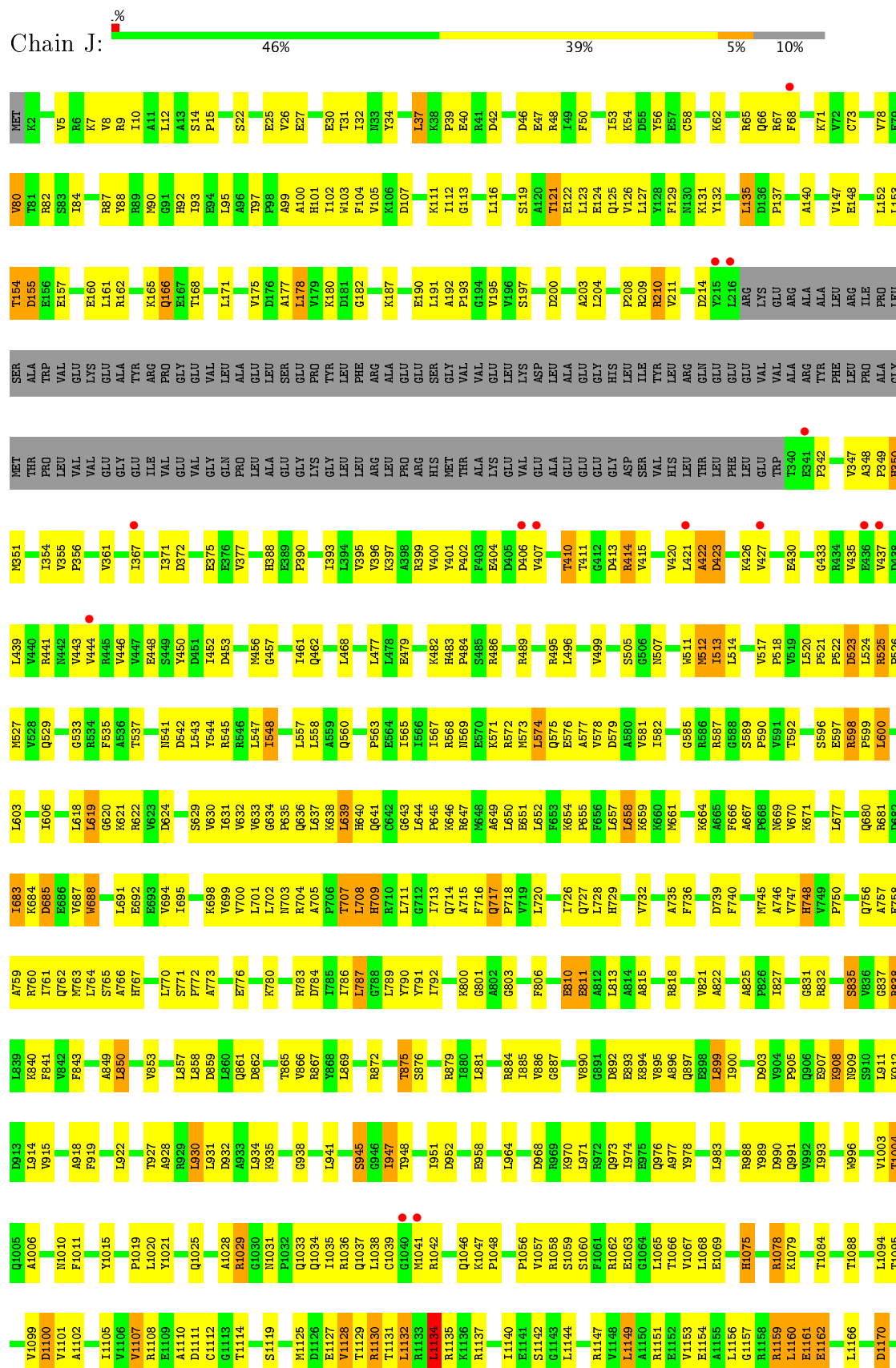


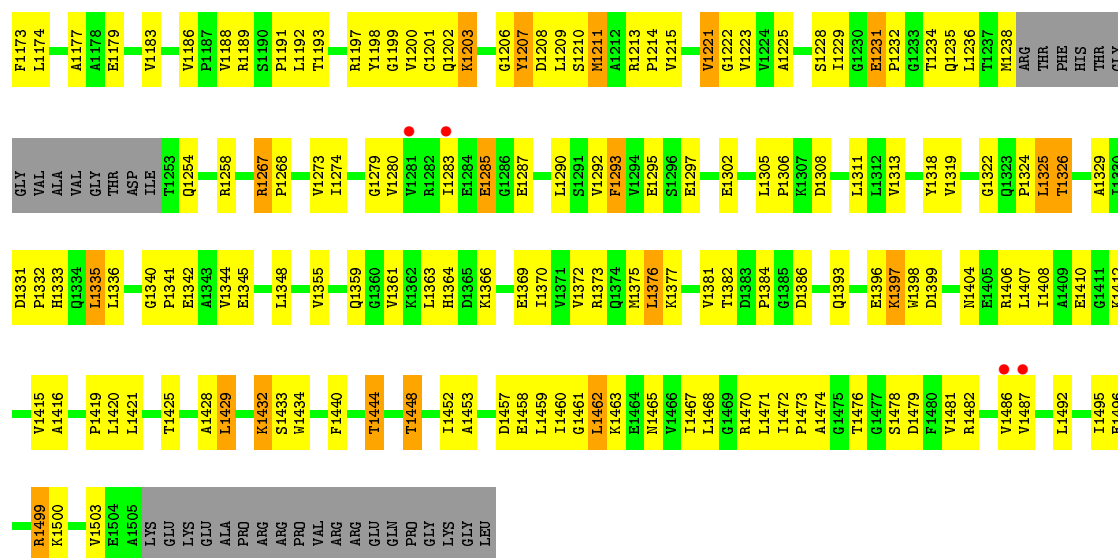


• Molecule 3: DNA-directed RNA polymerase subunit beta'

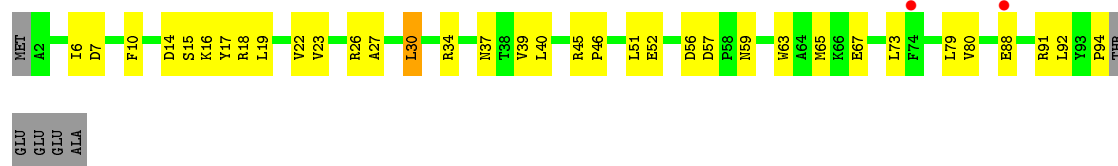




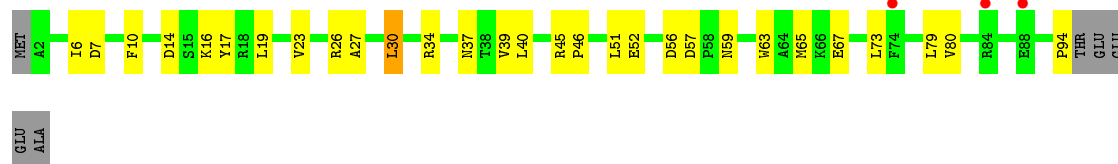




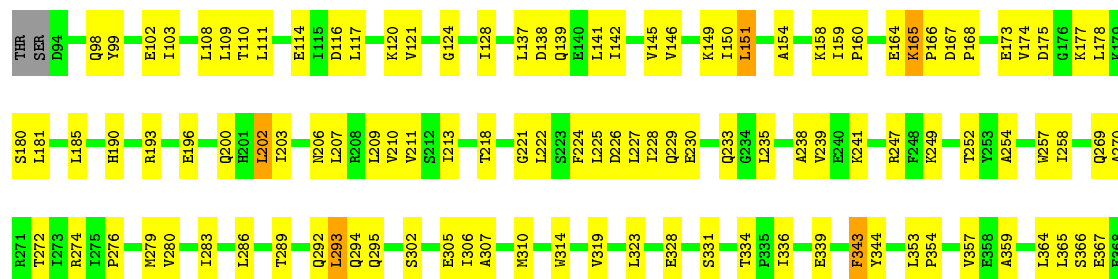
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega

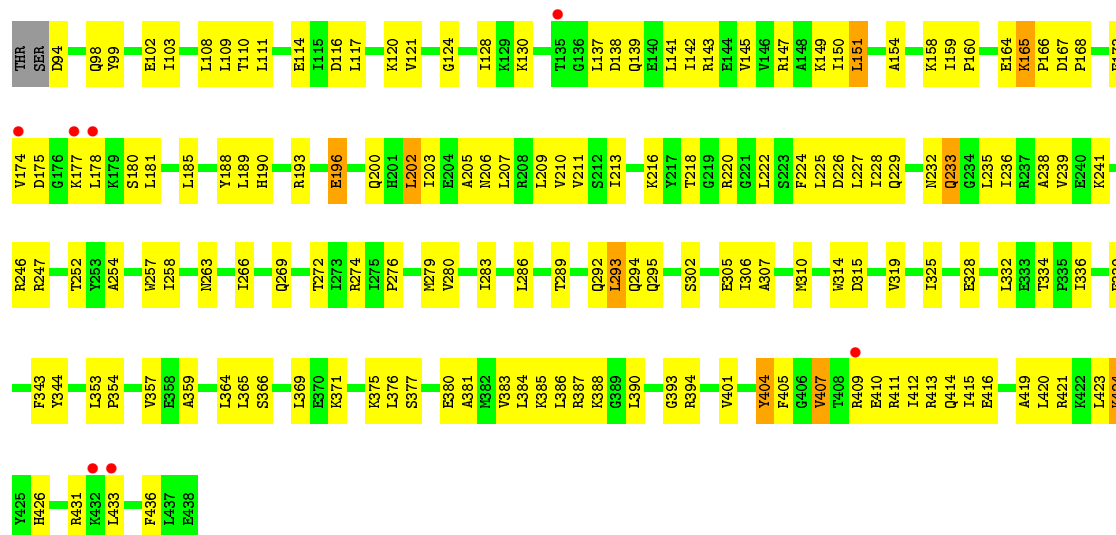


• Molecule 5: RNA polymerase sigma factor SigA





• Molecule 5: RNA polymerase sigma factor SigA



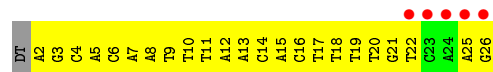
• Molecule 6: DNA (30-MER)



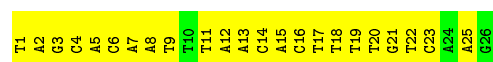
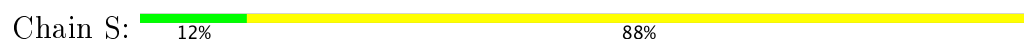
• Molecule 6: DNA (30-MER)



• Molecule 7: DNA (26-MER)



• Molecule 7: DNA (26-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.23Å 288.23Å 535.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 4.60 49.81 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.81-4.60) 98.6 (49.81-4.60)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.245 , 0.281 0.240 , 0.279	Depositor DCC
$R_{free}$ test set	6217 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	154.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 174.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	56477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/1804	0.64	1/2455 (0.0%)
1	B	0.30	0/1804	0.61	0/2455
1	G	0.31	0/1804	0.64	1/2455 (0.0%)
1	H	0.30	0/1804	0.61	0/2455
2	C	0.27	0/8905	0.55	2/12040 (0.0%)
2	I	0.27	0/8905	0.55	2/12040 (0.0%)
3	D	0.28	0/11963	0.55	3/16165 (0.0%)
3	J	0.28	0/10959	0.57	1/14802 (0.0%)
4	E	0.25	0/783	0.54	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.55	1/3804 (0.0%)
5	L	0.27	0/2829	0.55	1/3804 (0.0%)
6	O	0.50	0/687	0.92	0/1059
6	R	0.50	0/687	0.91	0/1059
7	P	0.54	0/571	0.93	0/878
7	S	0.54	0/590	0.93	0/908
All	All	0.29	0/57707	0.59	12/78487 (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
2	C	0	3
2	I	0	3
3	D	0	1
3	J	0	1
All	All	0	8

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	311	LEU	CA-CB-CG	7.45	132.43	115.30
3	D	1134	LEU	CA-CB-CG	6.98	131.36	115.30
2	I	417	GLY	N-CA-C	6.42	129.14	113.10
2	C	417	GLY	N-CA-C	6.40	129.09	113.10
3	J	1134	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	52	ALA	C-N-CA	5.63	135.77	121.70
1	G	52	ALA	C-N-CA	5.47	135.38	121.70
5	F	151	LEU	CA-CB-CG	5.32	127.53	115.30
3	D	964	LEU	CA-CB-CG	5.31	127.50	115.30
2	I	242	LEU	CA-CB-CG	5.19	127.23	115.30
2	C	242	LEU	CA-CB-CG	5.16	127.17	115.30
5	L	151	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	415	PRO	Peptide
2	C	423	ALA	Peptide
2	C	737	LEU	Peptide
3	D	1208	ASP	Peptide
2	I	415	PRO	Peptide
2	I	423	ALA	Peptide
2	I	737	LEU	Peptide
3	J	1359	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1799	89	0
1	B	1770	0	1799	101	0
1	G	1770	0	1799	103	0
1	H	1770	0	1799	95	0
2	C	8739	0	8841	499	0
2	I	8739	0	8841	485	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11761	0	11976	585	0
3	J	10779	0	10993	503	0
4	E	768	0	784	37	0
4	K	768	0	784	29	0
5	F	2787	0	2866	120	0
5	L	2787	0	2866	133	0
6	O	613	0	343	28	0
6	R	613	0	343	26	0
7	P	510	0	284	27	0
7	S	527	0	297	25	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56477	0	56414	2598	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 23.

All (2598) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:707:ARG:HE	2:C:824:ARG:HE	1.17	0.90
6:R:24:DC:H42	7:S:3:DG:H1	1.18	0.90
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.88
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.39	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.39	0.87
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.19	0.87
1:A:158:ILE:HB	1:A:166:PRO:HG3	1.57	0.86
2:I:707:ARG:HE	2:I:824:ARG:HE	1.17	0.86
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.21	0.86
2:I:557:ARG:HG3	2:I:879:ARG:HB3	1.57	0.86
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.59	0.85
2:C:557:ARG:HG3	2:C:879:ARG:HB3	1.59	0.85
3:D:231:VAL:H	3:D:243:ALA:HA	1.43	0.84
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.44	0.83
1:G:158:ILE:HB	1:G:166:PRO:HG3	1.58	0.83
2:C:313:LEU:HD13	2:C:321:GLU:HA	1.61	0.83
2:I:313:LEU:HD13	2:I:321:GLU:HA	1.61	0.82
2:C:857:ASP:HB3	2:C:978:ARG:HG2	1.62	0.82
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:750:LYS:HD3	3:D:681:ARG:HG3	1.60	0.82
2:I:857:ASP:HB3	2:I:978:ARG:HG2	1.62	0.82
3:D:835:SER:HB3	3:D:838:ARG:HE	1.44	0.81
2:C:716:LYS:HG3	3:D:37:LEU:HD11	1.62	0.81
2:I:15:LEU:H	2:I:586:ARG:HH22	1.27	0.81
2:C:494:TYR:HB3	2:C:530:GLU:HG3	1.62	0.81
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.63	0.80
2:I:1033:GLY:HA2	3:J:620:GLY:HA3	1.64	0.80
2:C:1033:GLY:HA2	3:D:620:GLY:HA3	1.63	0.80
2:C:15:LEU:H	2:C:586:ARG:HH22	1.29	0.80
2:C:808:ARG:HH11	2:C:815:LEU:H	1.29	0.80
2:I:716:LYS:HG3	3:J:37:LEU:HD11	1.63	0.80
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.63	0.80
2:I:808:ARG:HH11	2:I:815:LEU:H	1.30	0.79
3:J:97:THR:HG21	3:J:571:LYS:HG3	1.64	0.79
1:B:151:VAL:HG13	1:B:155:ARG:HB2	1.64	0.79
3:J:1142:SER:O	3:J:1364:HIS:ND1	2.13	0.79
3:D:166:GLN:HB3	3:D:396:VAL:HG13	1.64	0.79
3:D:708:LEU:HD12	3:D:1231:GLU:HG2	1.66	0.78
2:I:1036:GLU:HA	3:J:707:THR:HG21	1.66	0.78
5:L:164:GLU:HG3	5:L:165:LYS:HD2	1.66	0.78
2:C:1008:ARG:HD3	2:C:1028:GLY:HA2	1.66	0.78
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.65	0.78
1:G:97:THR:HG23	1:G:98:THR:H	1.49	0.77
2:I:494:TYR:HB3	2:I:530:GLU:HG3	1.64	0.77
3:J:1202:GLN:NE2	3:J:1215:VAL:O	2.12	0.77
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.64	0.77
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.66	0.77
2:I:595:LEU:HD23	2:I:639:GLN:HE22	1.49	0.77
3:J:47:GLU:HG3	3:J:53:ILE:HG13	1.67	0.77
1:A:27:PRO:HD3	1:A:186:LEU:HD22	1.64	0.77
2:I:129:ILE:HD13	2:I:134:ARG:HB2	1.66	0.77
3:J:208:PRO:HA	3:J:390:PRO:HA	1.67	0.77
3:J:563:PRO:HB3	5:L:200:GLN:HB3	1.66	0.77
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.65	0.77
1:A:222:LEU:HD13	1:B:218:LEU:HD23	1.66	0.76
7:P:13:DA:H1'	7:P:14:DC:H5'	1.67	0.76
1:H:151:VAL:HG13	1:H:155:ARG:HB2	1.64	0.76
7:P:15:DA:H1'	7:P:16:DC:H5'	1.66	0.76
3:D:270:ILE:HB	3:D:282:TYR:HB2	1.67	0.76
2:C:32:ALA:HA	2:C:73:ILE:HG21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:LYS:HB3	2:I:997:LEU:HB2	1.68	0.76
2:I:32:ALA:HA	2:I:73:ILE:HG21	1.68	0.76
3:D:47:GLU:HG3	3:D:53:ILE:HG13	1.68	0.76
1:A:97:THR:HG23	1:A:98:THR:H	1.48	0.76
3:D:879:ARG:HH12	3:D:905:PRO:HA	1.50	0.76
2:I:710:ILE:HG21	2:I:756:VAL:HG21	1.66	0.76
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.68	0.76
5:F:164:GLU:HG3	5:F:165:LYS:HD2	1.66	0.76
1:G:222:LEU:HD13	1:H:218:LEU:HD23	1.65	0.76
3:J:1486:VAL:HG11	4:K:26:ARG:HB2	1.68	0.75
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.68	0.75
1:A:184:THR:HB	1:A:194:LYS:HB3	1.67	0.75
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.67	0.75
3:J:1147:ARG:HB3	3:J:1188:VAL:HG11	1.66	0.75
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.67	0.75
3:D:169:TYR:HE2	3:D:395:VAL:HG12	1.50	0.75
1:G:184:THR:HB	1:G:194:LYS:HB3	1.69	0.75
1:G:27:PRO:HD3	1:G:186:LEU:HD22	1.66	0.75
7:S:12:DA:H1'	7:S:13:DA:H5'	1.68	0.75
2:C:72:ARG:HB3	2:C:95:TYR:HB2	1.69	0.75
1:G:55:SER:HB2	1:G:158:ILE:HG12	1.68	0.74
3:D:1208:ASP:O	3:D:1210:SER:N	2.20	0.74
2:C:595:LEU:HD23	2:C:639:GLN:HE22	1.50	0.74
3:D:73:CYS:HB3	3:D:78:VAL:H	1.51	0.74
3:J:73:CYS:HB3	3:J:78:VAL:H	1.52	0.74
2:C:838:LYS:HB3	2:C:997:LEU:HB2	1.69	0.74
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.69	0.74
1:A:53:VAL:HG22	1:A:54:THR:H	1.52	0.74
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.70	0.74
2:C:86:LYS:HE2	2:C:813:VAL:HG23	1.70	0.74
3:D:1143:GLY:HA2	3:D:1364:HIS:CE1	2.22	0.74
2:I:370:ALA:HB1	5:L:295:GLN:HE22	1.53	0.74
2:C:419:THR:HG23	2:C:421:GLU:H	1.53	0.74
7:P:2:DA:H1'	7:P:3:DG:H5'	1.70	0.74
2:C:724:ARG:HG3	2:C:737:LEU:HD23	1.70	0.73
3:D:1223:VAL:HG21	3:D:1462:LEU:HD21	1.69	0.73
3:D:39:PRO:HB3	3:D:46:ASP:HA	1.70	0.73
4:E:30:LEU:HD12	4:E:37:ASN:ND2	2.03	0.73
1:G:53:VAL:HG22	1:G:54:THR:H	1.53	0.73
2:I:601:GLY:HA2	2:I:615:TYR:HA	1.70	0.73
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.70	0.73
1:H:57:TYR:CG	1:H:161:ARG:HG2	2.23	0.73
2:I:1064:ASN:HD22	5:L:359:ALA:HB2	1.53	0.73
3:J:165:LYS:H	3:J:397:LYS:HE2	1.52	0.73
2:C:662:GLU:HG2	2:C:663:GLU:HG2	1.69	0.73
2:C:710:ILE:HG21	2:C:756:VAL:HG21	1.69	0.73
2:C:498:GLN:HG3	3:D:1068:LEU:HD11	1.71	0.73
4:E:27:ALA:HA	4:E:30:LEU:HD22	1.71	0.73
2:I:724:ARG:HG3	2:I:737:LEU:HD23	1.71	0.73
2:I:662:GLU:HG2	2:I:663:GLU:HG2	1.71	0.73
3:D:39:PRO:HG2	3:D:47:GLU:HB2	1.71	0.73
2:I:1008:ARG:HD3	2:I:1028:GLY:HA2	1.71	0.73
2:C:541:SER:O	2:C:545:ASN:ND2	2.22	0.72
3:J:1336:LEU:HA	3:J:1344:VAL:HG21	1.71	0.72
3:D:596:SER:OG	3:D:597:GLU:N	2.20	0.72
3:J:680:GLN:HG2	3:J:681:ARG:H	1.54	0.72
3:D:680:GLN:HG2	3:D:681:ARG:H	1.53	0.72
1:A:55:SER:HB2	1:A:158:ILE:HG12	1.70	0.72
1:B:57:TYR:CG	1:B:161:ARG:HG2	2.25	0.72
2:I:541:SER:O	2:I:545:ASN:ND2	2.23	0.72
3:J:39:PRO:HG2	3:J:47:GLU:HB2	1.71	0.72
1:G:205:VAL:HG13	1:G:209:GLU:HB2	1.72	0.72
5:L:376:LEU:HD11	5:L:423:LEU:HD11	1.72	0.72
3:D:242:LEU:H	3:D:312:ARG:HA	1.53	0.72
3:J:39:PRO:HB3	3:J:46:ASP:HA	1.72	0.72
1:B:110:ARG:H	1:B:113:ASP:HB2	1.55	0.72
2:I:146:VAL:HG12	2:I:162:ILE:HG13	1.72	0.72
2:C:146:VAL:HG12	2:C:162:ILE:HG13	1.71	0.71
3:D:97:THR:HG21	3:D:571:LYS:HG3	1.71	0.71
3:J:1211:MET:HB3	3:J:1213:ARG:HG2	1.71	0.71
3:J:879:ARG:HH12	3:J:905:PRO:HA	1.55	0.71
3:J:410:THR:HG23	5:L:189:LEU:HD21	1.72	0.71
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.71	0.71
2:C:737:LEU:HG	2:C:741:GLY:HA2	1.72	0.71
2:I:1053:LEU:HA	3:J:621:LYS:HE3	1.72	0.71
6:O:7:DA:H61	7:P:20:DT:H3	1.38	0.71
3:D:214:ASP:OD1	3:D:214:ASP:N	2.22	0.71
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.72	0.71
3:D:226:PRO:HA	3:D:330:SER:HA	1.72	0.71
2:C:1053:LEU:HA	3:D:621:LYS:HE3	1.72	0.71
2:I:419:THR:HG23	2:I:421:GLU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:737:LEU:HG	2:I:741:GLY:HA2	1.72	0.71
3:D:618:LEU:HD23	3:D:1467:ILE:HG23	1.71	0.71
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.71	0.71
4:K:30:LEU:HD12	4:K:37:ASN:ND2	2.03	0.71
5:F:376:LEU:HD11	5:F:423:LEU:HD11	1.71	0.71
4:K:27:ALA:HA	4:K:30:LEU:HD22	1.72	0.70
3:J:367:ILE:HB	3:J:377:VAL:HB	1.73	0.70
2:C:601:GLY:HA2	2:C:615:TYR:HA	1.72	0.70
1:G:219:LYS:HA	1:G:222:LEU:HD23	1.74	0.70
1:B:186:LEU:HB2	1:B:192:LEU:HD11	1.72	0.70
3:J:1003:VAL:HG21	3:J:1041:MET:HG2	1.74	0.70
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.72	0.70
2:C:576:ALA:HB1	2:C:580:MET:HE3	1.73	0.70
3:J:1267:ARG:HE	3:J:1267:ARG:H	1.39	0.70
3:D:214:ASP:HA	3:D:342:PRO:HA	1.74	0.70
3:D:208:PRO:HA	3:D:390:PRO:HA	1.74	0.70
3:J:361:VAL:HG21	3:J:367:ILE:HD11	1.74	0.70
7:S:15:DA:H1'	7:S:16:DC:H5'	1.73	0.70
3:D:9:ARG:HG3	3:D:1456:LYS:HG2	1.74	0.70
2:I:576:ALA:HB1	2:I:580:MET:HE3	1.72	0.70
3:J:371:ILE:HG21	5:L:247:ARG:HH22	1.53	0.70
2:C:1101:THR:HG23	3:D:8:VAL:HG22	1.74	0.69
3:D:1192:LEU:HA	3:D:1373:ARG:HG3	1.73	0.69
2:I:498:GLN:HG3	3:J:1068:LEU:HD11	1.74	0.69
3:J:191:LEU:HD11	3:J:197:SER:HB2	1.73	0.69
6:O:17:DA:H1'	6:O:18:DA:H5'	1.73	0.69
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.73	0.69
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.74	0.69
3:D:1272:ALA:HB3	3:D:1330:ILE:HD13	1.75	0.69
3:D:563:PRO:HB3	5:F:200:GLN:HB3	1.74	0.69
3:J:371:ILE:HG23	3:J:372:ASP:H	1.55	0.69
3:J:761:ILE:O	3:J:767:HIS:ND1	2.23	0.69
2:I:72:ARG:HB3	2:I:95:TYR:HB2	1.75	0.69
3:D:236:TYR:HB3	3:D:313:LEU:HD22	1.74	0.69
1:H:110:ARG:H	1:H:113:ASP:HB2	1.58	0.69
2:I:542:LEU:HD12	2:I:542:LEU:H	1.58	0.69
3:J:1105:ILE:HD12	3:J:1373:ARG:HH12	1.58	0.69
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.75	0.69
2:I:468:ARG:HB3	2:I:485:TYR:O	1.93	0.69
2:I:833:LEU:HD11	2:I:839:LEU:HD11	1.75	0.69
3:D:93:ILE:HD13	3:D:548:ILE:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:18:DA:H1'	6:R:19:DT:H5'	1.74	0.68
2:I:969:LEU:HD23	2:I:971:LYS:HE3	1.74	0.68
6:O:10:DA:H1'	6:O:11:DG:H5'	1.75	0.68
7:P:17:DT:H1'	7:P:18:DT:H5'	1.73	0.68
3:J:560:GLN:O	5:L:147:ARG:NH1	2.26	0.68
3:D:520:LEU:O	3:D:525:ARG:NH2	2.26	0.68
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.75	0.68
3:D:977:ALA:HB2	3:J:831:GLY:H	1.59	0.68
1:B:59:GLU:HG3	1:B:139:TYR:HD2	1.57	0.68
2:C:200:LEU:HG	2:C:300:ASP:HB2	1.76	0.68
2:C:568:ALA:HB1	2:C:995:MET:SD	2.34	0.68
3:D:93:ILE:HB	3:D:517:VAL:HB	1.75	0.68
3:J:699:VAL:HG12	3:J:717:GLN:HG2	1.75	0.68
5:L:222:LEU:HD11	5:L:269:GLN:HG2	1.76	0.68
2:C:242:LEU:HD13	2:C:243:ARG:HB2	1.76	0.68
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.75	0.68
3:J:8:VAL:HG21	3:J:1468:LEU:HD11	1.76	0.68
3:D:371:ILE:HG23	3:D:372:ASP:H	1.59	0.67
2:I:568:ALA:HB1	2:I:995:MET:SD	2.34	0.67
3:D:45:PHE:HA	3:D:522:PRO:HB3	1.76	0.67
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.75	0.67
7:P:25:DA:H1'	7:P:26:DG:H5'	1.76	0.67
2:I:833:LEU:HD12	2:I:996:LYS:HE3	1.74	0.67
2:C:261:LEU:HB3	2:C:291:VAL:HG22	1.77	0.67
3:J:521:PRO:HD2	3:J:524:LEU:HD12	1.76	0.67
3:J:783:ARG:HD3	3:J:1028:ALA:O	1.94	0.67
2:C:230:ARG:HB3	2:C:231:PRO:HD2	1.76	0.67
2:C:542:LEU:HD12	2:C:542:LEU:H	1.59	0.67
2:C:995:MET:HE2	2:C:996:LYS:H	1.60	0.67
1:G:39:PRO:HG2	1:H:39:PRO:HG3	1.76	0.67
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.77	0.67
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.25	0.67
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.77	0.67
2:I:211:LEU:HD13	2:I:218:VAL:HA	1.76	0.67
7:P:21:DG:H1'	7:P:22:DT:H5'	1.75	0.67
3:D:1382:THR:HG23	3:D:1417:TRP:HA	1.77	0.67
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.76	0.67
3:J:87:ARG:HG2	3:J:523:ASP:HB3	1.77	0.67
5:L:164:GLU:O	5:L:166:PRO:HD3	1.95	0.67
2:I:229:MET:HB3	2:I:234:ALA:HB2	1.76	0.67
2:I:397:GLU:HB2	2:I:632:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:140:ILE:HG22	2:I:412:ALA:HA	1.76	0.67
3:J:1140:ILE:HG23	3:J:1144:LEU:HD23	1.77	0.67
3:J:1273:VAL:HG22	3:J:1326:THR:HG22	1.77	0.67
3:J:618:LEU:HD23	3:J:1467:ILE:HG23	1.75	0.67
2:I:207:LEU:HD21	2:I:221:LEU:HB3	1.76	0.66
6:O:9:DA:H1'	6:O:10:DA:H5'	1.77	0.66
2:C:229:MET:HB3	2:C:234:ALA:HB2	1.75	0.66
5:F:164:GLU:O	5:F:166:PRO:HD3	1.95	0.66
3:J:100:ALA:HA	3:J:513:ILE:HA	1.77	0.66
2:C:1042:ALA:HA	3:D:1224:VAL:HG22	1.75	0.66
2:I:200:LEU:HG	2:I:300:ASP:HB2	1.77	0.66
2:I:688:ILE:HB	2:I:849:VAL:HA	1.76	0.66
3:D:783:ARG:HD3	3:D:1028:ALA:O	1.96	0.66
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.77	0.66
3:J:423:ASP:HB3	3:J:426:LYS:HB3	1.76	0.66
2:C:833:LEU:HD12	2:C:996:LYS:HE3	1.75	0.66
3:D:569:ASN:HD22	5:F:229:GLN:HE21	1.44	0.66
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.76	0.66
2:C:64:LEU:HD13	2:C:359:MET:HG2	1.78	0.66
2:C:777:ILE:HA	5:F:420:LEU:HD11	1.77	0.66
2:C:969:LEU:HD23	2:C:971:LYS:HE3	1.76	0.66
2:I:230:ARG:HB3	2:I:231:PRO:HD2	1.76	0.66
2:I:708:TYR:CE1	2:I:827:VAL:HB	2.31	0.66
6:O:12:DT:H1'	6:O:13:DG:H5'	1.78	0.66
2:C:468:ARG:HB3	2:C:485:TYR:O	1.95	0.66
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.61	0.66
3:D:354:ILE:HD11	3:D:369:ALA:HB2	1.77	0.66
2:I:242:LEU:HD13	2:I:243:ARG:HB2	1.76	0.66
2:I:1101:THR:HG23	3:J:8:VAL:HG22	1.78	0.66
2:I:332:ARG:HB2	2:I:465:GLY:HA3	1.77	0.66
2:C:762:LYS:HB3	2:C:786:LYS:HB2	1.78	0.66
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.77	0.66
2:I:537:LYS:HZ3	2:I:905:VAL:N	1.91	0.66
2:C:101:ILE:HG23	2:C:108:ILE:HA	1.77	0.66
2:I:101:ILE:HG23	2:I:108:ILE:HA	1.79	0.65
6:O:24:DC:H42	7:P:3:DG:H1	1.43	0.65
2:C:211:LEU:HD13	2:C:218:VAL:HA	1.77	0.65
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.77	0.65
3:D:594:PRO:HB3	5:F:221:GLY:HA2	1.78	0.65
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.78	0.65
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HA	1:A:222:LEU:HD23	1.77	0.65
2:C:140:ILE:HG22	2:C:412:ALA:HA	1.77	0.65
3:J:582:ILE:HD13	3:J:603:LEU:HD12	1.79	0.65
2:I:458:TYR:HD1	2:I:538:GLN:HB3	1.61	0.65
3:J:100:ALA:HB2	3:J:513:ILE:HD13	1.78	0.65
6:R:9:DA:H1'	6:R:10:DA:H5'	1.77	0.65
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.29	0.65
2:I:710:ILE:HB	2:I:790:LEU:HD22	1.79	0.65
2:C:397:GLU:HB2	2:C:632:ASN:HB2	1.79	0.65
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.79	0.65
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.79	0.65
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.77	0.65
2:I:995:MET:HE2	2:I:996:LYS:H	1.60	0.65
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.78	0.65
3:D:8:VAL:HG21	3:D:1468:LEU:HD11	1.78	0.65
6:R:10:DA:H1'	6:R:11:DG:H5'	1.78	0.65
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.78	0.64
5:F:222:LEU:HD11	5:F:269:GLN:HG2	1.79	0.64
3:J:1285:GLU:HB3	3:J:1290:LEU:HA	1.79	0.64
6:R:2:DT:H3	7:S:25:DA:H2	1.42	0.64
2:C:207:LEU:HD21	2:C:221:LEU:HB3	1.77	0.64
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.79	0.64
3:D:242:LEU:HD23	3:D:285:PRO:HB3	1.79	0.64
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.79	0.64
2:C:1051:GLU:HG2	2:C:1055:ILE:HD12	1.79	0.64
1:H:59:GLU:HB2	1:H:139:TYR:HB3	1.79	0.64
7:S:13:DA:H1'	7:S:14:DC:H5'	1.78	0.64
2:C:139:GLN:HB2	2:C:391:LEU:HD21	1.79	0.64
3:D:268:HIS:HB2	3:D:284:LEU:HD22	1.78	0.64
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.78	0.64
2:C:217:LEU:HD13	2:C:311:PHE:HB3	1.80	0.64
2:C:467:ILE:HD12	2:C:467:ILE:H	1.63	0.64
5:L:149:LYS:HD3	5:L:193:ARG:HH22	1.61	0.64
2:I:773:LEU:HB2	5:L:388:LYS:HG3	1.80	0.64
3:D:573:MET:HA	3:D:576:GLU:HG2	1.78	0.64
2:I:64:LEU:HD13	2:I:359:MET:HG2	1.80	0.64
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.80	0.64
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.79	0.64
3:J:67:ARG:HD2	5:L:394:ARG:HB2	1.78	0.64
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.78	0.64
1:H:186:LEU:HB2	1:H:192:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.80	0.64
2:I:139:GLN:HB2	2:I:391:LEU:HD21	1.80	0.64
2:I:86:LYS:HE2	2:I:813:VAL:HG23	1.79	0.64
3:J:887:GLY:HA3	3:J:893:GLU:HA	1.79	0.64
2:C:688:ILE:HB	2:C:849:VAL:HA	1.79	0.63
1:H:24:VAL:HG22	1:H:196:THR:HG23	1.79	0.63
2:I:261:LEU:HB3	2:I:291:VAL:HG22	1.80	0.63
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.79	0.63
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.62	0.63
5:F:364:LEU:HD12	5:F:436:PHE:HZ	1.63	0.63
2:I:101:ILE:HA	2:I:107:LEU:O	1.98	0.63
2:I:577:PRO:HA	2:I:671:ASN:HD21	1.63	0.63
3:D:618:LEU:HB3	3:D:1467:ILE:HG12	1.79	0.63
3:J:102:ILE:HB	3:J:579:ASP:HB3	1.79	0.63
6:O:18:DA:H1'	6:O:19:DT:H5'	1.78	0.63
2:C:708:TYR:CE1	2:C:827:VAL:HB	2.33	0.63
1:A:39:PRO:HG2	1:B:39:PRO:HG3	1.81	0.63
2:C:1064:ASN:HD22	5:F:359:ALA:HB2	1.64	0.63
3:D:887:GLY:HA3	3:D:893:GLU:HA	1.80	0.63
3:J:65:ARG:NH1	5:L:393:GLY:O	2.32	0.63
2:C:723:THR:O	2:C:757:GLY:HA3	1.99	0.63
2:C:833:LEU:HD11	2:C:839:LEU:HD11	1.79	0.63
2:I:217:LEU:HD13	2:I:311:PHE:HB3	1.81	0.63
6:O:4:DG:H1'	6:O:5:DA:H5'	1.80	0.63
3:D:1472:ILE:HG12	3:D:1474:ALA:H	1.63	0.63
2:C:1034:GLU:HG2	3:D:619:LEU:HB3	1.81	0.63
5:L:383:VAL:HA	5:L:386:LEU:HD12	1.79	0.63
1:B:44:LEU:HD23	1:B:174:VAL:HG21	1.81	0.63
1:B:73:GLU:HB2	1:B:78:ILE:HD11	1.80	0.63
3:D:514:LEU:HD21	3:D:518:PRO:HD3	1.81	0.63
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.80	0.63
3:D:701:LEU:HD21	3:D:763:MET:HG3	1.79	0.63
3:J:974:ILE:HG12	3:J:991:GLN:HE21	1.63	0.63
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.79	0.62
4:E:79:LEU:HG	4:E:80:VAL:HG13	1.80	0.62
3:D:407:VAL:HG22	3:D:409:VAL:H	1.63	0.62
2:I:467:ILE:HD12	2:I:467:ILE:H	1.63	0.62
3:J:835:SER:HB3	3:J:838:ARG:HE	1.63	0.62
3:D:761:ILE:O	3:D:767:HIS:ND1	2.26	0.62
3:D:367:ILE:HB	3:D:377:VAL:HB	1.80	0.62
5:F:383:VAL:HA	5:F:386:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:773:LEU:HB2	5:F:388:LYS:HG3	1.80	0.62
2:I:607:ASP:O	2:I:609:THR:N	2.33	0.62
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.82	0.62
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.81	0.62
2:C:370:ALA:HB1	5:F:295:GLN:HE22	1.64	0.62
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.81	0.62
3:J:127:LEU:HD23	3:J:461:ILE:HG13	1.81	0.62
5:L:364:LEU:HD12	5:L:436:PHE:HZ	1.63	0.62
2:C:537:LYS:HZ3	2:C:905:VAL:N	1.93	0.62
2:I:123:GLU:HG2	2:I:592:LEU:HD13	1.81	0.62
3:J:1472:ILE:HG12	3:J:1474:ALA:H	1.65	0.62
3:J:701:LEU:HD21	3:J:763:MET:HG3	1.80	0.62
5:F:180:SER:O	5:F:181:LEU:HD12	2.00	0.62
2:I:762:LYS:HB3	2:I:786:LYS:HB2	1.80	0.62
2:I:691:SER:HB3	2:I:868:ASP:HA	1.82	0.62
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.82	0.62
2:C:101:ILE:HA	2:C:107:LEU:O	1.99	0.62
3:J:1004:THR:HG23	3:J:1036:ARG:HB2	1.81	0.62
1:B:59:GLU:HB2	1:B:139:TYR:HB3	1.82	0.62
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.35	0.62
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.82	0.62
1:G:46:SER:HB3	2:I:856:GLU:HG2	1.82	0.62
2:I:839:LEU:HG	2:I:996:LYS:HA	1.81	0.62
2:C:50:GLU:HA	2:C:265:LYS:HD2	1.82	0.61
3:D:1202:GLN:HE21	3:D:1217:ILE:HG12	1.65	0.61
1:H:73:GLU:HB2	1:H:78:ILE:HD11	1.82	0.61
2:C:107:LEU:HD12	2:C:109:LYS:HB2	1.82	0.61
3:D:168:THR:HA	3:D:394:LEU:HB2	1.81	0.61
3:D:974:ILE:HG12	3:D:991:GLN:HE21	1.65	0.61
1:H:44:LEU:HD23	1:H:174:VAL:HG21	1.82	0.61
3:J:772:PRO:HA	3:J:1209:LEU:HB2	1.82	0.61
6:R:10:DA:H2	7:S:17:DT:H3	1.47	0.61
2:C:607:ASP:O	2:C:609:THR:N	2.32	0.61
2:C:579:VAL:HG13	2:C:842:ARG:HH22	1.64	0.61
3:D:245:LEU:HB2	3:D:309:GLY:HA2	1.81	0.61
2:C:1090:LYS:NZ	2:C:1093:GLN:OE1	2.28	0.61
2:C:174:LEU:HD13	2:C:310:LEU:HD22	1.81	0.61
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.81	0.61
5:F:222:LEU:HB3	5:F:226:ASP:HB2	1.82	0.61
2:I:36:PRO:HA	2:I:39:ARG:HD2	1.83	0.61
2:I:723:THR:O	2:I:757:GLY:HA3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:112:ILE:HG23	3:J:512:MET:HG2	1.81	0.61
3:J:1313:VAL:HG21	3:J:1325:LEU:HD12	1.81	0.61
2:C:332:ARG:HB2	2:C:465:GLY:HA3	1.82	0.61
3:D:1143:GLY:HA2	3:D:1364:HIS:HE1	1.65	0.61
2:I:1016:ILE:O	3:J:87:ARG:NH2	2.34	0.61
6:R:11:DG:N2	7:S:16:DC:O2	2.34	0.61
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.81	0.61
1:G:35:THR:HG21	1:H:43:ILE:HG13	1.81	0.61
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.83	0.61
3:D:1100:ASP:HA	3:D:1463:LYS:HE2	1.82	0.61
1:H:59:GLU:HG3	1:H:139:TYR:HD2	1.66	0.61
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.83	0.61
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.81	0.61
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.83	0.61
1:G:51:THR:HG23	1:G:146:ARG:HG2	1.83	0.61
1:H:58:ILE:HD13	1:H:61:VAL:HB	1.82	0.61
2:C:191:PHE:HB2	2:C:195:LEU:HD22	1.82	0.61
2:I:1037:VAL:HG13	2:I:1049:LEU:HD11	1.82	0.61
2:I:262:ALA:HB2	2:I:291:VAL:HG23	1.83	0.61
2:I:1034:GLU:HG2	3:J:619:LEU:HB3	1.82	0.61
3:J:557:LEU:HD21	5:L:233:GLN:HG2	1.83	0.61
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.81	0.60
2:I:777:ILE:HA	5:L:420:LEU:HD11	1.83	0.60
3:J:703:ASN:HB2	3:J:713:ILE:HG12	1.82	0.60
4:K:79:LEU:HG	4:K:80:VAL:HG13	1.83	0.60
3:D:1111:ASP:OD1	3:D:1203:LYS:NZ	2.35	0.60
2:I:107:LEU:HD12	2:I:109:LYS:HB2	1.83	0.60
2:I:50:GLU:HA	2:I:265:LYS:HD2	1.83	0.60
2:I:1089:VAL:HG21	2:I:1111:ILE:HG21	1.83	0.60
2:I:36:PRO:HB2	2:I:70:GLU:HG2	1.83	0.60
2:C:1018:GLN:HB3	2:C:1063:ARG:NH1	2.15	0.60
3:D:270:ILE:HG12	3:D:284:LEU:HD11	1.82	0.60
2:I:174:LEU:HD13	2:I:310:LEU:HD22	1.82	0.60
3:J:7:LYS:NZ	3:J:1458:GLU:OE1	2.33	0.60
3:J:704:ARG:HB2	3:J:745:MET:HG2	1.83	0.60
5:L:180:SER:O	5:L:181:LEU:HD12	2.00	0.60
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.66	0.60
5:F:149:LYS:HD3	5:F:193:ARG:HH22	1.65	0.60
3:J:407:VAL:HG23	3:J:422:ALA:HB2	1.84	0.60
2:C:668:LEU:H	2:C:993:PHE:HZ	1.50	0.60
3:D:514:LEU:HG	3:D:516:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.82	0.60
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.82	0.60
5:L:222:LEU:HB3	5:L:226:ASP:HB2	1.83	0.60
2:C:839:LEU:HG	2:C:996:LYS:HA	1.83	0.60
1:A:46:SER:HB3	2:C:856:GLU:HG2	1.84	0.60
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.83	0.60
2:C:1005:MET:HG3	3:D:629:SER:HB2	1.83	0.60
1:G:54:THR:HB	1:G:143:ARG:O	2.02	0.60
1:H:51:THR:HB	1:H:87:VAL:O	2.01	0.60
2:I:118:LEU:HD13	2:I:382:LEU:HD23	1.82	0.60
3:J:1166:LEU:HD23	3:J:1174:LEU:HD11	1.81	0.60
1:B:58:ILE:HD13	1:B:61:VAL:HB	1.81	0.60
2:I:1005:MET:HG3	3:J:629:SER:HB2	1.82	0.60
2:I:668:LEU:H	2:I:993:PHE:HZ	1.50	0.60
2:I:1031:ARG:HG2	2:I:1033:GLY:H	1.67	0.60
3:J:759:ALA:HA	3:J:763:MET:HB3	1.83	0.60
3:D:1313:VAL:HG11	3:D:1325:LEU:HD23	1.83	0.59
1:G:42:ARG:NH1	2:I:978:ARG:HA	2.17	0.59
2:I:571:LEU:HD21	2:I:995:MET:HE1	1.84	0.59
3:J:1105:ILE:HB	3:J:1222:GLY:HA3	1.83	0.59
6:R:24:DC:N4	7:S:3:DG:H1	1.95	0.59
2:I:1051:GLU:HG2	2:I:1055:ILE:HD12	1.84	0.59
2:I:571:LEU:HG	2:I:700:TYR:HA	1.84	0.59
3:J:27:GLU:H	3:J:42:ASP:HB3	1.67	0.59
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.84	0.59
2:C:774:LEU:HG	5:F:365:LEU:HD21	1.84	0.59
3:J:101:HIS:NE2	3:J:582:ILE:HG21	2.17	0.59
3:D:1139:ASP:O	3:D:1142:SER:HB2	2.02	0.59
3:D:1188:VAL:HG12	3:D:1189:ARG:H	1.66	0.59
3:D:919:PHE:HA	3:D:927:THR:HG21	1.85	0.59
1:G:13:ALA:HB3	1:H:228:PRO:HB3	1.83	0.59
6:O:19:DT:H1'	6:O:20:DT:H5'	1.83	0.59
3:D:433:GLY:HA2	3:D:449:SER:HB2	1.85	0.59
3:D:92:HIS:HA	3:D:517:VAL:O	2.02	0.59
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.83	0.59
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.84	0.59
3:J:210:ARG:HD2	3:J:388:HIS:HB2	1.85	0.59
3:J:708:LEU:HG	3:J:709:HIS:H	1.67	0.59
3:J:978:TYR:HB2	3:J:988:ARG:HD3	1.83	0.59
2:C:408:ARG:NH2	2:C:456:ALA:O	2.35	0.59
2:I:408:ARG:NH2	2:I:456:ALA:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.84	0.59
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.85	0.59
1:B:51:THR:HB	1:B:87:VAL:O	2.02	0.59
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.37	0.59
3:D:9:ARG:HG2	3:D:10:ILE:H	1.66	0.59
2:C:716:LYS:HD2	3:D:37:LEU:HD21	1.85	0.59
3:D:1364:HIS:NE2	3:D:1366:LYS:HE2	2.17	0.59
1:A:54:THR:HB	1:A:143:ARG:O	2.02	0.59
2:C:911:GLU:OE1	3:D:1062:ARG:NH2	2.34	0.59
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	1.85	0.59
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.85	0.59
5:L:307:ALA:HB1	5:L:314:TRP:HB3	1.85	0.59
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.85	0.59
3:D:245:LEU:HD12	3:D:311:LEU:HD21	1.84	0.59
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.85	0.59
2:I:798:GLY:HA3	2:I:827:VAL:HG13	1.83	0.59
3:J:698:LYS:HG3	4:K:59:ASN:HD21	1.68	0.59
7:S:18:DT:H1'	7:S:19:DT:H5'	1.85	0.59
2:C:413:LEU:H	2:C:413:LEU:HD12	1.68	0.58
3:D:203:ALA:HA	3:D:395:VAL:HA	1.85	0.58
1:G:53:VAL:HG22	1:G:54:THR:N	2.18	0.58
2:I:704:HIS:CD2	2:I:831:ARG:HD2	2.37	0.58
3:J:125:GLN:HB3	3:J:131:LYS:HB3	1.84	0.58
2:C:15:LEU:HD11	2:C:457:ALA:HB1	1.85	0.58
1:G:101:LEU:HB3	1:G:140:MET:HB3	1.85	0.58
3:J:1280:VAL:O	3:J:1295:GLU:N	2.35	0.58
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.84	0.58
2:C:497:ALA:HB1	2:C:501:THR:HG21	1.85	0.58
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.86	0.58
3:J:1111:ASP:OD1	3:J:1203:LYS:NZ	2.36	0.58
3:J:971:LEU:HA	3:J:974:ILE:HD12	1.85	0.58
2:C:207:LEU:HD13	2:C:222:LEU:HD23	1.85	0.58
2:C:532:MET:HG2	2:C:533:ASP:H	1.68	0.58
3:D:125:GLN:HB3	3:D:131:LYS:HB3	1.85	0.58
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.84	0.58
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.86	0.58
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.85	0.58
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.86	0.58
3:D:907:GLU:O	3:D:911:LEU:HG	2.04	0.58
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.85	0.58
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG12	1:B:199:ILE:HG12	1.85	0.58
3:D:262:LYS:HB2	3:D:269:LEU:HB2	1.85	0.58
5:F:380:GLU:HB2	5:F:419:ALA:HB2	1.85	0.58
2:I:236:VAL:HG21	2:I:250:LYS:HG2	1.86	0.58
2:I:911:GLU:OE1	3:J:1062:ARG:NH2	2.36	0.58
3:J:461:ILE:HB	3:J:513:ILE:HD11	1.85	0.58
2:I:774:LEU:HG	5:L:365:LEU:HD21	1.84	0.58
2:C:571:LEU:HD21	2:C:995:MET:HE1	1.84	0.58
2:I:5:ARG:HA	2:I:902:ILE:HB	1.84	0.58
6:R:19:DT:H1'	6:R:20:DT:H5'	1.85	0.58
2:C:611:ILE:HG13	2:C:625:LEU:HD11	1.86	0.58
3:D:772:PRO:HG3	3:D:1210:SER:HB3	1.86	0.58
1:H:57:TYR:CD1	1:H:161:ARG:HG2	2.38	0.58
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.39	0.58
2:C:1071:ILE:O	3:D:659:LYS:HG2	2.04	0.58
2:C:571:LEU:HG	2:C:700:TYR:HA	1.85	0.58
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.18	0.58
3:J:1101:VAL:HB	3:J:1428:ALA:HB2	1.86	0.58
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.85	0.58
3:D:12:LEU:HD21	3:D:1452:ILE:HD13	1.86	0.58
2:I:579:VAL:HG13	2:I:842:ARG:HH22	1.69	0.58
3:J:520:LEU:O	3:J:525:ARG:NH2	2.37	0.58
6:R:17:DA:H1'	6:R:18:DA:H5'	1.86	0.58
7:S:8:DA:H2''	7:S:9:DT:H5''	1.86	0.58
1:A:51:THR:HG23	1:A:146:ARG:HG2	1.84	0.57
2:C:691:SER:HB3	2:C:868:ASP:HA	1.86	0.57
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.86	0.57
3:D:803:GLY:HA2	3:D:827:ILE:HG22	1.85	0.57
5:F:203:ILE:HG23	5:F:235:LEU:HD23	1.86	0.57
1:H:177:VAL:HG12	1:H:199:ILE:HG12	1.86	0.57
3:J:770:LEU:HB2	3:J:1210:SER:HA	1.85	0.57
3:J:9:ARG:HG2	3:J:10:ILE:H	1.68	0.57
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.68	0.57
2:C:236:VAL:HG21	2:C:250:LYS:HG2	1.86	0.57
3:D:205:TYR:HD1	3:D:393:ILE:HG12	1.68	0.57
3:D:25:GLU:HG2	3:D:93:ILE:HA	1.86	0.57
2:I:637:PHE:HA	2:I:659:PRO:HG3	1.86	0.57
5:L:225:LEU:HA	5:L:228:ILE:HD12	1.85	0.57
2:C:1089:VAL:HG21	2:C:1111:ILE:HG21	1.86	0.57
3:D:759:ALA:HA	3:D:763:MET:HB3	1.84	0.57
2:I:191:PHE:HB2	2:I:195:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:732:ALA:O	2:I:735:ARG:HG3	2.04	0.57
2:I:557:ARG:HB2	2:I:881:ASN:HD21	1.69	0.57
2:C:1031:ARG:HG2	2:C:1033:GLY:H	1.69	0.57
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.87	0.57
3:D:1087:ARG:NH2	3:D:1234:THR:O	2.37	0.57
3:D:443:VAL:HG22	3:D:445:ARG:H	1.69	0.57
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.86	0.57
1:H:188:GLN:HA	3:J:688:TRP:HD1	1.69	0.57
3:J:907:GLU:O	3:J:911:LEU:HG	2.05	0.57
2:C:162:ILE:HG22	2:C:172:ILE:HD13	1.85	0.57
2:C:975:TYR:HA	2:C:982:PRO:HA	1.87	0.57
3:D:171:LEU:HD21	3:D:393:ILE:HD12	1.87	0.57
2:C:1085:PHE:HA	3:D:618:LEU:HD21	1.87	0.57
2:I:532:MET:HG2	2:I:533:ASP:H	1.69	0.57
3:J:881:LEU:O	3:J:885:ILE:HG13	2.05	0.57
1:A:53:VAL:HG22	1:A:54:THR:N	2.18	0.57
1:A:35:THR:HG21	1:B:43:ILE:HG13	1.85	0.57
3:D:843:PHE:HB2	3:D:866:VAL:HG23	1.86	0.57
2:I:569:VAL:HB	2:I:635:THR:HG21	1.87	0.57
1:A:14:THR:OG1	1:B:231:SER:OG	2.21	0.57
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.05	0.57
2:C:5:ARG:HA	2:C:902:ILE:HB	1.86	0.57
3:D:1254:GLN:HB3	3:D:1258:ARG:CB	2.34	0.57
1:H:218:LEU:O	1:H:222:LEU:HG	2.05	0.57
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.37	0.57
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.86	0.57
3:D:1127:GLU:HG3	3:D:1128:VAL:HG23	1.85	0.57
3:D:244:GLU:O	3:D:310:LEU:N	2.36	0.57
5:F:225:LEU:HA	5:F:228:ILE:HD12	1.85	0.57
6:O:7:DA:H1'	6:O:8:DA:H5'	1.85	0.57
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.85	0.57
3:D:669:ASN:ND2	5:F:364:LEU:HD11	2.20	0.57
1:H:13:ALA:HB1	1:H:23:PHE:HD1	1.69	0.57
5:F:307:ALA:HB1	5:F:314:TRP:HB3	1.87	0.57
2:I:858:MET:H	2:I:977:GLY:HA3	1.70	0.57
1:B:57:TYR:CD1	1:B:161:ARG:HG2	2.39	0.56
3:D:95:LEU:HG	3:D:574:LEU:HD21	1.86	0.56
5:F:98:GLN:O	5:F:102:GLU:HG3	2.04	0.56
3:J:1100:ASP:HA	3:J:1463:LYS:HE2	1.86	0.56
5:L:150:ILE:HG12	5:L:193:ARG:HH11	1.69	0.56
3:D:56:TYR:HA	3:D:80:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.70	0.56
2:I:567:GLN:O	2:I:998:TYR:N	2.38	0.56
7:P:8:DA:H2"	7:P:9:DT:H5"	1.87	0.56
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.69	0.56
2:I:207:LEU:HD13	2:I:222:LEU:HD23	1.87	0.56
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.87	0.56
2:I:716:LYS:HD2	3:J:37:LEU:HD21	1.87	0.56
5:L:203:ILE:HG23	5:L:235:LEU:HD23	1.87	0.56
2:C:732:ALA:O	2:C:735:ARG:HG3	2.04	0.56
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.87	0.56
2:I:639:GLN:HB3	2:I:656:ALA:HB1	1.88	0.56
3:D:1176:LYS:HG3	3:J:1130:ARG:HD2	1.87	0.56
3:J:14:SER:HB3	3:J:511:TRP:CE2	2.40	0.56
2:C:1069:ALA:HB3	2:C:1076:VAL:HG12	1.86	0.56
2:C:262:ALA:HB2	2:C:291:VAL:HG23	1.87	0.56
3:D:881:LEU:O	3:D:885:ILE:HG13	2.05	0.56
3:D:698:LYS:HG3	4:E:59:ASN:HD21	1.69	0.56
2:I:162:ILE:HG22	2:I:172:ILE:HD13	1.86	0.56
2:I:497:ALA:HB1	2:I:501:THR:HG21	1.87	0.56
2:I:926:PHE:HE2	2:I:960:GLU:HG3	1.69	0.56
3:J:803:GLY:HA2	3:J:827:ILE:HG22	1.86	0.56
3:J:919:PHE:HA	3:J:927:THR:HG21	1.86	0.56
1:B:218:LEU:O	1:B:222:LEU:HG	2.05	0.56
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.40	0.56
3:D:191:LEU:HD13	3:D:195:VAL:HG12	1.87	0.56
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.86	0.56
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.88	0.56
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.86	0.56
2:I:774:LEU:HA	2:I:777:ILE:HD12	1.86	0.56
3:J:56:TYR:HA	3:J:80:VAL:HG23	1.88	0.56
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.87	0.56
6:O:2:DT:H2"	6:O:3:DT:H71	1.86	0.56
3:D:773:ALA:HB2	3:D:1228:SER:HB3	1.86	0.56
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.87	0.56
3:D:1500:LYS:HA	3:D:1503:VAL:HG22	1.88	0.56
1:G:40:LEU:O	1:G:44:LEU:HB2	2.05	0.56
3:D:977:ALA:HB2	3:J:831:GLY:N	2.19	0.56
7:S:17:DT:H1'	7:S:18:DT:H5'	1.87	0.56
1:A:54:THR:HG22	1:A:158:ILE:HD11	1.87	0.56
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.86	0.56
3:D:684:LYS:HD3	3:D:685:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLN:HA	3:D:688:TRP:HD1	1.71	0.56
4:E:30:LEU:HD23	4:E:63:TRP:HB3	1.88	0.56
2:C:114:PHE:HB3	5:F:295:GLN:HA	1.88	0.56
2:I:146:VAL:HG21	2:I:281:LEU:HD21	1.88	0.56
2:I:413:LEU:H	2:I:413:LEU:HD12	1.69	0.56
2:I:611:ILE:HG13	2:I:625:LEU:HD11	1.88	0.56
3:J:1088:THR:HA	3:J:1234:THR:HG22	1.87	0.56
3:J:191:LEU:HD13	3:J:195:VAL:HG12	1.88	0.56
3:J:974:ILE:HG22	3:J:988:ARG:HG3	1.86	0.56
3:D:406:ASP:OD1	3:D:407:VAL:N	2.38	0.56
4:K:30:LEU:HD23	4:K:63:TRP:HB3	1.86	0.56
6:R:5:DA:H1'	6:R:6:DC:H5'	1.87	0.56
1:A:40:LEU:O	1:A:44:LEU:HB2	2.06	0.56
2:C:202:TYR:HD1	2:C:206:THR:HG21	1.70	0.56
1:H:197:LEU:HG	1:H:199:ILE:HG13	1.88	0.56
2:I:15:LEU:HD11	2:I:457:ALA:HB1	1.87	0.56
6:O:21:DG:H1'	6:O:22:DT:H5''	1.88	0.56
1:A:13:ALA:HB3	1:B:228:PRO:HB3	1.87	0.56
2:C:831:ARG:HD3	2:C:1002:GLU:HG2	1.88	0.56
2:C:567:GLN:O	2:C:998:TYR:N	2.39	0.56
3:D:585:GLY:HA3	3:D:590:PRO:HG3	1.88	0.56
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.88	0.56
2:I:211:LEU:HB3	2:I:218:VAL:HG13	1.87	0.56
3:J:529:GLN:HA	3:J:535:PHE:HA	1.87	0.56
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.88	0.55
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.41	0.55
3:D:784:ASP:HA	3:D:787:LEU:HD23	1.88	0.55
3:D:9:ARG:HG2	3:D:10:ILE:N	2.21	0.55
6:O:11:DG:N2	7:P:16:DC:O2	2.39	0.55
1:B:68:ILE:HD12	1:B:69:PRO:HD2	1.88	0.55
2:I:975:TYR:HA	2:I:982:PRO:HA	1.88	0.55
7:S:2:DA:H1'	7:S:3:DG:H5'	1.88	0.55
1:B:197:LEU:HG	1:B:199:ILE:HG13	1.88	0.55
2:C:432:ARG:HH12	2:C:518:ARG:HE	1.53	0.55
2:C:328:LEU:HD21	2:C:434:HIS:HA	1.89	0.55
3:D:326:GLU:HB3	3:D:331:VAL:HG23	1.89	0.55
3:D:708:LEU:HG	3:D:709:HIS:H	1.70	0.55
3:D:947:ILE:HG22	3:D:1019:PRO:HB3	1.88	0.55
3:J:1166:LEU:H	3:J:1166:LEU:HD12	1.70	0.55
2:C:168:ARG:HD3	2:C:268:ASP:HB2	1.88	0.55
3:D:238:PRO:HB3	3:D:315:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.86	0.55
3:D:101:HIS:NE2	3:D:582:ILE:HG21	2.20	0.55
3:D:683:ILE:HG22	3:D:687:VAL:HG21	1.89	0.55
3:D:699:VAL:HG22	3:D:760:ARG:HG2	1.88	0.55
3:D:1216:SER:HB2	4:E:15:SER:HB2	1.87	0.55
1:B:182:GLU:HG3	1:B:194:LYS:HB3	1.89	0.55
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.07	0.55
3:D:875:THR:HG21	3:D:879:ARG:HG2	1.89	0.55
3:J:780:LYS:HB2	3:J:908:LYS:HZ1	1.72	0.55
1:A:178:ALA:HB3	1:A:198:ARG:HG3	1.89	0.55
1:G:54:THR:HG22	1:G:158:ILE:HD11	1.88	0.55
1:H:68:ILE:HD12	1:H:69:PRO:HD2	1.88	0.55
2:I:1018:GLN:HB3	2:I:1063:ARG:NH1	2.22	0.55
2:I:852:ILE:HG22	2:I:853:LEU:H	1.71	0.55
3:J:1331:ASP:O	3:J:1335:LEU:HD23	2.07	0.55
3:D:1380:GLU:HB3	3:D:1420:LEU:HD13	1.89	0.55
3:D:27:GLU:H	3:D:42:ASP:HB3	1.72	0.55
2:I:448:ASN:HA	2:I:451:LEU:HD22	1.89	0.55
3:J:400:VAL:HB	3:J:443:VAL:HG21	1.88	0.55
3:J:477:LEU:HD21	3:J:495:ARG:HD3	1.87	0.55
3:J:784:ASP:HA	3:J:787:LEU:HD23	1.89	0.55
3:D:973:GLN:HG3	3:J:831:GLY:HA2	1.89	0.55
3:J:843:PHE:HB2	3:J:866:VAL:HG23	1.87	0.55
3:J:911:LEU:O	3:J:915:VAL:HG23	2.05	0.55
2:C:48:PHE:O	2:C:52:PHE:HB2	2.07	0.55
2:C:123:GLU:HG2	2:C:592:LEU:HD13	1.87	0.55
2:C:668:LEU:HB3	2:C:995:MET:CG	2.37	0.55
3:D:1386:ASP:OD1	3:D:1386:ASP:N	2.39	0.55
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.89	0.55
2:I:712:ALA:HB3	2:I:820:ARG:HB2	1.89	0.55
6:R:12:DT:H1'	6:R:13:DG:H5'	1.89	0.55
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.70	0.55
3:D:238:PRO:HD3	3:D:318:THR:HG22	1.88	0.55
1:G:178:ALA:HB3	1:G:198:ARG:HG3	1.88	0.55
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.06	0.55
3:J:1345:GLU:HG2	3:J:1376:LEU:HD21	1.89	0.55
3:J:630:VAL:HG22	3:J:631:ILE:H	1.72	0.55
4:K:45:ARG:HD2	4:K:63:TRP:CH2	2.42	0.55
2:C:852:ILE:HG22	2:C:853:LEU:H	1.72	0.55
2:C:858:MET:H	2:C:977:GLY:HA3	1.72	0.55
3:D:31:THR:HG21	5:F:272:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:ILE:HG23	1:H:163:ASN:H	1.71	0.55
2:I:408:ARG:NH1	2:I:455:LEU:O	2.39	0.55
2:I:504:GLU:HG2	2:I:509:ALA:HB2	1.89	0.55
3:J:31:THR:HG21	5:L:272:THR:HG22	1.89	0.55
7:S:5:DA:H1'	7:S:6:DC:H5'	1.89	0.55
1:B:111:ALA:HB2	1:B:127:LEU:HB3	1.87	0.54
3:D:630:VAL:HG22	3:D:631:ILE:H	1.72	0.54
2:I:202:TYR:HD1	2:I:206:THR:HG21	1.72	0.54
3:J:708:LEU:HD12	3:J:1231:GLU:HG2	1.89	0.54
3:J:875:THR:HG21	3:J:879:ARG:HG2	1.89	0.54
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.89	0.54
6:R:4:DG:H1	7:S:23:DC:H42	1.55	0.54
1:A:101:LEU:HB3	1:A:140:MET:HB3	1.89	0.54
2:C:537:LYS:HD2	2:C:583:LEU:HD21	1.89	0.54
3:D:1470:ARG:HG2	3:D:1471:LEU:H	1.72	0.54
3:D:371:ILE:HG21	5:F:247:ARG:NH2	2.22	0.54
2:C:713:ARG:HD3	3:D:532:GLY:H	1.71	0.54
2:I:1103:ASP:OD1	2:I:1103:ASP:N	2.40	0.54
3:J:371:ILE:HG21	5:L:247:ARG:NH2	2.21	0.54
1:B:162:ILE:HG23	1:B:163:ASN:H	1.71	0.54
2:C:90:TYR:O	2:C:119:PRO:HA	2.08	0.54
2:C:798:GLY:HA2	2:C:829:GLN:HB3	1.89	0.54
3:D:371:ILE:HG21	5:F:247:ARG:HH22	1.72	0.54
3:J:684:LYS:HD3	3:J:685:ASP:H	1.72	0.54
2:C:194:VAL:HG23	2:C:195:LEU:HD12	1.88	0.54
2:I:168:ARG:HD3	2:I:268:ASP:HB2	1.89	0.54
2:I:754:ILE:HA	2:I:791:ARG:HA	1.88	0.54
3:J:119:SER:HB3	3:J:122:GLU:HG2	1.90	0.54
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.89	0.54
2:C:1103:ASP:OD1	2:C:1103:ASP:N	2.40	0.54
2:C:712:ALA:HB3	2:C:820:ARG:HB2	1.90	0.54
3:D:241:VAL:HG13	3:D:312:ARG:HG2	1.89	0.54
3:D:569:ASN:HA	3:D:572:ARG:NH2	2.22	0.54
2:I:149:THR:HA	2:I:322:VAL:HG13	1.88	0.54
2:I:215:GLY:O	2:I:218:VAL:HG23	2.08	0.54
2:I:537:LYS:HD2	2:I:583:LEU:HD21	1.89	0.54
3:J:415:VAL:HG21	3:J:446:VAL:HG11	1.89	0.54
5:L:280:VAL:HA	5:L:283:ILE:HD12	1.90	0.54
1:B:13:ALA:HB1	1:B:23:PHE:HD1	1.73	0.54
2:C:141:HIS:NE2	2:C:334:ARG:HD3	2.23	0.54
2:C:215:GLY:O	2:C:218:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:754:ILE:HG22	2:C:755:LEU:H	1.72	0.54
3:D:547:LEU:HD13	3:D:578:VAL:HG22	1.88	0.54
1:H:156:HIS:NE2	1:H:167:VAL:O	2.37	0.54
2:I:969:LEU:HG	3:J:952:ASP:HB2	1.90	0.54
3:J:1274:ILE:HG22	3:J:1324:PRO:HA	1.89	0.54
3:J:1377:LYS:O	3:J:1397:LYS:N	2.40	0.54
5:L:353:LEU:HD12	5:L:354:PRO:HD2	1.90	0.54
5:L:380:GLU:O	5:L:384:LEU:HB2	2.08	0.54
2:C:146:VAL:HG21	2:C:281:LEU:HD21	1.89	0.54
2:C:115:LEU:HB3	2:C:378:LEU:HD23	1.90	0.54
2:C:754:ILE:HA	2:C:791:ARG:HA	1.90	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HD12	1.90	0.54
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.43	0.54
3:D:102:ILE:HD11	3:D:587:ARG:HB2	1.89	0.54
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.72	0.54
5:F:154:ALA:O	5:F:158:LYS:HB2	2.07	0.54
5:F:376:LEU:HB2	5:F:381:ALA:HB2	1.89	0.54
1:H:62:LEU:HB3	1:H:163:ASN:ND2	2.23	0.54
2:I:343:GLN:HG3	2:I:385:PHE:HB2	1.89	0.54
3:J:1279:GLY:O	3:J:1319:VAL:HG22	2.08	0.54
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.89	0.54
3:D:147:VAL:HG21	3:D:153:LEU:HD21	1.89	0.54
3:D:233:LYS:HE3	3:D:234:GLU:H	1.72	0.54
2:I:1069:ALA:HB3	2:I:1076:VAL:HG12	1.88	0.54
2:I:194:VAL:HG23	2:I:195:LEU:HD12	1.90	0.54
3:J:423:ASP:HB2	3:J:427:VAL:HG12	1.89	0.54
2:C:206:THR:HG23	2:C:209:ARG:CZ	2.38	0.54
2:C:468:ARG:HD3	2:C:487:THR:HG22	1.90	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.90	0.54
3:D:614:PHE:O	3:D:619:LEU:HB2	2.08	0.54
5:F:150:ILE:HG12	5:F:193:ARG:HH11	1.72	0.54
1:H:78:ILE:HD12	1:H:129:ILE:O	2.07	0.54
3:J:647:ARG:HH12	3:J:683:ILE:HD11	1.73	0.54
1:B:176:ARG:HH11	3:D:884:ARG:HH22	1.55	0.54
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.90	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.07	0.54
1:H:161:ARG:HG3	1:H:162:ILE:N	2.23	0.54
1:G:14:THR:OG1	1:H:231:SER:OG	2.23	0.54
2:I:1112:PHE:HB3	3:J:88:TYR:CD2	2.43	0.54
2:I:668:LEU:HB3	2:I:995:MET:CG	2.38	0.54
1:H:176:ARG:HH11	3:J:884:ARG:HH22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:413:ARG:HE	7:S:22:DT:H2'	1.72	0.54
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.43	0.53
3:D:11:ALA:HA	3:D:1451:ALA:HA	1.90	0.53
3:D:154:THR:HG22	3:D:157:GLU:HG2	1.90	0.53
3:J:572:ARG:CZ	5:L:98:GLN:HG2	2.38	0.53
5:L:376:LEU:HB2	5:L:381:ALA:HB2	1.90	0.53
2:C:146:VAL:HG21	2:C:281:LEU:HD11	1.89	0.53
2:C:64:LEU:HD22	2:C:359:MET:SD	2.47	0.53
2:C:668:LEU:HB3	2:C:995:MET:HG3	1.90	0.53
2:C:759:THR:HB	2:C:785:VAL:HG21	1.90	0.53
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.89	0.53
2:C:114:PHE:HE1	5:F:294:GLN:HE21	1.55	0.53
1:G:63:HIS:HA	1:G:165:ILE:HD11	1.88	0.53
2:I:679:PHE:H	2:I:683:ASN:HD21	1.56	0.53
2:I:950:LEU:HD21	2:I:952:LEU:HD22	1.90	0.53
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.89	0.53
2:I:1071:ILE:O	3:J:659:LYS:HG2	2.08	0.53
2:C:926:PHE:HE2	2:C:960:GLU:HG3	1.72	0.53
3:D:1122:LEU:HD23	3:D:1140:ILE:HD13	1.91	0.53
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.23	0.53
2:I:1103:ASP:HA	3:J:5:VAL:HA	1.91	0.53
2:I:457:ALA:HB3	2:I:538:GLN:HA	1.89	0.53
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.90	0.53
2:I:889:HIS:CE1	2:I:970:GLY:HA3	2.44	0.53
2:I:971:LYS:HB3	2:I:986:PRO:HB2	1.90	0.53
3:J:147:VAL:HG21	3:J:153:LEU:HD21	1.90	0.53
5:L:98:GLN:O	5:L:102:GLU:HG3	2.09	0.53
7:S:7:DA:H1'	7:S:8:DA:H5'	1.90	0.53
1:B:59:GLU:HG3	1:B:139:TYR:CD2	2.42	0.53
3:D:229:ALA:HB1	3:D:245:LEU:H	1.74	0.53
3:D:523:ASP:HA	3:D:526:PRO:HG3	1.90	0.53
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.44	0.53
5:F:207:LEU:O	5:F:211:VAL:HG23	2.08	0.53
2:I:754:ILE:HG22	2:I:755:LEU:H	1.72	0.53
2:I:759:THR:HB	2:I:785:VAL:HG21	1.91	0.53
2:I:943:VAL:HG21	2:I:973:VAL:HG13	1.90	0.53
2:C:1086:ARG:HH11	2:C:1086:ARG:HG3	1.74	0.53
2:C:408:ARG:NH1	2:C:455:LEU:O	2.41	0.53
5:F:145:VAL:HG21	5:F:174:VAL:HG11	1.91	0.53
1:H:77:GLU:HB2	3:J:872:ARG:HH21	1.74	0.53
2:I:1086:ARG:HG3	2:I:1086:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:432:ARG:HH12	2:I:518:ARG:HE	1.55	0.53
3:J:104:PHE:CD2	3:J:512:MET:HG3	2.43	0.53
2:C:584:GLU:CD	2:C:584:GLU:H	2.11	0.53
3:D:1114:THR:HG21	3:D:1193:THR:O	2.09	0.53
3:D:119:SER:HB3	3:D:122:GLU:HG2	1.91	0.53
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.91	0.53
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.72	0.53
2:I:48:PHE:O	2:I:52:PHE:HB2	2.09	0.53
3:J:140:ALA:HB1	3:J:161:LEU:HD23	1.91	0.53
3:J:175:VAL:HG13	3:J:193:PRO:HD2	1.91	0.53
3:J:947:ILE:HG22	3:J:1019:PRO:HB3	1.90	0.53
1:A:23:PHE:CE2	1:A:199:ILE:HD12	2.44	0.53
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.90	0.53
3:D:729:HIS:HB3	3:D:732:VAL:HG22	1.91	0.53
4:E:45:ARG:HD2	4:E:63:TRP:CH2	2.43	0.53
2:I:90:TYR:O	2:I:119:PRO:HA	2.07	0.53
2:I:328:LEU:HD21	2:I:434:HIS:HA	1.91	0.53
3:J:166:GLN:HB3	3:J:396:VAL:HG13	1.91	0.53
3:J:99:ALA:HB2	3:J:574:LEU:HD21	1.91	0.53
1:B:78:ILE:HD12	1:B:129:ILE:O	2.09	0.53
2:C:149:THR:HA	2:C:322:VAL:HG13	1.91	0.53
1:G:70:GLY:HA2	1:G:133:GLU:HG2	1.91	0.53
2:I:64:LEU:HD22	2:I:359:MET:SD	2.48	0.53
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.24	0.53
3:J:764:LEU:HD23	3:J:767:HIS:CD2	2.43	0.53
1:B:62:LEU:HB3	1:B:163:ASN:ND2	2.24	0.53
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.42	0.53
5:F:380:GLU:O	5:F:384:LEU:HB2	2.09	0.53
1:G:16:GLN:HB3	1:G:20:TYR:HB3	1.91	0.53
2:I:584:GLU:H	2:I:584:GLU:CD	2.12	0.53
3:J:131:LYS:HG3	3:J:153:LEU:O	2.09	0.53
3:J:704:ARG:NE	3:J:705:ALA:O	2.42	0.53
2:C:37:GLU:HG2	2:C:38:LYS:N	2.24	0.53
2:C:448:ASN:HA	2:C:451:LEU:HD22	1.90	0.53
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.09	0.53
3:D:205:TYR:CD1	3:D:390:PRO:HG2	2.44	0.53
3:D:704:ARG:NE	3:D:705:ALA:O	2.42	0.53
3:D:757:ALA:O	3:D:761:ILE:HG13	2.09	0.53
3:D:668:PRO:HB2	5:F:432:LYS:HD3	1.91	0.53
1:G:27:PRO:HB3	1:G:186:LEU:O	2.09	0.53
2:I:577:PRO:HG2	2:I:580:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:683:ILE:HG22	3:J:687:VAL:HG21	1.91	0.53
5:L:154:ALA:O	5:L:158:LYS:HB2	2.08	0.53
1:A:72:LYS:HG3	2:C:641:PRO:HB2	1.91	0.52
5:F:137:LEU:HD22	5:F:178:LEU:HD11	1.91	0.52
2:I:206:THR:HG23	2:I:209:ARG:CZ	2.39	0.52
3:J:1293:PHE:HA	3:J:1302:GLU:HA	1.89	0.52
5:L:207:LEU:O	5:L:211:VAL:HG23	2.09	0.52
3:D:104:PHE:HB3	3:D:111:LYS:HB2	1.91	0.52
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.92	0.52
1:G:53:VAL:HA	1:G:144:VAL:HG22	1.90	0.52
3:J:1107:VAL:HG13	3:J:1200:VAL:HG23	1.91	0.52
1:B:45:LEU:HD21	1:B:177:VAL:HG22	1.91	0.52
2:C:162:ILE:HB	2:C:172:ILE:HB	1.92	0.52
2:C:304:LEU:HB2	2:C:305:PRO:HD3	1.92	0.52
2:C:851:LYS:HG2	2:C:852:ILE:H	1.75	0.52
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.75	0.52
3:D:264:LEU:HG	3:D:316:HIS:CE1	2.45	0.52
1:B:77:GLU:HB2	3:D:872:ARG:NH2	2.25	0.52
3:D:780:LYS:HB3	3:D:912:LYS:HZ1	1.74	0.52
3:J:154:THR:HG22	3:J:157:GLU:HG2	1.91	0.52
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.92	0.52
3:J:928:ALA:HA	3:J:931:LEU:HD12	1.92	0.52
3:J:968:ASP:OD1	3:J:1058:ARG:NH2	2.43	0.52
3:D:831:GLY:HA3	3:J:977:ALA:HB2	1.91	0.52
2:C:135:VAL:HG13	2:C:393:GLN:HG3	1.91	0.52
5:F:280:VAL:HA	5:F:283:ILE:HD12	1.91	0.52
2:I:468:ARG:HD3	2:I:487:THR:HG22	1.92	0.52
2:I:708:TYR:HE1	2:I:827:VAL:HB	1.75	0.52
3:J:1156:LEU:HD21	3:J:1177:ALA:HA	1.92	0.52
1:A:16:GLN:HB3	1:A:20:TYR:HB3	1.90	0.52
1:B:161:ARG:HG3	1:B:162:ILE:N	2.24	0.52
2:I:162:ILE:HB	2:I:172:ILE:HB	1.91	0.52
3:J:1470:ARG:HG2	3:J:1471:LEU:H	1.73	0.52
3:J:162:ARG:O	3:J:414:ARG:NH2	2.36	0.52
3:J:657:LEU:HG	3:J:661:MET:SD	2.49	0.52
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.91	0.52
2:C:290:LEU:HB3	2:C:303:PHE:CE1	2.45	0.52
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.91	0.52
2:C:798:GLY:HA3	2:C:827:VAL:HG13	1.91	0.52
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.45	0.52
3:D:1491:THR:HG22	4:E:92:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:304:LEU:HB2	2:I:305:PRO:HD3	1.92	0.52
1:A:27:PRO:HB3	1:A:186:LEU:O	2.09	0.52
3:D:348:ALA:HB1	3:D:349:PRO:HD2	1.92	0.52
3:D:650:LEU:HD11	3:D:688:TRP:CZ3	2.45	0.52
5:F:387:ARG:HD3	5:F:401:VAL:HG21	1.90	0.52
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.45	0.52
2:I:115:LEU:HB3	2:I:378:LEU:HD23	1.91	0.52
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.91	0.52
2:I:851:LYS:HG2	2:I:852:ILE:H	1.74	0.52
3:J:1344:VAL:O	3:J:1348:LEU:HG	2.10	0.52
3:J:791:TYR:CZ	3:J:945:SER:HB3	2.45	0.52
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.91	0.52
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.92	0.52
3:D:224:ARG:HB3	3:D:251:PHE:CE2	2.44	0.52
3:D:477:LEU:HD21	3:D:495:ARG:HD3	1.91	0.52
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.92	0.52
2:I:37:GLU:HG2	2:I:38:LYS:N	2.25	0.52
7:P:18:DT:H1'	7:P:19:DT:H5'	1.92	0.52
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.91	0.52
2:C:674:VAL:O	2:C:989:VAL:HA	2.10	0.52
2:C:940:GLU:HA	2:C:973:VAL:HG11	1.91	0.52
2:C:848:VAL:CG2	3:D:740:PHE:HB3	2.40	0.52
1:H:100:ILE:HD12	1:H:141:GLU:HG2	1.91	0.52
3:J:413:ASP:O	3:J:435:VAL:HG12	2.09	0.52
3:J:95:LEU:HG	3:J:574:LEU:HD11	1.91	0.52
3:J:757:ALA:O	3:J:761:ILE:HG13	2.10	0.52
1:B:156:HIS:NE2	1:B:167:VAL:O	2.38	0.52
2:C:211:LEU:HB3	2:C:218:VAL:HG13	1.91	0.52
2:C:484:VAL:HG12	2:C:486:MET:H	1.75	0.52
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.74	0.52
2:C:950:LEU:HD21	2:C:952:LEU:HD22	1.92	0.52
2:C:976:ASP:O	2:C:980:GLY:N	2.43	0.52
3:D:299:GLU:CD	3:D:300:VAL:H	2.13	0.52
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.91	0.52
2:I:1083:GLU:OE2	3:J:87:ARG:NH1	2.43	0.52
2:I:135:VAL:HG11	2:I:406:HIS:CE1	2.45	0.52
2:I:195:LEU:HA	2:I:198:ARG:HD3	1.92	0.52
2:I:146:VAL:HG21	2:I:281:LEU:HD11	1.92	0.52
3:J:542:ASP:OD1	3:J:545:ARG:NH2	2.43	0.52
2:C:756:VAL:O	2:C:789:SER:HB2	2.11	0.51
3:D:1261:GLU:OE2	3:D:1268:PRO:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:VAL:HG22	3:D:1326:THR:HG23	1.93	0.51
3:D:140:ALA:HB1	3:D:161:LEU:HD23	1.91	0.51
1:H:111:ALA:HB2	1:H:127:LEU:HB3	1.91	0.51
2:I:177:GLU:HG3	2:I:178:ALA:N	2.25	0.51
2:I:756:VAL:O	2:I:789:SER:HB2	2.09	0.51
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.44	0.51
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.09	0.51
3:D:71:LYS:O	3:D:80:VAL:HG12	2.10	0.51
2:I:940:GLU:HA	2:I:973:VAL:HG11	1.92	0.51
3:J:421:LEU:HD13	3:J:444:VAL:HB	1.92	0.51
2:C:969:LEU:HG	3:D:952:ASP:HB2	1.92	0.51
3:D:708:LEU:H	3:D:708:LEU:HD23	1.76	0.51
3:D:894:LYS:HG3	3:D:895:VAL:H	1.75	0.51
3:D:938:GLY:HA2	3:D:941:LEU:HD12	1.91	0.51
5:F:249:LYS:HG2	6:O:29:DC:OP2	2.10	0.51
5:F:353:LEU:HD12	5:F:354:PRO:HD2	1.91	0.51
2:I:135:VAL:HG13	2:I:393:GLN:HG3	1.92	0.51
2:I:136:ILE:HA	2:I:391:LEU:O	2.10	0.51
3:J:938:GLY:HA2	3:J:941:LEU:HD12	1.91	0.51
7:P:5:DA:H1'	7:P:6:DC:H5'	1.92	0.51
2:C:1103:ASP:HA	3:D:5:VAL:HA	1.92	0.51
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.92	0.51
2:C:881:ASN:O	2:C:883:GLY:N	2.44	0.51
3:D:131:LYS:HG3	3:D:153:LEU:O	2.10	0.51
3:D:572:ARG:CZ	5:F:98:GLN:HG2	2.40	0.51
1:G:87:VAL:HG11	1:G:144:VAL:HG11	1.92	0.51
2:I:876:VAL:HG13	2:I:884:GLN:HE21	1.76	0.51
2:I:770:GLU:HG2	5:L:366:SER:HA	1.92	0.51
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.93	0.51
3:D:1318:TYR:N	3:J:1157:GLY:O	2.43	0.51
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.45	0.51
3:J:1376:LEU:HA	3:J:1420:LEU:O	2.11	0.51
3:J:415:VAL:HG22	3:J:433:GLY:O	2.10	0.51
1:A:53:VAL:HA	1:A:144:VAL:HG22	1.92	0.51
2:C:408:ARG:HD3	2:C:542:LEU:HD21	1.92	0.51
3:D:122:GLU:HB2	3:D:152:LEU:HD21	1.93	0.51
2:I:141:HIS:NE2	2:I:334:ARG:HD3	2.25	0.51
2:I:18:LEU:H	2:I:18:LEU:HD22	1.75	0.51
2:I:290:LEU:HB3	2:I:303:PHE:CE1	2.45	0.51
2:I:484:VAL:HG12	2:I:486:MET:H	1.75	0.51
3:J:729:HIS:HB3	3:J:732:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:110:THR:HG22	5:L:111:LEU:H	1.75	0.51
5:L:137:LEU:HD22	5:L:178:LEU:HD11	1.93	0.51
1:B:181:VAL:HG12	1:B:195:LEU:HB2	1.93	0.51
2:C:637:PHE:HA	2:C:659:PRO:HG3	1.93	0.51
2:C:557:ARG:HB2	2:C:881:ASN:HD21	1.74	0.51
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.91	0.51
3:D:264:LEU:HG	3:D:316:HIS:NE2	2.26	0.51
4:E:34:ARG:HH21	4:E:94:PRO:HG2	1.76	0.51
2:I:1035:MET:HB2	3:J:707:THR:HB	1.92	0.51
2:I:195:LEU:HD23	2:I:238:LEU:HG	1.91	0.51
3:J:1110:ALA:O	3:J:1202:GLN:HB2	2.10	0.51
5:L:145:VAL:HG21	5:L:174:VAL:HG11	1.92	0.51
2:I:114:PHE:HE1	5:L:294:GLN:HE21	1.57	0.51
2:C:598:GLU:HG2	2:C:615:TYR:CZ	2.46	0.51
3:D:1170:ASP:O	3:D:1174:LEU:HG	2.11	0.51
3:D:1202:GLN:NE2	3:D:1217:ILE:HG12	2.26	0.51
3:J:773:ALA:HB2	3:J:1228:SER:HB3	1.93	0.51
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.11	0.51
5:L:218:THR:HA	5:L:227:LEU:HD11	1.93	0.51
5:L:380:GLU:HB2	5:L:419:ALA:HB2	1.93	0.51
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.92	0.51
2:C:198:ARG:HH22	2:C:238:LEU:HB2	1.75	0.51
2:C:436:GLY:HA2	2:C:538:GLN:O	2.11	0.51
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.91	0.51
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.75	0.51
2:C:9:ILE:HD12	2:C:907:ASP:HB2	1.92	0.51
3:D:1108:ARG:HB2	3:D:1108:ARG:NH1	2.26	0.51
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.92	0.51
5:F:110:THR:HG22	5:F:111:LEU:H	1.76	0.51
1:H:49:PRO:HA	1:H:147:GLY:O	2.10	0.51
2:I:831:ARG:HD3	2:I:1002:GLU:HG2	1.93	0.51
2:I:135:VAL:HG23	2:I:407:LYS:HG2	1.92	0.51
3:J:437:VAL:HG22	3:J:444:VAL:HG13	1.91	0.51
3:J:780:LYS:HB3	3:J:912:LYS:HZ1	1.76	0.51
3:D:1095:THR:HG22	3:D:1230:GLY:HA3	1.93	0.51
3:D:1135:ARG:HH21	3:D:1357:ARG:HH12	1.59	0.51
3:D:111:LYS:HD2	3:D:1452:ILE:HG13	1.93	0.51
3:D:647:ARG:HH12	3:D:683:ILE:HD11	1.76	0.51
5:F:412:ILE:HD13	5:F:415:ILE:HD12	1.93	0.51
2:I:277:ALA:HA	2:I:280:LYS:HD3	1.93	0.51
3:J:1047:LYS:HG2	3:J:1048:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:116:ASP:O	5:L:120:LYS:HG3	2.10	0.51
5:L:252:THR:HA	6:R:29:DC:H5	1.76	0.51
3:D:896:ALA:O	3:D:900:ILE:HG13	2.11	0.50
5:F:116:ASP:O	5:F:120:LYS:HG3	2.11	0.50
5:F:254:ALA:O	5:F:258:ILE:HG12	2.11	0.50
2:I:634:GLY:O	2:I:704:HIS:HA	2.11	0.50
3:J:1170:ASP:N	3:J:1170:ASP:OD2	2.43	0.50
1:B:149:GLY:O	1:B:171:PHE:HB2	2.12	0.50
1:A:14:THR:HG23	1:B:231:SER:O	2.11	0.50
2:C:408:ARG:HG2	2:C:455:LEU:HB3	1.93	0.50
3:D:1020:LEU:HD11	3:D:1035:ILE:HD12	1.94	0.50
3:D:657:LEU:HG	3:D:661:MET:SD	2.51	0.50
3:D:837:GLY:HA2	3:D:840:LYS:HB3	1.93	0.50
5:F:252:THR:OG1	6:O:28:DA:H2'	2.11	0.50
1:G:14:THR:HG23	1:H:231:SER:O	2.11	0.50
1:G:72:LYS:HG3	2:I:641:PRO:HB2	1.92	0.50
2:I:408:ARG:HD3	2:I:542:LEU:HD21	1.94	0.50
2:I:524:VAL:HG22	2:I:525:ALA:H	1.76	0.50
3:J:1344:VAL:HG12	3:J:1348:LEU:HD11	1.93	0.50
1:A:88:ARG:HD2	1:A:204:SER:O	2.11	0.50
2:C:18:LEU:HD22	2:C:18:LEU:H	1.76	0.50
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.94	0.50
3:D:1253:THR:HG22	3:D:1254:GLN:H	1.76	0.50
3:D:1343:ALA:HA	3:D:1346:ARG:HG3	1.94	0.50
5:F:410:GLU:O	5:F:413:ARG:HB3	2.10	0.50
1:G:20:TYR:HD2	1:G:21:GLY:H	1.59	0.50
1:H:45:LEU:HD21	1:H:177:VAL:HG22	1.94	0.50
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.93	0.50
2:I:683:ASN:HB2	2:I:872:ASN:H	1.77	0.50
2:I:668:LEU:HB3	2:I:995:MET:HG3	1.92	0.50
3:J:1285:GLU:HG2	3:J:1290:LEU:HG	1.93	0.50
3:J:420:VAL:HG22	3:J:421:LEU:O	2.11	0.50
3:J:479:GLU:O	3:J:482:LYS:HG2	2.12	0.50
4:K:34:ARG:HH21	4:K:94:PRO:HG2	1.75	0.50
5:L:165:LYS:HD2	5:L:165:LYS:H	1.76	0.50
1:B:100:ILE:HD12	1:B:141:GLU:HG2	1.94	0.50
1:H:182:GLU:HG3	1:H:194:LYS:HB3	1.93	0.50
1:G:218:LEU:HD21	1:H:222:LEU:HD22	1.94	0.50
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.93	0.50
2:I:706:GLU:HB3	2:I:708:TYR:CE1	2.46	0.50
3:J:543:LEU:HG	3:J:600:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:989:TYR:O	3:J:993:ILE:HB	2.11	0.50
1:B:89:PHE:HE1	1:B:97:THR:HG22	1.77	0.50
3:D:791:TYR:CZ	3:D:945:SER:HB3	2.47	0.50
2:I:501:THR:HG22	2:I:514:VAL:HG23	1.94	0.50
7:P:3:DG:H1'	7:P:4:DC:H5'	1.92	0.50
2:C:113:VAL:HG12	2:C:370:ALA:HA	1.94	0.50
2:C:403:SER:O	2:C:407:LYS:HE2	2.12	0.50
1:G:23:PHE:CE2	1:G:199:ILE:HD12	2.45	0.50
3:J:1231:GLU:HB3	3:J:1232:PRO:HD3	1.93	0.50
3:J:644:LEU:HG	3:J:649:ALA:HB2	1.93	0.50
3:J:654:LYS:O	3:J:658:LEU:HB2	2.11	0.50
3:J:650:LEU:HD11	3:J:688:TRP:CZ3	2.46	0.50
7:P:8:DA:H1'	7:P:9:DT:H5''	1.93	0.50
2:C:1112:PHE:HB3	3:D:88:TYR:CD2	2.46	0.50
2:C:195:LEU:HA	2:C:198:ARG:HD3	1.93	0.50
2:C:69:LEU:HG	2:C:98:LEU:HA	1.93	0.50
2:C:770:GLU:HG2	5:F:366:SER:HA	1.93	0.50
2:I:408:ARG:HG2	2:I:455:LEU:HB3	1.93	0.50
3:J:1425:THR:HG22	3:J:1429:LEU:HD12	1.94	0.50
5:L:431:ARG:HG2	5:L:431:ARG:O	2.12	0.50
1:B:29:GLU:HB3	1:B:32:PHE:CD1	2.47	0.50
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.92	0.50
3:D:112:ILE:HD12	3:D:113:GLY:N	2.27	0.50
3:D:1473:PRO:O	3:D:1478:SER:HA	2.11	0.50
2:I:173:ASP:O	2:I:184:MET:HG3	2.11	0.50
3:J:631:ILE:HD11	3:J:739:ASP:O	2.12	0.50
1:B:49:PRO:HA	1:B:147:GLY:O	2.12	0.50
2:C:177:GLU:HG3	2:C:178:ALA:N	2.27	0.50
2:C:23:VAL:HA	2:C:121:MET:SD	2.52	0.50
2:C:627:ARG:HD2	2:C:639:GLN:H	1.76	0.50
2:C:736:ASP:HB3	2:C:744:ARG:HG3	1.93	0.50
2:C:885:ILE:HG22	2:C:889:HIS:CD2	2.47	0.50
3:D:527:MET:HG3	3:D:537:THR:HB	1.92	0.50
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.94	0.50
1:H:149:GLY:O	1:H:171:PHE:HB2	2.11	0.50
2:I:387:SER:HB2	2:I:388:ARG:NH1	2.27	0.50
2:I:704:HIS:HD2	2:I:831:ARG:HD2	1.75	0.50
2:I:881:ASN:O	2:I:883:GLY:N	2.45	0.50
3:J:894:LYS:HG3	3:J:895:VAL:H	1.76	0.50
3:J:896:ALA:O	3:J:900:ILE:HG13	2.12	0.50
1:B:97:THR:OG1	1:B:98:THR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:ASN:O	2:C:451:LEU:HB2	2.12	0.49
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.94	0.49
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.93	0.49
3:D:274:GLN:HG3	3:D:279:VAL:HG21	1.94	0.49
3:D:317:MET:SD	3:D:337:LEU:HD22	2.52	0.49
1:G:56:VAL:HG21	1:G:82:LEU:HD13	1.94	0.49
2:I:537:LYS:HE3	2:I:583:LEU:HD11	1.94	0.49
2:I:729:LEU:HD12	2:I:734:LEU:HD13	1.94	0.49
3:J:1225:ALA:O	3:J:1229:ILE:HG13	2.12	0.49
3:J:402:PRO:HA	3:J:443:VAL:HA	1.93	0.49
2:I:1085:PHE:HA	3:J:618:LEU:HD21	1.94	0.49
2:I:848:VAL:HG11	3:J:630:VAL:HG21	1.94	0.49
1:H:77:GLU:HB2	3:J:872:ARG:NH2	2.26	0.49
6:R:7:DA:H61	7:S:20:DT:H3	1.60	0.49
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.94	0.49
2:C:37:GLU:HG2	2:C:38:LYS:H	1.77	0.49
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.24	0.49
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.94	0.49
3:D:1110:ALA:O	3:D:1202:GLN:HB2	2.12	0.49
3:D:1264:GLU:OE1	3:D:1425:THR:OG1	2.29	0.49
3:D:176:ASP:HA	3:D:389:GLU:HA	1.94	0.49
3:D:112:ILE:HG23	3:D:512:MET:SD	2.52	0.49
3:D:815:ALA:HA	3:D:818:ARG:HE	1.77	0.49
1:H:159:LYS:HA	1:H:164:ALA:HB3	1.94	0.49
2:I:976:ASP:O	2:I:980:GLY:N	2.44	0.49
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.47	0.49
1:A:63:HIS:HA	1:A:165:ILE:HD11	1.94	0.49
1:A:218:LEU:HD21	1:B:222:LEU:HD22	1.95	0.49
2:C:1083:GLU:O	2:C:1087:VAL:HG23	2.11	0.49
2:C:581:THR:OG1	2:C:584:GLU:OE2	2.30	0.49
3:D:18:ILE:HG12	3:D:518:PRO:HG3	1.94	0.49
5:F:209:LEU:HB2	6:O:30:DT:C2	2.47	0.49
5:F:289:THR:O	5:F:293:LEU:HG	2.12	0.49
3:J:650:LEU:HD21	3:J:683:ILE:HG21	1.94	0.49
3:J:711:LEU:HB3	3:J:735:ALA:HB1	1.94	0.49
2:I:848:VAL:CG2	3:J:740:PHE:HB3	2.41	0.49
2:C:277:ALA:HA	2:C:280:LYS:HD3	1.94	0.49
2:C:390:GLN:HG2	2:C:415:PRO:HD3	1.94	0.49
3:D:111:LYS:O	3:D:115:LEU:HB2	2.12	0.49
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.94	0.49
2:I:1083:GLU:O	2:I:1087:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.94	0.49
2:C:501:THR:HG22	2:C:514:VAL:HG23	1.94	0.49
2:C:707:ARG:HB2	2:C:707:ARG:HH11	1.78	0.49
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.94	0.49
3:D:644:LEU:HG	3:D:649:ALA:HB2	1.95	0.49
3:D:849:ALA:O	3:D:853:VAL:HG23	2.13	0.49
4:E:19:LEU:O	4:E:23:VAL:HG23	2.13	0.49
1:G:35:THR:HG23	1:H:42:ARG:HB2	1.94	0.49
2:I:588:VAL:HG21	2:I:664:GLY:HA2	1.93	0.49
3:J:132:TYR:HA	3:J:456:MET:HB3	1.94	0.49
2:C:1007:ALA:HB1	3:D:652:LEU:HD13	1.94	0.49
2:C:607:ASP:C	2:C:609:THR:H	2.15	0.49
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.27	0.49
3:D:245:LEU:CB	3:D:309:GLY:HA2	2.41	0.49
3:D:638:LYS:HG3	3:D:639:LEU:N	2.27	0.49
2:I:64:LEU:HD21	2:I:66:LEU:HB2	1.95	0.49
3:J:214:ASP:HA	3:J:342:PRO:HA	1.94	0.49
3:J:577:ALA:O	3:J:581:VAL:HG23	2.12	0.49
5:L:252:THR:HA	6:R:29:DC:C5	2.48	0.49
2:C:524:VAL:HG22	2:C:525:ALA:H	1.76	0.49
2:C:936:VAL:HB	2:C:941:LYS:HE2	1.95	0.49
3:D:471:GLU:O	3:D:474:GLU:HB3	2.12	0.49
5:F:149:LYS:HB2	5:F:193:ARG:HH12	1.78	0.49
2:I:598:GLU:HG2	2:I:615:TYR:CZ	2.47	0.49
2:I:9:ILE:HD12	2:I:907:ASP:HB2	1.94	0.49
3:J:1361:VAL:HG12	3:J:1363:LEU:H	1.78	0.49
5:L:241:LYS:HE2	6:R:24:DC:H3'	1.95	0.49
5:L:254:ALA:O	5:L:258:ILE:HG12	2.13	0.49
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.95	0.49
2:C:1067:TYR:O	2:C:1071:ILE:HB	2.12	0.49
2:C:729:LEU:HD12	2:C:734:LEU:HD13	1.94	0.49
3:D:1046:GLN:HE22	3:D:1079:LYS:HE2	1.78	0.49
3:D:1106:VAL:HB	3:D:1108:ARG:HH12	1.78	0.49
2:I:198:ARG:HH22	2:I:238:LEU:HB2	1.77	0.49
2:I:272:ALA:O	2:I:276:LYS:N	2.39	0.49
2:I:436:GLY:HA2	2:I:538:GLN:O	2.12	0.49
2:I:572:ILE:HD11	2:I:703:ILE:HG13	1.93	0.49
2:I:674:VAL:O	2:I:989:VAL:HA	2.12	0.49
2:C:65:VAL:HG12	2:C:101:ILE:HB	1.95	0.49
3:D:1131:THR:HA	3:J:1179:GLU:O	2.12	0.49
3:D:989:TYR:O	3:D:993:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.95	0.49
1:H:151:VAL:HG12	1:H:156:HIS:HD2	1.78	0.49
2:I:193:LEU:HA	2:I:196:LEU:HD13	1.94	0.49
3:J:815:ALA:HA	3:J:818:ARG:HE	1.78	0.49
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.95	0.49
5:L:238:ALA:HB2	5:L:257:TRP:HB2	1.95	0.49
5:L:387:ARG:HD3	5:L:401:VAL:HG21	1.95	0.49
5:L:412:ILE:O	5:L:416:GLU:HG2	2.13	0.49
1:A:87:VAL:HG11	1:A:144:VAL:HG11	1.95	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.13	0.49
3:D:1280:VAL:HG22	3:D:1295:GLU:O	2.12	0.49
3:D:1459:LEU:HD23	3:D:1470:ARG:HE	1.78	0.49
5:F:165:LYS:HD2	5:F:165:LYS:H	1.78	0.49
5:F:292:GLN:O	5:F:295:GLN:HG3	2.13	0.49
5:F:431:ARG:O	5:F:431:ARG:HG2	2.11	0.49
1:H:176:ARG:HG3	3:J:850:LEU:HD22	1.94	0.49
3:J:112:ILE:HD12	3:J:113:GLY:N	2.28	0.49
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.94	0.49
2:C:952:LEU:HD23	2:C:966:LEU:HD11	1.95	0.48
3:D:112:ILE:HD12	3:D:113:GLY:H	1.78	0.48
3:D:1377:LYS:O	3:D:1397:LYS:N	2.39	0.48
1:G:15:THR:O	1:H:232:LEU:HD23	2.13	0.48
2:I:497:ALA:HB3	2:I:532:MET:HG3	1.94	0.48
2:I:65:VAL:HG12	2:I:101:ILE:HB	1.95	0.48
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.78	0.48
3:J:638:LYS:HG3	3:J:639:LEU:N	2.28	0.48
3:J:927:THR:HA	3:J:930:LEU:HB3	1.95	0.48
5:L:124:GLY:O	5:L:128:ILE:HG13	2.13	0.48
5:L:336:ILE:HD11	5:L:344:TYR:HA	1.95	0.48
5:L:220:ARG:HH22	7:S:1:DT:H3'	1.78	0.48
3:D:1107:VAL:HG13	3:D:1200:VAL:HG23	1.95	0.48
3:D:1170:ASP:N	3:D:1170:ASP:OD2	2.43	0.48
3:D:974:ILE:HG22	3:D:988:ARG:HG3	1.94	0.48
2:I:22:GLN:HA	2:I:336:VAL:HG21	1.95	0.48
2:I:736:ASP:HB3	2:I:744:ARG:HG3	1.94	0.48
2:I:751:PRO:HB3	2:I:794:PRO:HA	1.94	0.48
3:J:122:GLU:O	3:J:126:VAL:HG23	2.12	0.48
3:J:666:PHE:CE1	3:J:687:VAL:HG12	2.48	0.48
3:J:702:LEU:HD12	3:J:746:ALA:O	2.12	0.48
5:F:241:LYS:HE2	6:O:24:DC:H3'	1.96	0.48
2:C:11:GLU:HG3	2:C:535:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:410:ILE:O	2:C:452:ILE:HA	2.13	0.48
1:A:63:HIS:HB3	2:C:746:GLY:HA3	1.95	0.48
5:F:336:ILE:HD11	5:F:344:TYR:HA	1.94	0.48
2:I:713:ARG:NH1	3:J:533:GLY:HA2	2.28	0.48
7:P:8:DA:C2'	7:P:9:DT:H5''	2.44	0.48
1:B:151:VAL:HG12	1:B:156:HIS:HD2	1.79	0.48
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.95	0.48
3:D:397:LYS:HE2	3:D:448:GLU:HB3	1.94	0.48
3:D:806:PHE:CD1	3:D:811:GLU:HB3	2.48	0.48
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.46	0.48
2:I:885:ILE:HG22	2:I:889:HIS:CD2	2.49	0.48
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.94	0.48
3:J:15:PRO:HG3	3:J:514:LEU:HD12	1.95	0.48
3:J:71:LYS:O	3:J:80:VAL:HG12	2.13	0.48
6:O:14:DT:H1'	6:O:15:DT:H5'	1.95	0.48
6:R:7:DA:H1'	6:R:8:DA:H5'	1.94	0.48
1:B:176:ARG:HG3	3:D:850:LEU:HD22	1.94	0.48
2:C:1035:MET:HB2	3:D:707:THR:HB	1.94	0.48
2:C:135:VAL:HG11	2:C:406:HIS:CE1	2.48	0.48
2:C:816:LYS:HG3	2:C:817:PRO:HD2	1.94	0.48
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.49	0.48
3:D:780:LYS:HB2	3:D:908:LYS:HZ1	1.79	0.48
1:G:36:LEU:O	1:G:39:PRO:HD2	2.14	0.48
1:H:156:HIS:ND1	1:H:156:HIS:O	2.46	0.48
2:I:1112:PHE:HB2	2:I:1115:LEU:HB2	1.96	0.48
2:I:11:GLU:HG3	2:I:535:SER:HB2	1.94	0.48
2:I:572:ILE:HD12	2:I:572:ILE:H	1.77	0.48
2:I:69:LEU:HG	2:I:98:LEU:HA	1.94	0.48
1:A:30:ARG:HG3	2:C:938:LYS:NZ	2.28	0.48
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.96	0.48
2:C:679:PHE:H	2:C:683:ASN:HD21	1.60	0.48
3:D:1065:LEU:HB3	3:D:1069:GLU:HB2	1.95	0.48
3:D:1098:LEU:HD11	3:D:1263:PHE:CD2	2.48	0.48
3:D:127:LEU:HD23	3:D:461:ILE:HG13	1.95	0.48
2:I:37:GLU:HG2	2:I:38:LYS:H	1.78	0.48
2:I:772:ARG:HG2	5:L:388:LYS:HD2	1.96	0.48
2:I:816:LYS:HG3	2:I:817:PRO:HD2	1.95	0.48
3:J:1283:ILE:HA	3:J:1292:VAL:HG22	1.96	0.48
3:J:122:GLU:HB2	3:J:152:LEU:HD21	1.95	0.48
3:J:716:PHE:CZ	3:J:728:LEU:HD11	2.48	0.48
3:J:699:VAL:HG22	3:J:760:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:862:ASP:O	3:J:876:SER:HA	2.13	0.48
3:J:25:GLU:HG2	3:J:93:ILE:HA	1.94	0.48
1:A:24:VAL:HA	1:A:195:LEU:O	2.14	0.48
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.95	0.48
2:C:71:TYR:HD1	2:C:94:LEU:HD11	1.78	0.48
2:C:848:VAL:HG11	3:D:630:VAL:HG21	1.95	0.48
3:D:103:TRP:HE3	3:D:1448:THR:HG23	1.77	0.48
3:D:521:PRO:HD2	3:D:524:LEU:HD12	1.95	0.48
1:B:187:GLY:H	4:E:51:LEU:HD11	1.79	0.48
2:I:1089:VAL:HG11	2:I:1112:PHE:HE2	1.78	0.48
3:J:1500:LYS:HA	3:J:1503:VAL:HG22	1.95	0.48
5:L:165:LYS:O	5:L:165:LYS:HG2	2.13	0.48
1:A:57:TYR:HB3	1:A:141:GLU:HG3	1.95	0.48
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.95	0.48
2:C:157:ARG:CZ	2:C:314:THR:HB	2.43	0.48
2:C:578:VAL:HG23	2:C:671:ASN:ND2	2.28	0.48
1:A:42:ARG:NH1	2:C:857:ASP:OD1	2.46	0.48
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.49	0.48
1:G:66:SER:O	1:G:75:VAL:HG23	2.14	0.48
2:I:432:ARG:HG3	2:I:432:ARG:H	1.48	0.48
2:I:448:ASN:O	2:I:451:LEU:HB2	2.14	0.48
3:J:123:LEU:HG	3:J:127:LEU:HD11	1.96	0.48
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.48	0.48
2:C:135:VAL:HG23	2:C:407:LYS:HG2	1.95	0.48
2:C:660:ALA:O	2:C:667:ALA:N	2.41	0.48
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	1.96	0.48
2:I:113:VAL:HG12	2:I:370:ALA:HA	1.96	0.48
2:I:627:ARG:HD2	2:I:639:GLN:H	1.79	0.48
2:I:941:LYS:HZ2	2:I:959:PRO:HG2	1.78	0.48
3:J:1127:GLU:HG3	3:J:1128:VAL:HG23	1.96	0.48
3:J:1473:PRO:O	3:J:1478:SER:HA	2.13	0.48
3:J:876:SER:O	3:J:879:ARG:HB3	2.14	0.48
2:C:173:ASP:O	2:C:184:MET:HG3	2.14	0.48
2:C:387:SER:HB2	2:C:388:ARG:NH1	2.29	0.48
2:C:399:ASN:HD21	2:C:566:THR:HA	1.79	0.48
2:C:714:ASP:HA	2:C:719:PRO:HA	1.95	0.48
3:D:862:ASP:O	3:D:876:SER:HA	2.14	0.48
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.95	0.48
4:E:26:ARG:O	4:E:30:LEU:HD13	2.14	0.48
5:F:165:LYS:O	5:F:165:LYS:HG2	2.14	0.48
1:G:42:ARG:NH2	1:H:31:GLY:O	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1047:HIS:HA	2:I:1050:GLN:HG2	1.94	0.48
2:I:798:GLY:HA3	2:I:827:VAL:CG1	2.43	0.48
1:G:42:ARG:NH1	2:I:857:ASP:OD1	2.47	0.48
7:P:10:DT:H1'	7:P:11:DT:H5'	1.96	0.48
1:A:36:LEU:O	1:A:39:PRO:HD2	2.14	0.47
2:C:572:ILE:HD12	2:C:572:ILE:H	1.79	0.47
3:D:46:ASP:O	3:D:50:PHE:HB2	2.14	0.47
3:D:638:LYS:HG2	3:D:640:HIS:CE1	2.49	0.47
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.49	0.47
1:G:88:ARG:HD2	1:G:204:SER:O	2.13	0.47
1:H:64:GLU:HG3	1:H:165:ILE:HG21	1.96	0.47
3:J:1335:LEU:HD12	3:J:1344:VAL:HG22	1.96	0.47
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.95	0.47
3:J:760:ARG:HH21	4:K:65:MET:HG3	1.79	0.47
5:L:178:LEU:HA	5:L:181:LEU:HD13	1.96	0.47
5:L:412:ILE:HD13	5:L:415:ILE:HD12	1.96	0.47
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.96	0.47
2:C:209:ARG:HG3	2:C:210:GLU:N	2.29	0.47
2:C:569:VAL:HB	2:C:635:THR:HG21	1.96	0.47
3:D:475:ARG:HA	3:D:478:LEU:HD12	1.96	0.47
2:I:1047:HIS:HA	2:I:1050:GLN:CG	2.43	0.47
2:I:22:GLN:HG3	2:I:407:LYS:HB3	1.96	0.47
2:I:607:ASP:C	2:I:609:THR:H	2.18	0.47
2:I:769:PRO:HG3	3:J:65:ARG:HH12	1.78	0.47
2:I:705:ILE:HG12	2:I:828:ALA:HB2	1.96	0.47
3:J:544:TYR:O	3:J:548:ILE:HG13	2.13	0.47
3:J:560:GLN:HE22	5:L:236:ILE:HD13	1.79	0.47
6:O:28:DA:H1'	6:O:29:DC:H5'	1.96	0.47
1:A:181:VAL:O	1:A:182:GLU:HG3	2.14	0.47
1:A:20:TYR:HD2	1:A:21:GLY:H	1.62	0.47
2:C:876:VAL:HG13	2:C:884:GLN:HE21	1.79	0.47
3:D:1225:ALA:HB1	3:D:1367:HIS:HB3	1.96	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.47
3:D:650:LEU:HD21	3:D:683:ILE:HG21	1.95	0.47
1:G:177:VAL:HG13	1:G:199:ILE:HG12	1.95	0.47
1:G:209:GLU:O	1:G:213:GLN:HG2	2.15	0.47
1:G:44:LEU:HD13	1:G:177:VAL:HG21	1.97	0.47
2:I:157:ARG:CZ	2:I:314:THR:HB	2.44	0.47
2:I:403:SER:O	2:I:407:LYS:HE2	2.13	0.47
2:I:410:ILE:O	2:I:452:ILE:HA	2.14	0.47
2:I:1085:PHE:HE2	3:J:1468:LEU:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:977:ALA:HB3	3:J:983:LEU:HD12	1.96	0.47
4:K:26:ARG:O	4:K:30:LEU:HD13	2.15	0.47
2:C:374:ASN:OD1	2:C:375:SER:N	2.47	0.47
2:C:700:TYR:HB3	2:C:833:LEU:HD13	1.96	0.47
3:D:1153:VAL:O	3:D:1159:ARG:HB2	2.14	0.47
3:D:1188:VAL:HG12	3:D:1189:ARG:N	2.30	0.47
3:D:250:LEU:HD23	3:D:306:GLU:HG3	1.96	0.47
3:D:517:VAL:O	3:D:519:VAL:HG23	2.15	0.47
1:G:41:ARG:HD3	1:G:45:LEU:HD11	1.96	0.47
2:I:209:ARG:HG3	2:I:210:GLU:N	2.29	0.47
3:J:131:LYS:HE2	3:J:152:LEU:HB3	1.96	0.47
3:J:708:LEU:H	3:J:708:LEU:HD23	1.79	0.47
5:L:117:LEU:O	5:L:121:VAL:HG23	2.15	0.47
2:C:578:VAL:HG13	2:C:900:ARG:HG2	1.97	0.47
3:D:1302:GLU:OE2	3:D:1304:LYS:HE3	2.14	0.47
3:D:841:PHE:CE2	3:D:858:LEU:HD13	2.50	0.47
3:D:918:ALA:O	3:D:922:LEU:HB2	2.15	0.47
3:D:971:LEU:HA	3:D:974:ILE:HD12	1.95	0.47
3:D:977:ALA:HB3	3:D:983:LEU:HD12	1.97	0.47
1:H:150:TYR:HD2	3:J:857:LEU:HD12	1.80	0.47
2:I:45:GLN:HE21	2:I:45:GLN:HA	1.79	0.47
2:I:570:PRO:HD2	2:I:635:THR:HG21	1.97	0.47
2:I:707:ARG:HB2	2:I:707:ARG:HH11	1.79	0.47
3:J:1114:THR:HG21	3:J:1193:THR:O	2.15	0.47
3:J:1151:ARG:HA	3:J:1162:GLU:HG3	1.96	0.47
3:J:1366:LYS:O	3:J:1370:ILE:HG13	2.14	0.47
3:J:9:ARG:HG2	3:J:10:ILE:N	2.28	0.47
3:J:1495:ILE:HD13	4:K:80:VAL:HB	1.95	0.47
5:L:286:LEU:HD23	5:L:310:MET:HG3	1.95	0.47
5:L:383:VAL:HG22	5:L:404:TYR:HE2	1.77	0.47
1:B:156:HIS:O	1:B:156:HIS:ND1	2.48	0.47
2:C:136:ILE:HA	2:C:391:LEU:O	2.14	0.47
2:C:64:LEU:HD21	2:C:66:LEU:HB2	1.95	0.47
2:C:772:ARG:HG2	5:F:388:LYS:HD2	1.96	0.47
3:D:1464:GLU:CD	3:D:1464:GLU:H	2.15	0.47
4:E:45:ARG:HD2	4:E:63:TRP:HH2	1.80	0.47
5:F:238:ALA:HB2	5:F:257:TRP:HB2	1.96	0.47
1:G:57:TYR:HB3	1:G:141:GLU:HG3	1.95	0.47
1:H:54:THR:OG1	1:H:55:SER:N	2.47	0.47
2:I:214:TYR:HB3	2:I:217:LEU:HD12	1.97	0.47
2:I:874:LEU:O	2:I:877:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1444:THR:O	3:J:1448:THR:OG1	2.33	0.47
3:J:849:ALA:O	3:J:853:VAL:HG23	2.13	0.47
2:C:1048:THR:O	2:C:1052:MET:HG2	2.15	0.47
2:C:888:THR:HG22	2:C:989:VAL:O	2.15	0.47
3:D:122:GLU:O	3:D:126:VAL:HG23	2.15	0.47
3:D:226:PRO:HD2	3:D:245:LEU:HD21	1.97	0.47
3:D:517:VAL:HG11	3:D:547:LEU:HD21	1.96	0.47
3:D:25:GLU:HA	3:D:92:HIS:O	2.14	0.47
1:H:187:GLY:H	4:K:51:LEU:HD11	1.79	0.47
1:H:34:VAL:HG11	2:I:978:ARG:HB3	1.97	0.47
2:I:754:ILE:HG12	2:I:791:ARG:HD3	1.95	0.47
2:I:71:TYR:HD1	2:I:94:LEU:HD11	1.79	0.47
3:J:135:LEU:O	3:J:453:ASP:HB3	2.14	0.47
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.97	0.47
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.14	0.47
3:D:1211:MET:HB3	3:D:1213:ARG:HG2	1.96	0.47
3:D:548:ILE:HG13	3:D:548:ILE:H	1.54	0.47
3:D:635:PRO:O	3:D:935:LYS:HE2	2.15	0.47
3:D:711:LEU:HB3	3:D:735:ALA:HB1	1.95	0.47
3:D:810:GLU:O	3:D:813:LEU:HB3	2.14	0.47
3:D:930:LEU:O	3:D:934:LEU:HD12	2.15	0.47
5:F:124:GLY:O	5:F:128:ILE:HG13	2.13	0.47
3:D:557:LEU:HD11	5:F:229:GLN:OE1	2.14	0.47
1:G:30:ARG:HG3	2:I:938:LYS:NZ	2.30	0.47
1:H:40:LEU:O	1:H:44:LEU:HB2	2.15	0.47
2:I:1088:LEU:O	2:I:1092:LEU:HG	2.15	0.47
2:I:952:LEU:HD23	2:I:966:LEU:HD11	1.96	0.47
3:J:1102:ALA:HB1	3:J:1222:GLY:C	2.35	0.47
3:J:1459:LEU:HB3	3:J:1465:ASN:ND2	2.30	0.47
3:J:46:ASP:O	3:J:50:PHE:HB2	2.13	0.47
3:J:698:LYS:HG3	4:K:59:ASN:ND2	2.29	0.47
6:O:5:DA:H1'	6:O:6:DC:H5'	1.96	0.47
7:S:21:DG:H1'	7:S:22:DT:H5'	1.97	0.47
1:B:159:LYS:HA	1:B:164:ALA:HB3	1.97	0.47
2:C:430:VAL:HG12	2:C:434:HIS:CD2	2.50	0.47
3:D:1135:ARG:NH2	3:D:1357:ARG:HH22	2.13	0.47
3:D:233:LYS:HB3	3:D:236:TYR:CE1	2.49	0.47
2:I:609:THR:O	2:I:625:LEU:HG	2.15	0.47
2:I:952:LEU:HD21	2:I:971:LYS:HZ2	1.80	0.47
3:J:1021:TYR:CE1	3:J:1025:GLN:HG3	2.50	0.47
3:J:486:ARG:HA	3:J:489:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:28:DA:H1'	6:R:29:DC:H5'	1.97	0.47
1:A:177:VAL:HG13	1:A:199:ILE:HG12	1.96	0.47
2:C:1019:GLN:OE1	2:C:1057:SER:OG	2.32	0.47
2:C:202:TYR:CD1	2:C:206:THR:HG21	2.50	0.47
2:C:111:ASP:HB3	2:C:369:PRO:HG2	1.97	0.47
2:C:456:ALA:HB1	2:C:538:GLN:O	2.15	0.47
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.96	0.47
3:D:1006:ALA:O	3:D:1010:ASN:HB2	2.15	0.47
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.48	0.47
1:G:35:THR:CG2	1:H:39:PRO:HA	2.45	0.47
2:I:1007:ALA:HB1	3:J:652:LEU:HD13	1.97	0.47
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.50	0.47
2:I:299:LYS:HG3	2:I:300:ASP:H	1.80	0.47
2:I:15:LEU:O	2:I:586:ARG:NH1	2.47	0.47
2:I:714:ASP:HA	2:I:719:PRO:HA	1.96	0.47
3:J:1209:LEU:H	3:J:1209:LEU:HD12	1.80	0.47
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.15	0.47
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.15	0.47
3:J:918:ALA:O	3:J:922:LEU:HB2	2.14	0.47
6:O:7:DA:N6	7:P:20:DT:H3	2.10	0.47
1:B:54:THR:HG22	1:B:143:ARG:O	2.15	0.47
2:C:1047:HIS:HA	2:C:1050:GLN:CG	2.45	0.47
2:C:118:LEU:HD13	2:C:382:LEU:HD23	1.96	0.47
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.43	0.47
2:C:676:ILE:HA	2:C:871:LEU:O	2.14	0.47
3:D:123:LEU:HG	3:D:127:LEU:HD11	1.96	0.47
3:D:1373:ARG:O	3:D:1377:LYS:HB3	2.14	0.47
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.30	0.47
3:D:632:VAL:O	3:D:727:GLN:HA	2.15	0.47
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.50	0.47
2:I:1048:THR:O	2:I:1052:MET:HG2	2.15	0.47
2:I:1047:HIS:O	2:I:1051:GLU:HG3	2.15	0.47
2:I:456:ALA:HB1	2:I:538:GLN:O	2.15	0.47
2:I:72:ARG:O	2:I:94:LEU:HD12	2.15	0.47
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.50	0.47
3:J:560:GLN:NE2	5:L:236:ILE:HG21	2.30	0.47
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.96	0.47
1:A:55:SER:CB	1:A:158:ILE:HG12	2.44	0.46
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.96	0.46
2:C:1083:GLU:HA	2:C:1086:ARG:HG3	1.97	0.46
2:C:537:LYS:HE3	2:C:583:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:720:GLU:HB2	2:C:759:THR:O	2.15	0.46
3:D:1197:ARG:HG3	3:D:1398:TRP:CG	2.50	0.46
1:G:24:VAL:HA	1:G:195:LEU:O	2.14	0.46
2:I:1083:GLU:HA	2:I:1086:ARG:HG3	1.96	0.46
3:J:514:LEU:HD21	3:J:518:PRO:HD3	1.96	0.46
3:J:930:LEU:O	3:J:934:LEU:HD12	2.15	0.46
3:J:996:TRP:CE2	3:J:1056:PRO:HD3	2.49	0.46
1:A:63:HIS:CD2	1:A:66:SER:HB2	2.50	0.46
2:C:1102:LEU:HA	2:C:1107:ASN:O	2.15	0.46
2:C:890:LEU:HD21	2:C:914:ILE:HG12	1.97	0.46
2:C:941:LYS:HZ2	2:C:959:PRO:HG2	1.81	0.46
3:D:1465:ASN:HA	3:D:1468:LEU:HB2	1.96	0.46
1:H:97:THR:OG1	1:H:98:THR:N	2.46	0.46
2:I:23:VAL:HA	2:I:121:MET:SD	2.54	0.46
3:J:1188:VAL:HG12	3:J:1189:ARG:H	1.80	0.46
4:K:46:PRO:HB2	4:K:57:ASP:HB3	1.98	0.46
7:S:3:DG:H1'	7:S:4:DC:H5'	1.97	0.46
1:A:190:THR:OG1	1:A:191:ASP:N	2.47	0.46
2:C:1047:HIS:HA	2:C:1050:GLN:HG2	1.97	0.46
2:C:397:GLU:HG3	2:C:632:ASN:HD22	1.80	0.46
2:C:532:MET:HG2	2:C:533:ASP:N	2.29	0.46
2:C:880:MET:CE	3:D:1037:GLN:HB2	2.46	0.46
2:C:537:LYS:NZ	2:C:905:VAL:H	2.02	0.46
3:D:1331:ASP:HA	3:D:1332:PRO:HD3	1.82	0.46
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.96	0.46
3:D:698:LYS:HG3	4:E:59:ASN:ND2	2.29	0.46
3:D:876:SER:O	3:D:879:ARG:HB3	2.15	0.46
1:G:35:THR:HG22	1:H:39:PRO:HA	1.97	0.46
1:H:59:GLU:HG3	1:H:139:TYR:CD2	2.47	0.46
2:I:578:VAL:HG23	2:I:671:ASN:ND2	2.29	0.46
2:I:971:LYS:HG2	2:I:988:VAL:HG12	1.98	0.46
3:J:1020:LEU:HD11	3:J:1035:ILE:HD12	1.95	0.46
2:C:886:LEU:HA	2:C:889:HIS:HB2	1.97	0.46
3:D:716:PHE:CZ	3:D:728:LEU:HD11	2.51	0.46
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.97	0.46
3:J:1364:HIS:NE2	3:J:1366:LYS:HE3	2.31	0.46
3:J:82:ARG:HB2	3:J:84:ILE:HG22	1.98	0.46
7:P:9:DT:H1'	7:P:10:DT:H5'	1.98	0.46
1:B:185:ARG:NH2	1:B:187:GLY:O	2.49	0.46
2:C:446:GLY:O	2:C:449:ILE:HG13	2.16	0.46
3:D:1166:LEU:H	3:D:1166:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:264:LEU:HG	3:D:316:HIS:HE2	1.80	0.46
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.96	0.46
5:F:413:ARG:NH1	5:F:414:GLN:HG2	2.31	0.46
3:J:592:THR:HB	3:J:598:ARG:O	2.14	0.46
6:R:14:DT:H1'	6:R:15:DT:H5'	1.97	0.46
1:B:89:PHE:CE1	1:B:97:THR:HG22	2.51	0.46
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.50	0.46
2:C:151:ASP:HB2	2:C:154:ARG:O	2.14	0.46
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.46
2:C:718:GLY:HA2	2:C:719:PRO:HD3	1.78	0.46
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.96	0.46
3:D:493:ARG:HH11	3:D:494:LYS:HE3	1.81	0.46
5:F:235:LEU:O	5:F:239:VAL:HG23	2.16	0.46
5:F:413:ARG:HD2	7:P:22:DT:H72	1.98	0.46
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.84	0.46
2:C:423:ALA:O	2:C:428:ARG:HG3	2.16	0.46
2:C:798:GLY:HA3	2:C:827:VAL:CG1	2.45	0.46
2:C:85:GLU:HA	2:C:824:ARG:HH22	1.79	0.46
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.16	0.46
2:C:1085:PHE:HE2	3:D:1468:LEU:HD22	1.81	0.46
3:D:927:THR:HA	3:D:930:LEU:HB3	1.97	0.46
5:F:178:LEU:HA	5:F:181:LEU:HD13	1.98	0.46
1:G:29:GLU:O	1:G:32:PHE:HB2	2.15	0.46
1:H:10:VAL:HG12	1:H:12:THR:HG23	1.98	0.46
1:H:54:THR:HG22	1:H:143:ARG:O	2.16	0.46
2:I:1056:LYS:O	3:J:624:ASP:N	2.35	0.46
3:J:1154:GLU:HG2	3:J:1159:ARG:HB3	1.98	0.46
3:J:1397:LYS:HA	3:J:1397:LYS:NZ	2.30	0.46
3:J:350:HIS:HB3	5:L:247:ARG:HH12	1.81	0.46
3:J:646:LYS:HA	3:J:720:LEU:HD22	1.98	0.46
3:J:87:ARG:HG2	3:J:523:ASP:CB	2.45	0.46
2:C:45:GLN:HE21	2:C:45:GLN:HA	1.80	0.46
2:C:15:LEU:O	2:C:586:ARG:NH1	2.48	0.46
2:C:609:THR:O	2:C:625:LEU:HG	2.15	0.46
2:C:897:LEU:HD23	2:C:899:GLN:H	1.80	0.46
3:D:169:TYR:CE2	3:D:395:VAL:HG12	2.40	0.46
3:D:474:GLU:O	3:D:478:LEU:HG	2.16	0.46
5:F:319:VAL:O	5:F:323:LEU:HB2	2.15	0.46
5:F:383:VAL:HG22	5:F:404:TYR:HE2	1.81	0.46
2:I:405:ARG:O	2:I:409:ARG:HG3	2.16	0.46
2:I:436:GLY:O	2:I:459:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:532:MET:HG2	2:I:533:ASP:N	2.30	0.46
2:I:660:ALA:O	2:I:667:ALA:N	2.41	0.46
3:J:1119:SER:HA	3:J:1186:VAL:O	2.16	0.46
3:J:397:LYS:HE3	3:J:448:GLU:O	2.16	0.46
3:J:527:MET:HG3	3:J:537:THR:HB	1.97	0.46
5:L:302:SER:O	5:L:306:ILE:HG22	2.16	0.46
5:L:410:GLU:O	5:L:413:ARG:HB3	2.15	0.46
1:A:66:SER:O	1:A:75:VAL:HG23	2.16	0.46
5:F:376:LEU:HG	5:F:423:LEU:HD21	1.98	0.46
3:J:1095:THR:O	3:J:1099:VAL:HG23	2.16	0.46
3:J:104:PHE:HB3	3:J:111:LYS:HB2	1.98	0.46
3:J:1254:GLN:HB3	3:J:1258:ARG:CB	2.45	0.46
3:J:93:ILE:HB	3:J:517:VAL:HB	1.98	0.46
5:L:235:LEU:O	5:L:239:VAL:HG23	2.16	0.46
1:A:29:GLU:O	1:A:32:PHE:HB2	2.16	0.46
1:B:150:TYR:HD2	3:D:857:LEU:HD12	1.80	0.46
2:C:436:GLY:O	2:C:459:ALA:HB2	2.16	0.46
3:D:414:ARG:HA	3:D:414:ARG:HD2	1.68	0.46
3:D:584:ASN:OD1	3:D:591:VAL:HG12	2.16	0.46
3:D:702:LEU:HD12	3:D:746:ALA:O	2.16	0.46
5:F:412:ILE:O	5:F:416:GLU:HG2	2.16	0.46
2:I:744:ARG:NE	2:I:747:ALA:HB2	2.30	0.46
1:G:63:HIS:HB2	2:I:799:ILE:HD12	1.97	0.46
2:I:1067:TYR:CE2	5:L:357:VAL:HA	2.52	0.46
2:C:711:GLU:HA	2:C:822:VAL:HG12	1.98	0.45
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.98	0.45
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.52	0.45
3:D:175:VAL:HG13	3:D:193:PRO:HD2	1.99	0.45
3:D:892:ASP:HB2	3:D:894:LYS:HG2	1.99	0.45
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.16	0.45
5:F:202:LEU:HD21	5:F:239:VAL:HG22	1.98	0.45
5:F:218:THR:HA	5:F:227:LEU:HD11	1.98	0.45
1:H:29:GLU:HB3	1:H:32:PHE:CD1	2.51	0.45
2:I:1102:LEU:HA	2:I:1107:ASN:O	2.16	0.45
2:I:430:VAL:HG12	2:I:434:HIS:CD2	2.51	0.45
3:J:483:HIS:CG	3:J:484:PRO:HD2	2.50	0.45
3:J:522:PRO:HA	3:J:525:ARG:NH1	2.31	0.45
3:J:565:ILE:H	3:J:565:ILE:HD12	1.80	0.45
3:J:634:GLY:O	3:J:637:LEU:N	2.30	0.45
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.51	0.45
2:C:570:PRO:HD2	2:C:635:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:ARG:HG2	2:C:642:ARG:HH12	1.81	0.45
3:D:102:ILE:HB	3:D:579:ASP:HB3	1.98	0.45
3:D:1277:ILE:HG12	3:D:1278:ASP:H	1.81	0.45
3:D:264:LEU:O	3:D:267:GLY:N	2.47	0.45
3:D:293:VAL:HB	3:D:296:GLU:HB2	1.98	0.45
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.45
3:D:990:ASP:O	3:D:993:ILE:HG22	2.17	0.45
1:G:76:VAL:HA	1:G:79:ILE:HD12	1.98	0.45
2:I:122:THR:HG23	2:I:128:ILE:HD11	1.98	0.45
2:I:816:LYS:HA	2:I:817:PRO:HD3	1.83	0.45
2:I:880:MET:CE	3:J:1037:GLN:HB2	2.46	0.45
3:J:112:ILE:HD12	3:J:113:GLY:H	1.79	0.45
3:J:1293:PHE:H	3:J:1293:PHE:HD1	1.63	0.45
3:J:633:VAL:C	3:J:635:PRO:HD3	2.36	0.45
2:C:193:LEU:HA	2:C:196:LEU:HD13	1.97	0.45
2:C:272:ALA:O	2:C:276:LYS:N	2.39	0.45
3:D:1135:ARG:HB3	3:D:1139:ASP:HB3	1.98	0.45
3:D:350:HIS:HB2	3:D:371:ILE:HG22	1.98	0.45
3:D:44:LEU:HG	3:D:525:ARG:HH12	1.81	0.45
3:D:698:LYS:HB3	3:D:756:GLN:NE2	2.31	0.45
5:F:252:THR:HG1	6:O:28:DA:H8	1.64	0.45
5:F:385:LYS:HA	5:F:390:LEU:HD12	1.98	0.45
1:H:179:PHE:HB3	1:H:197:LEU:HD13	1.99	0.45
2:I:374:ASN:OD1	2:I:375:SER:N	2.47	0.45
2:I:456:ALA:HB3	2:I:459:ALA:HB2	1.98	0.45
2:I:640:ARG:HG2	2:I:642:ARG:HH12	1.82	0.45
2:I:726:ILE:HD12	2:I:729:LEU:HG	1.99	0.45
3:J:1046:GLN:HE22	3:J:1079:LYS:HE2	1.81	0.45
3:J:1223:VAL:HG21	3:J:1462:LEU:HD21	1.98	0.45
3:J:102:ILE:HD11	3:J:587:ARG:HB2	1.97	0.45
5:L:292:GLN:O	5:L:295:GLN:HG3	2.17	0.45
5:L:376:LEU:HB3	5:L:380:GLU:HG3	1.98	0.45
5:L:412:ILE:HA	5:L:415:ILE:HD12	1.97	0.45
7:S:4:DC:H2"	7:S:5:DA:C8	2.51	0.45
1:A:44:LEU:HD13	1:A:177:VAL:HG21	1.99	0.45
2:C:1056:LYS:NZ	3:D:748:HIS:HB3	2.32	0.45
2:C:185:LYS:HA	2:C:189:ARG:O	2.16	0.45
2:C:242:LEU:HD11	2:C:256:TYR:CE2	2.52	0.45
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.31	0.45
2:C:99:GLN:HB3	2:C:110:GLU:HG3	1.99	0.45
3:D:1088:THR:HA	3:D:1234:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1482:ARG:HE	3:D:1483:PHE:HE1	1.65	0.45
3:D:654:LYS:O	3:D:658:LEU:HB2	2.16	0.45
3:D:974:ILE:HG12	3:D:991:GLN:HG2	1.97	0.45
1:G:181:VAL:O	1:G:182:GLU:HG3	2.16	0.45
2:I:357:GLU:HG2	5:L:216:LYS:HE2	1.99	0.45
2:I:897:LEU:HD21	2:I:899:GLN:HG2	1.97	0.45
3:J:990:ASP:O	3:J:993:ILE:HG22	2.16	0.45
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.99	0.45
1:B:211:LEU:O	1:B:215:VAL:HG13	2.15	0.45
2:C:405:ARG:O	2:C:409:ARG:HG3	2.16	0.45
2:C:644:ARG:HD2	2:C:647:GLN:HB3	1.98	0.45
2:C:639:GLN:HB3	2:C:656:ALA:HB1	1.99	0.45
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.16	0.45
3:D:1221:VAL:HG23	3:D:1222:GLY:H	1.82	0.45
3:D:187:LYS:N	3:D:200:ASP:OD2	2.49	0.45
4:E:18:ARG:O	4:E:22:VAL:HG23	2.17	0.45
5:F:141:LEU:O	5:F:145:VAL:HG23	2.17	0.45
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.97	0.45
1:H:44:LEU:HA	1:H:48:ILE:HD13	1.98	0.45
2:I:242:LEU:HD11	2:I:256:TYR:CE2	2.52	0.45
2:I:897:LEU:HD23	2:I:899:GLN:H	1.80	0.45
2:I:937:ASP:HB3	2:I:940:GLU:HG3	1.97	0.45
3:J:1135:ARG:HB2	3:J:1140:ILE:HD11	1.98	0.45
3:J:1381:VAL:HG21	3:J:1393:GLN:HB3	1.98	0.45
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.97	0.45
3:J:684:LYS:O	3:J:687:VAL:HG22	2.17	0.45
6:R:2:DT:H2"	6:R:3:DT:OP2	2.16	0.45
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.99	0.45
1:B:23:PHE:HE2	1:B:199:ILE:HB	1.81	0.45
1:B:202:ASP:OD1	1:B:203:GLY:N	2.49	0.45
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.97	0.45
3:D:1161:GLU:OE2	3:D:1164:ARG:HB2	2.16	0.45
3:D:225:ILE:O	3:D:331:VAL:HG12	2.17	0.45
3:D:522:PRO:HA	3:D:525:ARG:NH1	2.32	0.45
3:D:638:LYS:HG2	3:D:640:HIS:NE2	2.32	0.45
5:F:286:LEU:HD23	5:F:310:MET:HG3	1.98	0.45
3:D:593:ASN:ND2	5:F:331:SER:OG	2.50	0.45
1:G:190:THR:OG1	1:G:191:ASP:N	2.48	0.45
2:I:1012:PRO:HB2	2:I:1021:LEU:HD11	1.98	0.45
2:I:111:ASP:HB3	2:I:369:PRO:HG2	1.98	0.45
2:I:151:ASP:HB2	2:I:154:ARG:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:140:ILE:HD12	2:I:332:ARG:O	2.17	0.45
2:I:878:SER:O	3:J:1034:GLN:NE2	2.49	0.45
2:I:890:LEU:HD21	2:I:914:ILE:HG12	1.99	0.45
3:J:1434:TRP:CD1	3:J:1457:ASP:HB2	2.52	0.45
3:J:638:LYS:HG2	3:J:640:HIS:CE1	2.51	0.45
2:I:1044:GLY:HA3	4:K:17:TYR:HE1	1.81	0.45
4:K:45:ARG:HD2	4:K:63:TRP:HH2	1.82	0.45
5:L:413:ARG:NH1	5:L:414:GLN:HG2	2.31	0.45
1:A:35:THR:HG23	1:B:42:ARG:HB2	1.99	0.45
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.79	0.45
2:C:291:VAL:HG13	2:C:303:PHE:CE1	2.52	0.45
2:C:440:PRO:O	3:D:1078:ARG:HG3	2.17	0.45
3:D:300:VAL:HG12	3:D:301:GLY:H	1.82	0.45
3:D:525:ARG:HG2	3:D:540:LEU:HD23	1.98	0.45
3:D:815:ALA:HB1	3:D:821:VAL:HG23	1.99	0.45
5:F:302:SER:O	5:F:306:ILE:HG22	2.16	0.45
1:H:211:LEU:O	1:H:215:VAL:HG13	2.16	0.45
2:I:1019:GLN:OE1	2:I:1057:SER:OG	2.34	0.45
2:I:440:PRO:O	3:J:1078:ARG:HG3	2.17	0.45
3:J:65:ARG:HG2	5:L:393:GLY:O	2.16	0.45
3:J:767:HIS:CE1	4:K:6:ILE:HD13	2.52	0.45
7:S:8:DA:C2'	7:S:9:DT:H5''	2.46	0.45
1:B:62:LEU:HD12	1:B:62:LEU:H	1.82	0.45
1:B:81:ASN:OD1	3:D:867:ARG:NH2	2.49	0.45
1:B:87:VAL:HG12	1:B:122:ILE:HG12	1.97	0.45
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.99	0.45
2:C:584:GLU:HB3	2:C:666:LEU:HB3	1.99	0.45
3:D:14:SER:HB3	3:D:511:TRP:CD2	2.51	0.45
3:D:684:LYS:O	3:D:687:VAL:HG22	2.17	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.45
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.52	0.45
1:H:185:ARG:NH2	1:H:187:GLY:O	2.50	0.45
2:I:207:LEU:HD13	2:I:227:LEU:HD11	1.97	0.45
2:I:710:ILE:HD13	2:I:790:LEU:HD13	1.98	0.45
3:J:618:LEU:HB3	3:J:1467:ILE:HG12	1.98	0.45
3:J:597:GLU:O	3:J:599:PRO:HD3	2.17	0.45
2:C:751:PRO:HA	2:C:792:VAL:HG13	1.99	0.45
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.99	0.45
3:D:129:PHE:CE1	3:D:571:LYS:HG2	2.52	0.45
3:D:565:ILE:H	3:D:565:ILE:HD12	1.81	0.45
3:D:701:LEU:HD21	3:D:763:MET:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:160:GLU:CD	3:J:165:LYS:HD3	2.38	0.45
1:A:209:GLU:O	1:A:213:GLN:HG2	2.17	0.45
2:C:1088:LEU:O	2:C:1092:LEU:HG	2.17	0.45
2:C:634:GLY:O	2:C:704:HIS:HA	2.17	0.45
2:C:673:LEU:HA	2:C:990:GLY:O	2.16	0.45
2:C:771:GLU:O	2:C:775:ARG:HG3	2.17	0.45
3:D:633:VAL:C	3:D:635:PRO:HD3	2.37	0.45
3:D:701:LEU:HD22	3:D:713:ILE:HG22	1.98	0.45
3:D:794:GLN:HG3	3:D:795:VAL:N	2.32	0.45
5:F:159:ILE:N	5:F:160:PRO:HD3	2.32	0.45
1:G:231:SER:H	1:H:14:THR:HG22	1.81	0.45
2:I:1058:ASP:OD1	2:I:1058:ASP:N	2.49	0.45
2:I:429:ASP:OD1	2:I:430:VAL:N	2.43	0.45
2:I:446:GLY:O	2:I:449:ILE:HG13	2.16	0.45
3:J:632:VAL:O	3:J:727:GLN:HA	2.17	0.45
3:J:841:PHE:CE2	3:J:858:LEU:HD13	2.52	0.45
4:K:79:LEU:HD23	4:K:80:VAL:HG22	1.99	0.45
5:L:149:LYS:HB2	5:L:193:ARG:HH12	1.82	0.45
5:L:202:LEU:HD21	5:L:239:VAL:HG22	1.98	0.45
5:L:289:THR:O	5:L:293:LEU:HG	2.17	0.45
7:P:19:DT:H1'	7:P:20:DT:H5'	1.99	0.45
2:C:299:LYS:HG3	2:C:300:ASP:H	1.82	0.44
2:C:807:ARG:HB3	2:C:810:ASP:OD1	2.17	0.44
3:D:1179:GLU:HG2	3:J:1131:THR:HG22	1.99	0.44
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.52	0.44
3:D:259:VAL:HG13	3:D:298:VAL:HG21	2.00	0.44
5:F:181:LEU:HD23	5:F:185:LEU:HD13	1.98	0.44
1:G:28:LEU:HD11	1:G:36:LEU:HD12	1.98	0.44
2:I:1030:GLN:O	3:J:622:ARG:HA	2.17	0.44
2:I:549:PHE:HB3	2:I:552:HIS:HD2	1.82	0.44
2:I:737:LEU:HA	2:I:737:LEU:HD12	1.61	0.44
3:J:1006:ALA:O	3:J:1010:ASN:HB2	2.16	0.44
3:J:1479:ASP:HA	3:J:1482:ARG:HG2	1.99	0.44
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.98	0.44
2:I:770:GLU:HB3	5:L:369:LEU:HD12	1.99	0.44
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.99	0.44
2:C:432:ARG:HH12	2:C:518:ARG:NE	2.15	0.44
3:D:1144:LEU:HA	3:D:1144:LEU:HD12	1.53	0.44
3:D:1312:LEU:HG	3:D:1325:LEU:O	2.17	0.44
2:C:370:ALA:O	5:F:295:GLN:NE2	2.50	0.44
1:G:89:PHE:CE1	1:G:120:VAL:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1009:SER:HB3	3:J:651:GLU:O	2.18	0.44
2:I:142:ARG:HA	2:I:331:ARG:HA	2.00	0.44
2:I:423:ALA:O	2:I:428:ARG:HG3	2.16	0.44
2:I:564:MET:HG2	2:I:567:GLN:NE2	2.32	0.44
3:J:1191:PRO:O	3:J:1373:ARG:HD2	2.17	0.44
3:J:1406:ARG:O	3:J:1410:GLU:HG3	2.16	0.44
3:J:810:GLU:O	3:J:813:LEU:HB3	2.17	0.44
3:J:806:PHE:CD1	3:J:811:GLU:HB3	2.52	0.44
4:K:19:LEU:O	4:K:23:VAL:HG23	2.17	0.44
1:A:28:LEU:HD22	1:A:32:PHE:HD2	1.82	0.44
2:C:41:ASN:HA	2:C:45:GLN:HB3	1.99	0.44
2:C:670:GLN:O	2:C:672:VAL:HG23	2.17	0.44
2:C:744:ARG:NE	2:C:747:ALA:HB2	2.33	0.44
2:C:971:LYS:HG2	2:C:988:VAL:HG12	1.99	0.44
2:C:1030:GLN:O	3:D:622:ARG:HA	2.17	0.44
3:D:638:LYS:HG3	3:D:640:HIS:H	1.81	0.44
1:G:73:GLU:HB3	1:G:77:GLU:HG3	1.99	0.44
1:H:87:VAL:HG12	1:H:122:ILE:HG12	1.99	0.44
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.32	0.44
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.99	0.44
2:I:69:LEU:C	2:I:70:GLU:HG3	2.37	0.44
1:H:176:ARG:NH1	3:J:884:ARG:HH12	2.16	0.44
5:L:159:ILE:N	5:L:160:PRO:HD3	2.33	0.44
5:L:411:ARG:HD3	6:R:1:DC:C6	2.52	0.44
1:A:79:ILE:HD13	1:A:167:VAL:HG12	2.00	0.44
1:A:22:GLU:HA	1:A:197:LEU:O	2.17	0.44
2:C:333:ILE:HB	2:C:461:VAL:HG11	2.00	0.44
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.44
3:D:1078:ARG:HH11	3:D:1078:ARG:HB3	1.82	0.44
3:D:1127:GLU:C	3:D:1129:THR:H	2.21	0.44
3:D:1288:ASP:OD2	3:D:1288:ASP:N	2.50	0.44
3:D:213:VAL:HB	3:D:345:TYR:HE1	1.82	0.44
3:D:631:ILE:HD11	3:D:739:ASP:O	2.18	0.44
1:G:63:HIS:CD2	1:G:66:SER:HB2	2.53	0.44
2:I:550:LEU:HD11	2:I:558:ALA:HB1	1.98	0.44
3:J:1293:PHE:CD1	3:J:1293:PHE:N	2.85	0.44
3:J:701:LEU:HD22	3:J:713:ILE:HG22	1.98	0.44
6:O:2:DT:H2"	6:O:3:DT:OP2	2.18	0.44
1:A:231:SER:H	1:B:14:THR:HG22	1.82	0.44
2:C:97:ARG:HB2	2:C:112:GLU:HG3	1.99	0.44
2:C:682:TYR:HA	3:D:633:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:634:GLY:O	3:D:637:LEU:N	2.28	0.44
4:E:6:ILE:HG23	4:E:7:ASP:H	1.83	0.44
2:I:194:VAL:O	2:I:198:ARG:HG3	2.17	0.44
2:I:526:PRO:O	2:I:529:VAL:HG12	2.17	0.44
2:I:644:ARG:HD2	2:I:647:GLN:HB3	2.00	0.44
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.53	0.44
3:J:1078:ARG:HH11	3:J:1078:ARG:HB3	1.83	0.44
3:J:1144:LEU:HD13	3:J:1144:LEU:HA	1.77	0.44
3:J:22:SER:HB2	3:J:92:HIS:HB3	1.97	0.44
3:J:90:MET:HE1	3:J:518:PRO:HB3	1.98	0.44
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.52	0.44
1:A:232:LEU:H	1:A:232:LEU:HD12	1.82	0.44
1:B:23:PHE:HE1	1:B:208:LEU:HD12	1.82	0.44
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.99	0.44
2:C:878:SER:HB2	3:D:1029:ARG:HG3	1.99	0.44
3:D:155:ASP:N	3:D:155:ASP:OD2	2.49	0.44
1:H:202:ASP:OD1	1:H:203:GLY:N	2.51	0.44
2:I:1086:ARG:NH1	2:I:1086:ARG:HG3	2.32	0.44
2:I:1090:LYS:NZ	2:I:1093:GLN:OE1	2.35	0.44
2:I:670:GLN:O	2:I:672:VAL:HG23	2.17	0.44
2:I:761:PHE:HA	2:I:785:VAL:HA	1.99	0.44
2:I:994:ILE:HG22	2:I:995:MET:H	1.82	0.44
3:J:558:LEU:CD2	3:J:567:ILE:HG23	2.48	0.44
3:J:84:ILE:HD11	3:J:88:TYR:HE1	1.83	0.44
5:L:99:TYR:O	5:L:103:ILE:HG12	2.17	0.44
1:A:227:ASN:HA	1:A:228:PRO:HD2	1.75	0.44
1:A:58:ILE:HG22	1:A:60:ASP:H	1.81	0.44
3:D:1141:GLU:OE1	3:D:1168:LEU:HD11	2.18	0.44
3:D:117:ASP:HB2	3:D:495:ARG:CZ	2.47	0.44
3:D:638:LYS:HB3	3:D:641:GLN:HE21	1.83	0.44
1:G:182:GLU:O	1:G:193:ASP:HA	2.18	0.44
1:G:22:GLU:HA	1:G:197:LEU:O	2.18	0.44
1:H:41:ARG:HG3	1:H:177:VAL:HG21	2.00	0.44
1:H:34:VAL:HG22	1:H:181:VAL:HG21	2.00	0.44
2:I:714:ASP:HB2	2:I:818:GLY:O	2.18	0.44
2:I:834:GLN:HG2	2:I:835:VAL:H	1.82	0.44
3:J:1202:GLN:O	3:J:1206:GLY:N	2.51	0.44
3:J:1499:ARG:HH21	3:J:1500:LYS:HG3	1.83	0.44
3:J:496:LEU:HD12	3:J:499:VAL:HB	1.99	0.44
5:F:398:LEU:HB3	7:P:21:DG:OP2	2.18	0.44
1:A:182:GLU:O	1:A:193:ASP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:O	1:B:44:LEU:HB2	2.18	0.44
1:B:78:ILE:O	1:B:82:LEU:HG	2.18	0.44
2:C:1112:PHE:HB2	2:C:1115:LEU:HB2	1.99	0.44
2:C:588:VAL:HG23	2:C:596:TYR:OH	2.17	0.44
2:C:834:GLN:HG2	2:C:835:VAL:H	1.82	0.44
3:D:1199:GLY:O	3:D:1373:ARG:NH1	2.51	0.44
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.83	0.44
5:F:173:GLU:O	5:F:177:LYS:HB2	2.18	0.44
2:I:1089:VAL:HG13	2:I:1099:VAL:HG11	2.00	0.44
2:I:269:LEU:HB2	2:I:288:ARG:O	2.18	0.44
2:I:399:ASN:HD21	2:I:566:THR:HA	1.83	0.44
3:J:523:ASP:HA	3:J:526:PRO:HG3	2.00	0.44
3:J:537:THR:O	5:L:332:LEU:HG	2.18	0.44
3:J:568:ARG:HA	3:J:571:LYS:HE2	1.98	0.44
2:I:1115:LEU:HD21	3:J:84:ILE:HG23	2.00	0.44
2:C:458:TYR:CD1	2:C:538:GLN:HB3	2.49	0.44
2:C:5:ARG:HB2	2:C:5:ARG:HE	1.70	0.44
3:D:1068:LEU:H	3:D:1068:LEU:HD12	1.83	0.44
3:D:1189:ARG:HE	3:D:1203:LYS:HB2	1.82	0.44
3:D:1258:ARG:HG3	3:D:1258:ARG:O	2.18	0.44
3:D:1370:ILE:H	3:D:1370:ILE:HG13	1.66	0.44
3:D:529:GLN:HA	3:D:535:PHE:HA	1.99	0.44
2:I:581:THR:OG1	2:I:584:GLU:OE2	2.36	0.44
2:I:700:TYR:HB3	2:I:833:LEU:HD13	2.00	0.44
2:I:537:LYS:NZ	2:I:905:VAL:H	2.01	0.44
3:J:1033:GLN:O	3:J:1037:GLN:HG3	2.18	0.44
3:J:1038:LEU:O	3:J:1060:SER:OG	2.22	0.44
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.18	0.44
3:J:439:LEU:HD21	5:L:190:HIS:HB3	2.00	0.44
1:A:44:LEU:HD11	1:A:199:ILE:HD13	1.99	0.43
1:A:35:THR:CG2	1:B:39:PRO:HA	2.47	0.43
1:A:76:VAL:HA	1:A:79:ILE:HD12	1.99	0.43
2:C:1012:PRO:HB2	2:C:1021:LEU:HD11	2.00	0.43
2:C:321:GLU:HG2	2:C:322:VAL:H	1.83	0.43
2:C:675:ALA:O	2:C:870:ILE:HA	2.18	0.43
2:C:714:ASP:HB2	2:C:818:GLY:O	2.18	0.43
2:C:775:ARG:CZ	2:C:782:ALA:HB2	2.48	0.43
3:D:1368:ILE:HG13	3:D:1368:ILE:H	1.67	0.43
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.53	0.43
3:D:701:LEU:HD11	3:D:763:MET:HG2	2.00	0.43
1:G:44:LEU:HD11	1:G:199:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:332:ARG:HH11	2:I:334:ARG:HD2	1.82	0.43
2:I:376:ARG:HB2	2:I:377:PRO:HD3	2.00	0.43
2:I:588:VAL:HG23	2:I:596:TYR:OH	2.18	0.43
2:I:807:ARG:HB3	2:I:810:ASP:OD1	2.18	0.43
2:I:709:GLU:HA	2:I:823:VAL:O	2.18	0.43
3:J:638:LYS:HG2	3:J:640:HIS:NE2	2.33	0.43
3:J:792:ILE:HD13	3:J:881:LEU:HD23	1.99	0.43
3:J:635:PRO:O	3:J:935:LYS:HE2	2.18	0.43
2:C:140:ILE:HD12	2:C:332:ARG:O	2.17	0.43
2:C:713:ARG:O	2:C:720:GLU:HG2	2.18	0.43
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.18	0.43
3:D:154:THR:HG23	3:D:156:GLU:H	1.83	0.43
1:G:28:LEU:HD22	1:G:32:PHE:HD2	1.83	0.43
1:G:46:SER:OG	1:G:47:SER:N	2.51	0.43
2:I:269:LEU:H	2:I:288:ARG:HB3	1.82	0.43
1:G:178:ALA:HB2	2:I:864:GLY:HA3	2.01	0.43
3:D:1180:ALA:O	3:J:1132:LEU:HD12	2.18	0.43
3:J:1200:VAL:HG22	3:J:1221:VAL:HG21	1.99	0.43
3:J:505:SER:HB3	3:J:1453:ALA:HA	1.99	0.43
3:J:637:LEU:HG	3:J:641:GLN:HB3	2.01	0.43
3:J:560:GLN:HE22	5:L:236:ILE:HG21	1.82	0.43
5:L:407:VAL:HG12	6:R:1:DC:H3'	2.00	0.43
5:L:246:ARG:HD3	6:R:26:DA:C6	2.54	0.43
1:B:107:LYS:O	1:B:132:LEU:HB2	2.17	0.43
1:B:51:THR:HG21	1:B:86:VAL:HG23	2.00	0.43
2:C:1050:GLN:HE22	3:D:1470:ARG:C	2.21	0.43
2:C:1047:HIS:O	2:C:1051:GLU:HG3	2.18	0.43
2:C:1089:VAL:HG11	2:C:1112:PHE:HE2	1.82	0.43
2:C:332:ARG:HH11	2:C:334:ARG:HD2	1.83	0.43
2:C:69:LEU:C	2:C:70:GLU:HG3	2.38	0.43
2:C:897:LEU:HD21	2:C:899:GLN:HG2	1.99	0.43
3:D:1269:LYS:HG3	3:D:1270:ALA:H	1.82	0.43
5:F:377:SER:HB3	5:F:380:GLU:HG2	2.00	0.43
2:I:390:GLN:HG2	2:I:415:PRO:HD3	1.99	0.43
3:J:1333:HIS:O	3:J:1336:LEU:HB3	2.18	0.43
3:J:34:TYR:HB2	5:L:325:ILE:HG23	2.00	0.43
4:K:30:LEU:HA	4:K:37:ASN:HD21	1.83	0.43
5:L:141:LEU:O	5:L:145:VAL:HG23	2.18	0.43
5:F:252:THR:HA	6:O:29:DC:H5	1.83	0.43
1:A:57:TYR:C	1:A:58:ILE:HD12	2.39	0.43
1:B:55:SER:HB2	1:B:166:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:THR:HG23	2:C:128:ILE:HD11	1.99	0.43
2:C:84:ARG:HA	2:C:131:GLY:HA2	2.00	0.43
2:C:65:VAL:CG1	2:C:101:ILE:HB	2.48	0.43
2:C:994:ILE:HG22	2:C:995:MET:H	1.83	0.43
3:D:589:SER:HA	3:D:590:PRO:HD3	1.86	0.43
3:D:67:ARG:HD2	5:F:394:ARG:HB2	1.99	0.43
3:D:858:LEU:HD12	3:D:859:ASP:H	1.83	0.43
3:D:790:TYR:CD1	3:D:907:GLU:HB3	2.54	0.43
3:D:996:TRP:CE2	3:D:1056:PRO:HD3	2.53	0.43
5:F:276:PRO:HB2	5:F:279:MET:HG2	1.99	0.43
1:H:37:GLY:HA3	1:H:179:PHE:CE1	2.53	0.43
2:I:202:TYR:CD1	2:I:206:THR:HG21	2.53	0.43
2:I:170:PRO:HD2	2:I:267:TYR:HD1	1.83	0.43
2:I:327:HIS:O	2:I:331:ARG:HG3	2.18	0.43
2:I:333:ILE:HB	2:I:461:VAL:HG11	2.00	0.43
2:I:713:ARG:O	2:I:720:GLU:HG2	2.18	0.43
3:J:1042:ARG:HB3	3:J:1057:VAL:CG2	2.48	0.43
3:J:1065:LEU:HB3	3:J:1069:GLU:HB2	1.99	0.43
3:J:1068:LEU:H	3:J:1068:LEU:HD12	1.83	0.43
3:J:1108:ARG:NH2	3:J:1198:TYR:O	2.50	0.43
3:J:32:ILE:HA	3:J:40:GLU:HG2	2.00	0.43
3:J:592:THR:OG1	3:J:596:SER:O	2.29	0.43
3:J:892:ASP:HB2	3:J:894:LYS:HG2	2.01	0.43
5:L:109:LEU:HD22	5:L:205:ALA:HB1	2.00	0.43
5:L:376:LEU:HG	5:L:423:LEU:HD21	1.99	0.43
6:O:5:DA:H2	7:P:22:DT:H3	1.65	0.43
7:S:11:DT:H1'	7:S:12:DA:H5'	2.01	0.43
1:A:65:PHE:CD2	2:C:799:ILE:HD11	2.54	0.43
1:B:160:ASP:O	1:B:161:ARG:HB2	2.18	0.43
1:A:42:ARG:NH2	1:B:31:GLY:O	2.41	0.43
2:C:1018:GLN:HG2	2:C:1083:GLU:HG2	2.00	0.43
2:C:124:ASP:HB2	2:C:407:LYS:NZ	2.34	0.43
2:C:269:LEU:HB2	2:C:288:ARG:O	2.18	0.43
2:C:495:THR:H	2:C:530:GLU:CG	2.31	0.43
2:C:710:ILE:HD13	2:C:790:LEU:HD13	2.00	0.43
3:D:1142:SER:HB3	3:D:1353:GLN:NE2	2.33	0.43
3:D:242:LEU:HB3	3:D:311:LEU:O	2.19	0.43
3:D:970:LYS:O	3:D:973:GLN:HB3	2.18	0.43
4:E:79:LEU:HD23	4:E:80:VAL:HG22	2.00	0.43
3:D:30:GLU:HB3	5:F:274:ARG:HB2	2.00	0.43
1:G:150:TYR:CZ	1:G:152:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:LEU:HD12	1:G:232:LEU:H	1.83	0.43
1:H:176:ARG:HB3	1:H:200:TRP:CE3	2.53	0.43
1:H:213:GLN:HE21	1:H:217:ILE:HD11	1.83	0.43
2:I:41:ASN:HA	2:I:45:GLN:HB3	2.01	0.43
3:J:121:THR:O	3:J:124:GLU:HB3	2.18	0.43
2:I:1056:LYS:NZ	3:J:748:HIS:HB3	2.34	0.43
3:J:698:LYS:HB3	3:J:756:GLN:NE2	2.34	0.43
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.18	0.43
2:C:390:GLN:CG	2:C:415:PRO:HD3	2.48	0.43
3:D:1288:ASP:CG	3:D:1289:ARG:H	2.22	0.43
3:D:132:TYR:HB3	3:D:454:ALA:HB1	1.99	0.43
3:D:1361:VAL:HG12	3:D:1363:LEU:H	1.84	0.43
1:G:55:SER:CB	1:G:158:ILE:HG12	2.43	0.43
1:G:64:GLU:HA	1:G:75:VAL:HG11	1.99	0.43
2:I:160:ALA:HB3	2:I:174:LEU:HD11	2.01	0.43
2:I:181:VAL:HG22	2:I:182:VAL:H	1.84	0.43
2:I:321:GLU:HG2	2:I:322:VAL:H	1.84	0.43
2:I:343:GLN:HG3	2:I:385:PHE:CB	2.48	0.43
2:I:577:PRO:HB3	2:I:993:PHE:CG	2.53	0.43
3:J:1059:SER:HB3	3:J:1063:GLU:HB2	1.99	0.43
3:J:1149:LEU:HG	3:J:1160:LEU:HD12	2.01	0.43
3:J:1336:LEU:HD11	3:J:1419:PRO:HB2	1.99	0.43
3:J:1434:TRP:NE1	3:J:1457:ASP:HB2	2.33	0.43
3:J:209:ARG:HA	3:J:347:VAL:HB	1.99	0.43
3:J:354:ILE:HG23	3:J:355:VAL:HG13	2.01	0.43
1:A:28:LEU:HD11	1:A:36:LEU:HD12	2.00	0.43
1:A:89:PHE:CE1	1:A:120:VAL:HG12	2.54	0.43
2:C:424:GLY:O	2:C:425:PHE:HD1	2.00	0.43
2:C:690:ILE:HG13	2:C:852:ILE:HG23	2.00	0.43
3:D:1110:ALA:HB2	3:D:1217:ILE:HD13	2.01	0.43
3:D:82:ARG:HB2	3:D:84:ILE:HG22	2.01	0.43
5:F:117:LEU:O	5:F:121:VAL:HG23	2.18	0.43
1:H:89:PHE:HE1	1:H:97:THR:HG22	1.83	0.43
2:I:1067:TYR:O	2:I:1071:ILE:HB	2.19	0.43
2:I:676:ILE:O	2:I:987:ILE:HG23	2.18	0.43
2:I:768:SER:O	2:I:772:ARG:N	2.50	0.43
3:J:56:TYR:CA	3:J:80:VAL:HG23	2.49	0.43
5:L:181:LEU:HD23	5:L:185:LEU:HD13	1.99	0.43
5:L:263:ASN:HA	5:L:266:ILE:CD1	2.49	0.43
2:C:537:LYS:CE	2:C:583:LEU:HD11	2.49	0.43
3:D:56:TYR:CA	3:D:80:VAL:HG23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:PHE:HE2	1:H:199:ILE:HB	1.83	0.43
2:I:549:PHE:HB3	2:I:552:HIS:CD2	2.54	0.43
3:J:1170:ASP:O	3:J:1174:LEU:HG	2.18	0.43
3:J:187:LYS:N	3:J:200:ASP:OD2	2.49	0.43
3:J:406:ASP:CG	3:J:407:VAL:H	2.21	0.43
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.48	0.43
4:K:6:ILE:HG23	4:K:7:ASP:H	1.82	0.43
5:L:109:LEU:HD12	5:L:114:GLU:HA	2.01	0.43
5:L:167:ASP:HB2	5:L:168:PRO:HD3	2.01	0.43
3:J:569:ASN:ND2	5:L:229:GLN:HE21	2.16	0.43
5:L:377:SER:HB3	5:L:380:GLU:HG2	2.01	0.43
2:C:1086:ARG:NH1	2:C:1086:ARG:HG3	2.33	0.43
2:C:160:ALA:HB3	2:C:174:LEU:HD11	2.01	0.43
2:C:343:GLN:HG3	2:C:385:PHE:CB	2.49	0.43
2:C:64:LEU:HD21	2:C:66:LEU:CB	2.49	0.43
2:C:683:ASN:HB2	2:C:872:ASN:H	1.84	0.43
3:D:1042:ARG:HB3	3:D:1057:VAL:CG2	2.49	0.43
3:D:1238:MET:C	3:D:1253:THR:HB	2.38	0.43
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.76	0.43
3:D:210:ARG:HD2	3:D:388:HIS:HB2	2.00	0.43
3:D:553:ARG:HH11	5:F:230:GLU:HG2	1.83	0.43
1:G:53:VAL:CG2	1:G:54:THR:H	2.28	0.43
1:H:101:LEU:HD22	1:H:102:ARG:H	1.84	0.43
2:I:99:GLN:HB3	2:I:110:GLU:HG3	2.00	0.43
2:I:495:THR:H	2:I:530:GLU:CG	2.32	0.43
2:I:584:GLU:HB3	2:I:666:LEU:HB3	2.00	0.43
2:I:124:ASP:HA	2:I:592:LEU:HD12	2.01	0.43
2:I:536:PRO:HB3	3:J:1067:VAL:HG11	2.01	0.43
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	2.00	0.43
3:J:155:ASP:N	3:J:155:ASP:OD2	2.52	0.43
3:J:354:ILE:HG22	3:J:367:ILE:O	2.19	0.43
3:J:349:PRO:HB2	5:L:111:LEU:HD23	2.01	0.43
2:C:182:VAL:O	2:C:192:PRO:HA	2.19	0.43
2:C:543:ASN:HA	2:C:546:LEU:HD12	2.01	0.43
2:C:564:MET:SD	2:C:846:LYS:HG2	2.59	0.43
2:C:858:MET:SD	2:C:859:PRO:HD2	2.59	0.43
2:C:892:LEU:HD13	2:C:970:GLY:HA2	2.01	0.43
3:D:1289:ARG:HD3	3:D:1304:LYS:HD2	2.01	0.43
3:D:1293:PHE:HA	3:D:1302:GLU:HA	2.01	0.43
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.75	0.43
3:D:218:LYS:HA	3:D:337:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:439:LEU:HD21	5:F:190:HIS:HB3	2.01	0.43
3:D:84:ILE:HD11	3:D:88:TYR:HE1	1.84	0.43
3:D:792:ILE:HD13	3:D:881:LEU:HD23	2.00	0.43
4:E:26:ARG:NH2	4:E:37:ASN:HD22	2.17	0.43
1:H:160:ASP:O	1:H:161:ARG:HB2	2.19	0.43
1:H:201:THR:HG21	1:H:205:VAL:HG23	2.01	0.43
2:I:185:LYS:HA	2:I:189:ARG:O	2.19	0.43
2:I:679:PHE:CE2	2:I:853:LEU:HD21	2.54	0.43
3:J:1149:LEU:HD22	3:J:1166:LEU:HD11	2.00	0.43
3:J:791:TYR:CE2	3:J:945:SER:HB3	2.54	0.43
5:L:143:ARG:NH1	5:L:196:GLU:OE2	2.52	0.43
7:P:11:DT:H1'	7:P:12:DA:H5'	2.01	0.43
6:R:21:DG:H1'	6:R:22:DT:H5''	2.00	0.43
1:B:159:LYS:HG3	1:B:164:ALA:HB3	2.01	0.42
2:C:181:VAL:HG22	2:C:182:VAL:H	1.83	0.42
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.01	0.42
1:B:34:VAL:HG11	2:C:978:ARG:HB3	2.01	0.42
3:D:369:ALA:HA	3:D:376:GLU:HG2	2.01	0.42
3:D:397:LYS:O	3:D:447:VAL:HG23	2.19	0.42
3:D:789:LEU:HD13	3:D:934:LEU:HD23	2.01	0.42
5:F:167:ASP:HB2	5:F:168:PRO:HD3	2.01	0.42
1:G:48:ILE:HG22	1:G:173:PRO:HD2	2.00	0.42
1:G:97:THR:HG23	1:G:98:THR:N	2.27	0.42
1:H:62:LEU:HD12	1:H:62:LEU:H	1.83	0.42
2:I:397:GLU:HG3	2:I:632:ASN:HD22	1.84	0.42
2:I:424:GLY:O	2:I:425:PHE:HD1	2.01	0.42
2:I:720:GLU:HB2	2:I:759:THR:O	2.19	0.42
2:I:711:GLU:HA	2:I:822:VAL:HG12	2.01	0.42
2:I:878:SER:HB2	3:J:1029:ARG:HG3	2.00	0.42
3:J:1384:PRO:O	3:J:1415:VAL:HG22	2.19	0.42
3:J:701:LEU:HD11	3:J:763:MET:HG2	2.01	0.42
3:J:837:GLY:HA2	3:J:840:LYS:HB3	2.00	0.42
1:B:23:PHE:CE2	1:B:199:ILE:HB	2.54	0.42
2:C:437:ARG:HD3	2:C:467:ILE:O	2.19	0.42
2:C:547:ILE:HG21	2:C:550:LEU:HD13	2.02	0.42
2:C:607:ASP:HB3	2:C:610:ARG:O	2.19	0.42
2:C:737:LEU:HA	2:C:737:LEU:HD12	1.60	0.42
3:D:1167:SER:H	3:D:1170:ASP:CG	2.22	0.42
3:D:576:GLU:HG3	3:D:577:ALA:N	2.35	0.42
5:F:142:ILE:HA	5:F:145:VAL:HB	2.02	0.42
5:F:302:SER:H	5:F:305:GLU:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ILE:HG13	1:H:35:THR:HG21	2.01	0.42
1:H:55:SER:HB2	1:H:166:PRO:HA	2.00	0.42
2:I:1019:GLN:HA	2:I:1020:PRO:HD3	1.87	0.42
2:I:941:LYS:NZ	2:I:959:PRO:HG2	2.33	0.42
3:J:1161:GLU:HG2	3:J:1161:GLU:H	1.58	0.42
3:J:30:GLU:HB3	5:L:274:ARG:HB2	2.00	0.42
5:L:209:LEU:HB2	6:R:30:DT:C2	2.54	0.42
1:A:34:VAL:HG22	1:A:181:VAL:HG21	2.02	0.42
1:B:28:LEU:O	1:B:193:ASP:N	2.51	0.42
2:C:564:MET:HG2	2:C:567:GLN:NE2	2.34	0.42
2:C:67:ASP:O	2:C:98:LEU:HB2	2.19	0.42
3:D:1122:LEU:HD12	3:D:1184:ARG:O	2.19	0.42
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.54	0.42
3:D:313:LEU:HD12	3:D:314:PRO:HD2	2.01	0.42
3:D:100:ALA:HA	3:D:513:ILE:HA	2.02	0.42
3:D:698:LYS:HG2	3:D:756:GLN:HG2	2.01	0.42
2:I:328:LEU:HD23	2:I:437:ARG:HD2	2.01	0.42
2:I:537:LYS:CE	2:I:583:LEU:HD11	2.49	0.42
2:I:458:TYR:CD1	2:I:538:GLN:HB3	2.48	0.42
3:J:103:TRP:O	3:J:107:ASP:HB2	2.19	0.42
3:J:1267:ARG:NE	3:J:1267:ARG:H	2.14	0.42
3:J:1481:VAL:HG21	4:K:17:TYR:HB2	2.00	0.42
3:J:177:ALA:HB2	3:J:393:ILE:HD11	2.01	0.42
3:J:603:LEU:O	3:J:606:ILE:HG22	2.19	0.42
3:J:58:CYS:HB2	3:J:78:VAL:HB	2.01	0.42
3:J:853:VAL:HG22	3:J:858:LEU:HD23	2.00	0.42
1:A:173:PRO:HB3	1:A:202:ASP:OD1	2.20	0.42
2:C:639:GLN:HA	2:C:657:ASP:O	2.20	0.42
2:C:726:ILE:HD12	2:C:729:LEU:HG	2.01	0.42
2:C:806:LEU:HB2	2:C:822:VAL:HG22	2.01	0.42
2:C:839:LEU:HA	2:C:995:MET:O	2.19	0.42
3:D:1021:TYR:O	3:D:1025:GLN:HB2	2.19	0.42
3:D:1229:ILE:O	3:D:1232:PRO:HD2	2.19	0.42
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.20	0.42
3:D:1460:ILE:HG13	3:D:1461:GLY:N	2.33	0.42
3:D:544:TYR:O	3:D:548:ILE:HG13	2.20	0.42
3:D:577:ALA:O	3:D:581:VAL:HG23	2.18	0.42
3:D:643:GLY:O	3:D:726:ILE:HG23	2.19	0.42
5:F:99:TYR:O	5:F:103:ILE:HG12	2.20	0.42
2:C:770:GLU:HB3	5:F:369:LEU:HD12	2.01	0.42
1:G:20:TYR:HD2	1:G:21:GLY:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:LEU:HB3	1:H:193:ASP:HB2	2.01	0.42
2:I:751:PRO:HA	2:I:792:VAL:HG13	2.01	0.42
2:I:775:ARG:CZ	2:I:782:ALA:HB2	2.49	0.42
3:J:1229:ILE:O	3:J:1232:PRO:HD2	2.19	0.42
3:J:1311:LEU:H	3:J:1311:LEU:HD23	1.83	0.42
3:J:12:LEU:HD21	3:J:1452:ILE:HD13	2.01	0.42
3:J:677:LEU:HD23	3:J:677:LEU:HA	1.87	0.42
5:L:421:ARG:HA	5:L:424:LYS:HG3	2.02	0.42
1:B:101:LEU:HD22	1:B:102:ARG:H	1.85	0.42
2:C:194:VAL:O	2:C:198:ARG:HG3	2.19	0.42
2:C:143:SER:H	2:C:331:ARG:HA	1.85	0.42
2:C:142:ARG:HA	2:C:331:ARG:HG2	2.01	0.42
2:C:418:LEU:HD21	2:C:427:VAL:HG11	2.01	0.42
2:C:572:ILE:HD11	2:C:703:ILE:HG13	2.00	0.42
2:C:709:GLU:HA	2:C:823:VAL:O	2.19	0.42
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.49	0.42
3:D:211:VAL:O	3:D:345:TYR:HD1	2.02	0.42
3:D:220:ARG:O	3:D:281:ARG:HD3	2.20	0.42
3:D:471:GLU:O	3:D:475:ARG:HG2	2.19	0.42
3:D:909:ASN:O	3:D:912:LYS:HB3	2.20	0.42
5:F:109:LEU:HD12	5:F:114:GLU:HA	2.02	0.42
5:F:412:ILE:HA	5:F:415:ILE:HD12	2.00	0.42
2:I:200:LEU:HA	2:I:200:LEU:HD12	1.69	0.42
2:I:390:GLN:CG	2:I:415:PRO:HD3	2.49	0.42
2:I:971:LYS:HA	2:I:988:VAL:HA	2.00	0.42
3:J:1021:TYR:O	3:J:1025:GLN:HB2	2.19	0.42
6:O:3:DT:H2'	6:O:3:DT:H6	1.65	0.42
1:B:115:THR:HA	1:B:116:PRO:HD3	1.85	0.42
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.54	0.42
2:C:1010:THR:HG23	2:C:1013:TYR:OH	2.20	0.42
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.53	0.42
2:C:550:LEU:HD11	2:C:558:ALA:HB1	2.00	0.42
3:D:160:GLU:CD	3:D:165:LYS:HD3	2.40	0.42
3:D:44:LEU:HG	3:D:525:ARG:NH1	2.35	0.42
3:D:695:ILE:HG23	3:D:718:PRO:HB2	2.02	0.42
4:E:30:LEU:HA	4:E:37:ASN:HD21	1.85	0.42
5:F:376:LEU:HB3	5:F:380:GLU:HG3	2.01	0.42
1:G:38:ASN:HB2	1:G:179:PHE:CZ	2.54	0.42
1:G:58:ILE:HG22	1:G:60:ASP:H	1.84	0.42
1:H:156:HIS:CG	1:H:156:HIS:O	2.72	0.42
2:I:135:VAL:CG2	2:I:407:LYS:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:399:ASN:HB2	2:I:400:PRO:HD2	2.00	0.42
2:I:437:ARG:HH22	2:I:491:GLU:CD	2.21	0.42
2:I:470:PRO:HA	2:I:484:VAL:O	2.20	0.42
2:I:892:LEU:HD13	2:I:970:GLY:HA2	2.02	0.42
2:I:888:THR:HG22	2:I:989:VAL:O	2.19	0.42
3:J:95:LEU:HA	3:J:95:LEU:HD12	1.91	0.42
5:L:142:ILE:HA	5:L:145:VAL:HB	2.02	0.42
5:L:385:LYS:HA	5:L:390:LEU:HD12	2.02	0.42
1:B:156:HIS:CG	1:B:156:HIS:O	2.72	0.42
2:C:22:GLN:HA	2:C:336:VAL:HG21	2.01	0.42
2:C:498:GLN:H	2:C:501:THR:HG23	1.85	0.42
2:C:926:PHE:CE2	2:C:960:GLU:HG3	2.55	0.42
2:C:971:LYS:HA	2:C:988:VAL:HA	2.00	0.42
3:D:1479:ASP:HA	3:D:1482:ARG:HG2	2.01	0.42
3:D:218:LYS:NZ	3:D:338:GLU:HB3	2.35	0.42
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.83	0.42
3:D:637:LEU:HG	3:D:641:GLN:HB3	2.01	0.42
3:D:1481:VAL:HG21	4:E:17:TYR:HB2	2.00	0.42
5:F:375:LYS:HD3	5:F:426:HIS:CG	2.55	0.42
2:I:858:MET:SD	2:I:859:PRO:HD2	2.60	0.42
2:I:889:HIS:HA	2:I:892:LEU:HD12	2.01	0.42
3:J:116:LEU:HD23	3:J:468:LEU:HD22	2.00	0.42
3:J:1188:VAL:HG12	3:J:1189:ARG:N	2.35	0.42
3:J:95:LEU:HD21	3:J:578:VAL:HG21	2.01	0.42
5:L:302:SER:H	5:L:305:GLU:CG	2.33	0.42
2:C:207:LEU:HD13	2:C:227:LEU:HD11	2.00	0.42
2:C:526:PRO:O	2:C:529:VAL:HG12	2.19	0.42
2:C:720:GLU:CD	2:C:760:SER:HB3	2.40	0.42
2:C:816:LYS:HG3	2:C:817:PRO:CD	2.50	0.42
3:D:1059:SER:HB3	3:D:1063:GLU:HB2	2.00	0.42
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.19	0.42
3:D:217:ARG:HG3	3:D:341:GLU:OE1	2.20	0.42
3:D:508:ARG:HB2	3:D:511:TRP:NE1	2.35	0.42
2:C:713:ARG:NH1	3:D:533:GLY:HA2	2.34	0.42
3:D:646:LYS:HE3	3:D:688:TRP:CZ2	2.55	0.42
1:G:88:ARG:HB2	1:G:204:SER:HA	2.02	0.42
1:G:44:LEU:HD11	1:G:199:ILE:CD1	2.49	0.42
1:G:219:LYS:HE3	1:H:219:LYS:HD3	2.02	0.42
2:I:603:VAL:O	2:I:646:GLY:HA2	2.19	0.42
3:J:100:ALA:N	3:J:575:GLN:HE22	2.17	0.42
3:J:1011:PHE:HZ	3:J:1039:CYS:HG	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:789:LEU:O	3:J:792:ILE:HG13	2.19	0.42
5:L:173:GLU:O	5:L:177:LYS:HB2	2.20	0.42
5:L:334:THR:O	5:L:344:TYR:HB2	2.19	0.42
1:A:104:GLU:HG3	1:A:137:LYS:HG2	2.00	0.42
1:B:188:GLN:HA	3:D:688:TRP:CD1	2.54	0.42
1:B:54:THR:OG1	1:B:55:SER:N	2.50	0.42
2:C:1056:LYS:O	3:D:624:ASP:N	2.35	0.42
2:C:1102:LEU:HD12	2:C:1107:ASN:N	2.34	0.42
2:C:269:LEU:H	2:C:288:ARG:HB3	1.84	0.42
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.42
2:C:437:ARG:HH22	2:C:491:GLU:CD	2.21	0.42
2:C:499:ALA:N	2:C:533:ASP:HB3	2.35	0.42
2:C:603:VAL:O	2:C:646:GLY:HA2	2.19	0.42
3:D:1254:GLN:HG3	3:D:1258:ARG:HD3	2.01	0.42
3:D:1255:GLY:O	3:D:1259:VAL:HG23	2.20	0.42
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.02	0.42
3:D:750:PRO:HG2	3:D:756:GLN:HE22	1.85	0.42
3:D:895:VAL:O	3:D:899:LEU:HG	2.19	0.42
4:E:88:GLU:HG2	4:E:91:ARG:NH2	2.35	0.42
1:G:89:PHE:HE1	1:G:120:VAL:HG12	1.85	0.42
1:G:44:LEU:O	1:G:174:VAL:HG11	2.20	0.42
2:I:1050:GLN:HE22	3:J:1470:ARG:C	2.23	0.42
2:I:432:ARG:HH22	2:I:518:ARG:NH2	2.18	0.42
2:I:926:PHE:O	2:I:930:GLN:HG2	2.19	0.42
3:J:178:LEU:HD11	3:J:190:GLU:O	2.20	0.42
5:L:206:ASN:O	5:L:209:LEU:HB3	2.20	0.42
2:C:380:ALA:O	2:C:383:ARG:HG2	2.20	0.42
2:C:399:ASN:HB2	2:C:400:PRO:HD2	2.01	0.42
2:C:525:ALA:HB1	2:C:527:GLU:OE2	2.20	0.42
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.55	0.42
2:C:761:PHE:HA	2:C:785:VAL:HA	2.01	0.42
3:D:205:TYR:CD1	3:D:393:ILE:HG12	2.53	0.42
5:F:160:PRO:HG2	5:F:164:GLU:HG2	2.01	0.42
1:H:48:ILE:HG22	1:H:173:PRO:HD2	2.02	0.42
2:I:549:PHE:HB3	2:I:886:LEU:HD12	2.01	0.42
2:I:648:ARG:HG2	2:I:648:ARG:H	1.69	0.42
3:J:12:LEU:HD12	3:J:507:ASN:HB3	2.02	0.42
3:J:815:ALA:HB1	3:J:821:VAL:HG23	2.02	0.42
3:J:790:TYR:CD1	3:J:907:GLU:HB3	2.55	0.42
1:A:44:LEU:HD11	1:A:199:ILE:CD1	2.49	0.41
1:B:75:VAL:O	1:B:79:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:PRO:HD2	2:C:267:TYR:HD1	1.85	0.41
2:C:339:LEU:O	2:C:342:ASP:HB2	2.19	0.41
3:D:1215:VAL:HG21	3:D:1221:VAL:CG1	2.50	0.41
3:D:1216:SER:HB2	4:E:16:LYS:H	1.85	0.41
3:D:15:PRO:HG3	3:D:514:LEU:HD12	2.02	0.41
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.84	0.41
5:F:343:PHE:HD2	5:F:343:PHE:HA	1.75	0.41
2:I:98:LEU:HD22	2:I:113:VAL:HG22	2.02	0.41
2:I:950:LEU:HD11	2:I:952:LEU:HD13	2.02	0.41
3:J:1047:LYS:CG	3:J:1048:PRO:HD2	2.50	0.41
3:J:1206:GLY:HA2	3:J:1215:VAL:HG12	2.02	0.41
3:J:1274:ILE:HD12	3:J:1322:GLY:HA2	2.02	0.41
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.95	0.41
3:J:643:GLY:HA3	3:J:727:GLN:HB2	2.02	0.41
3:J:643:GLY:O	3:J:726:ILE:HG23	2.20	0.41
3:J:771:SER:HA	3:J:772:PRO:HD3	1.93	0.41
4:K:10:PHE:CE1	4:K:16:LYS:HG2	2.55	0.41
2:C:124:ASP:HB2	2:C:407:LYS:HZ2	1.85	0.41
2:C:191:PHE:HA	2:C:192:PRO:HD3	1.89	0.41
2:C:399:ASN:O	2:C:402:SER:HB2	2.20	0.41
2:C:535:SER:O	2:C:538:GLN:HG2	2.20	0.41
2:C:72:ARG:O	2:C:94:LEU:HD12	2.20	0.41
2:C:952:LEU:HD21	2:C:971:LYS:HZ2	1.84	0.41
3:D:1307:LYS:HB3	3:D:1307:LYS:HE3	1.76	0.41
3:D:216:LEU:HB3	3:D:218:LYS:HE2	2.01	0.41
3:D:638:LYS:HB3	3:D:641:GLN:NE2	2.35	0.41
3:D:666:PHE:CE1	3:D:687:VAL:HG12	2.55	0.41
3:D:698:LYS:HG3	4:E:59:ASN:OD1	2.20	0.41
3:D:1475:GLY:HA2	4:E:17:TYR:CZ	2.55	0.41
5:F:181:LEU:HB3	5:F:185:LEU:HB2	2.03	0.41
1:G:227:ASN:HA	1:G:228:PRO:HD2	1.75	0.41
2:I:291:VAL:HG13	2:I:303:PHE:CE1	2.56	0.41
2:I:5:ARG:HE	2:I:5:ARG:HB2	1.72	0.41
2:I:838:LYS:HG2	2:I:997:LEU:HD12	2.02	0.41
3:J:1207:TYR:H	3:J:1214:PRO:HA	1.84	0.41
3:J:1465:ASN:OD1	3:J:1470:ARG:HB3	2.20	0.41
5:L:315:ASP:O	5:L:319:VAL:HG12	2.20	0.41
2:I:1064:ASN:ND2	5:L:359:ALA:HB2	2.27	0.41
1:A:99:LEU:HD13	1:A:144:VAL:HG23	2.02	0.41
1:A:53:VAL:CG2	1:A:54:THR:H	2.27	0.41
2:C:530:GLU:HG2	2:C:530:GLU:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:941:LYS:NZ	2:C:959:PRO:HG2	2.35	0.41
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.55	0.41
3:D:58:CYS:HB2	3:D:78:VAL:HB	2.01	0.41
3:D:869:LEU:HD21	3:D:893:GLU:HG3	2.02	0.41
5:F:146:VAL:HG12	5:F:150:ILE:HG13	2.02	0.41
5:F:398:LEU:HD12	5:F:412:ILE:HB	2.02	0.41
1:H:80:LEU:HD23	3:J:867:ARG:HB2	2.02	0.41
2:I:1034:GLU:H	2:I:1034:GLU:HG3	1.69	0.41
2:I:344:PHE:HA	2:I:382:LEU:HD11	2.01	0.41
2:I:537:LYS:NZ	2:I:905:VAL:HG22	2.35	0.41
3:J:1105:ILE:HG23	3:J:1199:GLY:HA2	2.02	0.41
3:J:1236:LEU:HD22	3:J:1355:VAL:HG12	2.02	0.41
2:I:1085:PHE:CE2	3:J:1468:LEU:HD22	2.56	0.41
3:J:203:ALA:HA	3:J:395:VAL:HA	2.02	0.41
3:J:569:ASN:HD22	5:L:229:GLN:HE21	1.66	0.41
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	2.02	0.41
1:B:49:PRO:HD2	1:B:213:GLN:HE22	1.86	0.41
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.84	0.41
3:D:1147:ARG:HB3	3:D:1188:VAL:CG1	2.51	0.41
3:D:789:LEU:O	3:D:792:ILE:HG13	2.21	0.41
1:B:176:ARG:NH1	3:D:884:ARG:HH12	2.18	0.41
4:E:52:GLU:HG3	4:E:52:GLU:H	1.59	0.41
5:F:367:GLU:O	5:F:370:GLU:N	2.51	0.41
1:G:57:TYR:C	1:G:58:ILE:HD12	2.41	0.41
2:I:198:ARG:HE	2:I:198:ARG:HB2	1.50	0.41
2:I:839:LEU:HA	2:I:995:MET:O	2.20	0.41
2:I:89:THR:HB	2:I:91:GLN:NE2	2.35	0.41
2:I:673:LEU:HA	2:I:990:GLY:O	2.20	0.41
3:J:1386:ASP:HB2	3:J:1412:LYS:HB3	2.02	0.41
5:L:94:ASP:O	5:L:98:GLN:HB2	2.21	0.41
1:A:38:ASN:HB2	1:A:179:PHE:CZ	2.56	0.41
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	2.02	0.41
2:C:429:ASP:OD1	2:C:430:VAL:N	2.43	0.41
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.92	0.41
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.41
3:D:1442:ASN:O	3:D:1446:VAL:HG23	2.20	0.41
3:D:1460:ILE:HG13	3:D:1461:GLY:H	1.85	0.41
3:D:231:VAL:N	3:D:243:ALA:HA	2.23	0.41
3:D:371:ILE:HG23	3:D:372:ASP:N	2.32	0.41
3:D:886:VAL:O	3:D:890:VAL:HG23	2.20	0.41
1:H:51:THR:HG21	1:H:86:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:530:GLU:H	2:I:530:GLU:HG2	1.59	0.41
2:I:676:ILE:HA	2:I:871:LEU:O	2.20	0.41
3:J:401:TYR:HE1	3:J:446:VAL:HB	1.85	0.41
3:J:525:ARG:HB2	3:J:541:ASN:OD1	2.20	0.41
5:L:276:PRO:HB2	5:L:279:MET:HG2	2.03	0.41
1:A:74:ASP:O	1:A:77:GLU:HB3	2.20	0.41
1:B:201:THR:HG21	1:B:205:VAL:HG23	2.03	0.41
2:C:1070:ILE:H	2:C:1070:ILE:HG13	1.55	0.41
2:C:215:GLY:O	2:C:217:LEU:N	2.54	0.41
2:C:307:LEU:HD12	2:C:310:LEU:HD23	2.03	0.41
2:C:508:ILE:HG21	2:C:526:PRO:HB3	2.02	0.41
3:D:1310:ARG:HH21	3:D:1327:ARG:NH1	2.18	0.41
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	2.03	0.41
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.19	0.41
1:G:149:GLY:O	1:G:171:PHE:HB2	2.21	0.41
1:G:48:ILE:HD13	1:G:48:ILE:HA	1.90	0.41
1:G:63:HIS:HD2	1:G:66:SER:HB2	1.86	0.41
2:I:418:LEU:HD21	2:I:427:VAL:HG11	2.01	0.41
2:I:64:LEU:HD21	2:I:66:LEU:CB	2.50	0.41
2:I:718:GLY:HA2	2:I:719:PRO:HD3	1.78	0.41
3:J:1031:ASN:O	3:J:1034:GLN:HB3	2.20	0.41
3:J:1382:THR:O	3:J:1416:ALA:HB3	2.20	0.41
3:J:786:ILE:CD1	3:J:908:LYS:HG2	2.48	0.41
4:K:52:GLU:H	4:K:52:GLU:HG3	1.60	0.41
5:L:421:ARG:O	5:L:424:LYS:HB2	2.21	0.41
1:B:32:PHE:O	1:B:36:LEU:HG	2.20	0.41
1:A:65:PHE:CE1	2:C:703:ILE:HD13	2.55	0.41
2:C:557:ARG:CG	2:C:879:ARG:HB3	2.40	0.41
2:C:98:LEU:HD22	2:C:113:VAL:HG22	2.01	0.41
3:D:1011:PHE:HZ	3:D:1039:CYS:HG	1.62	0.41
3:D:1117:TYR:HA	3:D:1193:THR:HG21	2.02	0.41
3:D:184:GLU:HG2	3:D:184:GLU:H	1.66	0.41
3:D:354:ILE:HG13	3:D:369:ALA:H	1.85	0.41
3:D:691:LEU:O	3:D:695:ILE:HG13	2.20	0.41
3:D:750:PRO:HB2	3:D:756:GLN:HA	2.03	0.41
5:F:210:VAL:HG21	5:F:235:LEU:HD22	2.03	0.41
2:I:167:LYS:HB3	2:I:167:LYS:HE3	1.93	0.41
2:I:237:ARG:HH22	2:I:241:LEU:HD21	1.86	0.41
2:I:291:VAL:HB	2:I:299:LYS:O	2.20	0.41
2:I:574:ALA:HA	2:I:670:GLN:CG	2.51	0.41
2:I:744:ARG:NH1	2:I:746:GLY:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:952:LEU:HD21	2:I:971:LYS:NZ	2.34	0.41
2:I:995:MET:HE3	2:I:995:MET:HA	2.02	0.41
3:J:1125:MET:HA	3:J:1132:LEU:HA	2.03	0.41
3:J:1465:ASN:HA	3:J:1468:LEU:HB2	2.02	0.41
3:J:67:ARG:HD2	5:L:394:ARG:CB	2.48	0.41
3:J:650:LEU:HD21	3:J:688:TRP:HZ3	1.85	0.41
3:J:970:LYS:O	3:J:973:GLN:HB3	2.21	0.41
5:L:232:ASN:O	5:L:236:ILE:HG13	2.20	0.41
3:J:669:ASN:HD22	5:L:364:LEU:HD11	1.86	0.41
7:P:14:DC:H2"	7:P:15:DA:OP2	2.21	0.41
1:A:149:GLY:O	1:A:171:PHE:HB2	2.21	0.41
2:C:696:LYS:NZ	2:C:855:VAL:HG11	2.36	0.41
2:C:889:HIS:HA	2:C:892:LEU:HD12	2.02	0.41
2:C:97:ARG:NH2	2:C:112:GLU:HB2	2.36	0.41
3:D:121:THR:O	3:D:124:GLU:HB3	2.20	0.41
3:D:213:VAL:HG13	3:D:384:VAL:O	2.21	0.41
3:D:760:ARG:HH21	4:E:65:MET:HG3	1.86	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.87	0.41
1:G:99:LEU:HD13	1:G:144:VAL:HG23	2.02	0.41
1:H:55:SER:HB2	1:H:158:ILE:HG23	2.03	0.41
2:I:525:ALA:HA	2:I:526:PRO:HD3	1.91	0.41
2:I:585:GLU:O	2:I:588:VAL:HG22	2.20	0.41
3:J:1366:LYS:O	3:J:1369:GLU:HB2	2.21	0.41
3:J:1396:GLU:HB3	3:J:1399:ASP:OD1	2.21	0.41
3:J:589:SER:HA	3:J:590:PRO:HD3	1.95	0.41
3:J:638:LYS:HG3	3:J:640:HIS:H	1.86	0.41
3:J:664:LYS:HE2	3:J:666:PHE:HE2	1.86	0.41
3:J:858:LEU:HD12	3:J:859:ASP:H	1.86	0.41
3:J:573:MET:HE3	5:L:225:LEU:HB3	2.01	0.41
5:L:381:ALA:O	5:L:385:LYS:HG3	2.21	0.41
7:S:14:DC:H2"	7:S:15:DA:OP2	2.20	0.41
2:C:1089:VAL:HG13	2:C:1099:VAL:HG11	2.03	0.41
2:C:229:MET:CB	2:C:234:ALA:HB2	2.46	0.41
2:C:328:LEU:HD23	2:C:437:ARG:HD2	2.03	0.41
2:C:474:VAL:HG23	2:C:478:VAL:O	2.21	0.41
2:C:537:LYS:NZ	2:C:905:VAL:HG22	2.36	0.41
3:D:1038:LEU:O	3:D:1060:SER:OG	2.23	0.41
3:D:229:ALA:HB1	3:D:245:LEU:N	2.36	0.41
2:C:1086:ARG:HB3	3:D:88:TYR:HE2	1.85	0.41
4:E:10:PHE:CE1	4:E:16:LYS:HG2	2.56	0.41
1:G:14:THR:O	1:G:14:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:PHE:O	1:G:172:SER:OG	2.37	0.41
1:G:52:ALA:O	1:G:53:VAL:HG12	2.21	0.41
2:I:1102:LEU:HD12	2:I:1107:ASN:N	2.35	0.41
2:I:55:GLU:HA	2:I:64:LEU:O	2.20	0.41
2:I:93:PRO:HG3	2:I:117:HIS:NE2	2.36	0.41
2:I:944:LEU:HD13	2:I:959:PRO:HB3	2.02	0.41
3:J:542:ASP:O	3:J:545:ARG:HB3	2.20	0.41
3:J:654:LYS:HB3	3:J:655:PRO:HD3	2.03	0.41
3:J:895:VAL:O	3:J:899:LEU:HG	2.20	0.41
7:P:16:DC:H2''	7:P:17:DT:OP2	2.21	0.41
1:A:14:THR:O	1:A:14:THR:HG22	2.21	0.41
2:C:45:GLN:HE21	2:C:48:PHE:HD2	1.69	0.41
2:C:525:ALA:HA	2:C:526:PRO:HD3	1.92	0.41
2:C:648:ARG:H	2:C:648:ARG:HG2	1.67	0.41
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.85	0.41
2:C:857:ASP:OD1	2:C:857:ASP:N	2.54	0.41
3:D:1271:LYS:HG3	3:D:1331:ASP:HB2	2.03	0.41
5:F:206:ASN:O	5:F:210:VAL:HG23	2.20	0.41
5:F:334:THR:O	5:F:344:TYR:HB2	2.21	0.41
1:H:13:ALA:CB	1:H:23:PHE:HD1	2.34	0.41
2:I:97:ARG:NH2	2:I:112:GLU:HB2	2.36	0.41
2:I:215:GLY:O	2:I:217:LEU:N	2.54	0.41
2:I:683:ASN:OD1	2:I:872:ASN:HB2	2.21	0.41
2:I:571:LEU:CD2	2:I:995:MET:HE1	2.51	0.41
3:J:1084:THR:O	3:J:1088:THR:HG23	2.21	0.41
3:J:1372:VAL:HA	3:J:1375:MET:SD	2.61	0.41
3:J:137:PRO:HG3	3:J:148:GLU:HA	2.02	0.41
3:J:1429:LEU:HG	3:J:1440:PHE:HD1	1.85	0.41
3:J:182:GLY:H	3:J:204:LEU:HD23	1.86	0.41
3:J:657:LEU:HD22	3:J:691:LEU:HD13	2.03	0.41
2:I:872:ASN:ND2	3:J:784:ASP:OD2	2.54	0.41
5:L:160:PRO:HG2	5:L:164:GLU:HG2	2.03	0.41
5:L:181:LEU:HB3	5:L:185:LEU:HB2	2.03	0.41
5:L:375:LYS:HD3	5:L:426:HIS:CG	2.56	0.41
6:O:24:DC:H1'	6:O:25:DT:H5'	2.01	0.41
1:A:33:GLY:O	1:A:195:LEU:HD21	2.21	0.41
1:A:43:ILE:HG13	1:B:35:THR:HG21	2.02	0.41
1:A:46:SER:OG	1:A:47:SER:N	2.54	0.41
2:C:291:VAL:HB	2:C:299:LYS:O	2.21	0.41
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	2.02	0.41
2:C:603:VAL:HA	2:C:613:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:988:VAL:H	3:D:948:THR:HG21	1.85	0.41
3:D:900:ILE:HG12	3:D:914:LEU:CD2	2.51	0.41
5:F:154:ALA:HB1	5:F:158:LYS:HE2	2.02	0.41
1:G:158:ILE:HG22	1:G:159:LYS:N	2.36	0.41
2:I:1085:PHE:O	2:I:1089:VAL:HG23	2.21	0.41
2:I:639:GLN:HA	2:I:657:ASP:O	2.21	0.41
3:J:1460:ILE:HG13	3:J:1461:GLY:N	2.36	0.41
3:J:691:LEU:O	3:J:695:ILE:HG13	2.20	0.41
3:J:886:VAL:O	3:J:890:VAL:HG23	2.21	0.41
6:O:6:DC:H2''	6:O:7:DA:OP2	2.21	0.41
1:A:107:LYS:HE2	1:A:113:ASP:OD2	2.21	0.40
1:A:97:THR:HG23	1:A:98:THR:N	2.27	0.40
1:B:90:LEU:HB2	1:B:119:ASP:HB3	2.03	0.40
2:C:223:ASP:OD1	2:C:226:VAL:HG23	2.21	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.97	0.40
2:C:512:ARG:H	2:C:512:ARG:HG2	1.54	0.40
2:C:529:VAL:HG13	2:C:529:VAL:O	2.21	0.40
2:C:585:GLU:O	2:C:588:VAL:HG22	2.22	0.40
2:C:865:THR:HA	2:C:866:PRO:HD2	1.94	0.40
3:D:1290:LEU:HB2	3:D:1307:LYS:HA	2.03	0.40
3:D:786:ILE:CD1	3:D:908:LYS:HG2	2.49	0.40
3:D:698:LYS:H	4:E:59:ASN:ND2	2.19	0.40
2:C:1063:ARG:HH21	5:F:353:LEU:HD23	1.86	0.40
5:F:99:TYR:HE2	5:F:211:VAL:HG22	1.86	0.40
1:H:159:LYS:HG3	1:H:164:ALA:HB3	2.03	0.40
1:H:188:GLN:HA	3:J:688:TRP:CD1	2.52	0.40
2:I:1010:THR:HG23	2:I:1013:TYR:OH	2.21	0.40
2:I:124:ASP:HB2	2:I:407:LYS:NZ	2.36	0.40
2:I:352:ALA:O	2:I:356:ARG:HG3	2.20	0.40
2:I:670:GLN:HE22	2:I:699:PHE:HA	1.86	0.40
2:I:6:PHE:HE1	2:I:901:TYR:HB3	1.86	0.40
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.83	0.40
3:J:547:LEU:HD13	3:J:578:VAL:HG22	2.03	0.40
3:J:698:LYS:HG2	3:J:756:GLN:HG2	2.03	0.40
3:J:974:ILE:HG12	3:J:991:GLN:HG2	2.03	0.40
5:L:206:ASN:O	5:L:210:VAL:HG23	2.22	0.40
7:P:7:DA:H1'	7:P:8:DA:H5'	2.02	0.40
7:S:19:DT:H1'	7:S:20:DT:H5'	2.02	0.40
1:A:40:LEU:HG	1:A:218:LEU:HD22	2.03	0.40
1:B:17:GLY:HA3	1:B:19:HIS:CE1	2.56	0.40
1:B:79:ILE:HA	1:B:82:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:ASP:OD1	2:C:1107:ASN:HB2	2.21	0.40
2:C:166:PRO:C	2:C:168:ARG:H	2.25	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.84	0.40
2:C:561:GLY:O	2:C:565:GLN:HG2	2.21	0.40
2:C:577:PRO:HD3	2:C:993:PHE:CZ	2.56	0.40
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	2.03	0.40
3:D:178:LEU:HD11	3:D:190:GLU:O	2.21	0.40
3:D:285:PRO:HD2	3:D:288:MET:SD	2.61	0.40
3:D:101:HIS:HE2	3:D:582:ILE:HG21	1.84	0.40
3:D:684:LYS:HB3	3:D:686:GLU:HG3	2.04	0.40
2:I:1070:ILE:H	2:I:1070:ILE:HG13	1.58	0.40
2:I:246:ASP:HA	2:I:247:PRO:HD3	1.94	0.40
2:I:360:VAL:HG21	5:L:216:LYS:NZ	2.37	0.40
2:I:399:ASN:O	2:I:402:SER:HB2	2.21	0.40
2:I:498:GLN:H	2:I:501:THR:HG23	1.87	0.40
3:J:1129:THR:C	3:J:1131:THR:H	2.25	0.40
3:J:1268:PRO:HB3	3:J:1329:ALA:HB3	2.04	0.40
1:B:182:GLU:CG	1:B:194:LYS:HB3	2.52	0.40
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.21	0.40
3:D:131:LYS:HE2	3:D:152:LEU:HB3	2.04	0.40
3:D:229:ALA:O	3:D:244:GLU:HB2	2.21	0.40
3:D:256:SER:HB3	3:D:300:VAL:HG23	2.03	0.40
3:D:388:HIS:C	3:D:389:GLU:HG3	2.41	0.40
3:D:551:ASN:O	3:D:555:LYS:HG3	2.22	0.40
3:D:640:HIS:O	3:D:717:GLN:HB2	2.21	0.40
3:D:545:ARG:NH1	5:F:269:GLN:O	2.54	0.40
5:F:418:LYS:O	5:F:422:LYS:HB2	2.21	0.40
1:G:34:VAL:HG22	1:G:181:VAL:HG21	2.03	0.40
1:H:23:PHE:CE2	1:H:199:ILE:HB	2.55	0.40
2:I:65:VAL:CG1	2:I:101:ILE:HB	2.50	0.40
2:I:607:ASP:HB3	2:I:610:ARG:O	2.21	0.40
3:J:1207:TYR:HA	3:J:1213:ARG:O	2.21	0.40
3:J:1396:GLU:OE2	3:J:1432:LYS:HD3	2.21	0.40
3:J:348:ALA:HB3	3:J:351:MET:HG3	2.03	0.40
3:J:669:ASN:ND2	5:L:364:LEU:HD11	2.36	0.40
3:J:692:GLU:HA	3:J:695:ILE:HD12	2.04	0.40
3:J:704:ARG:HB3	3:J:736:PHE:CD2	2.57	0.40
3:J:869:LEU:HD21	3:J:893:GLU:HG3	2.03	0.40
2:C:158:TYR:HD1	2:C:314:THR:HA	1.86	0.40
2:C:464:LEU:HD23	2:C:464:LEU:HA	1.95	0.40
3:D:1125:MET:N	3:D:1132:LEU:HD23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:654:LYS:HB3	3:D:655:PRO:HD3	2.03	0.40
1:G:195:LEU:HA	1:G:195:LEU:HD23	1.88	0.40
1:G:173:PRO:HB3	1:G:202:ASP:OD1	2.21	0.40
1:G:33:GLY:O	1:G:195:LEU:HD21	2.21	0.40
1:G:79:ILE:HD13	1:G:167:VAL:HG12	2.02	0.40
1:G:9:PRO:HB2	1:G:25:LEU:HD11	2.03	0.40
1:H:192:LEU:N	1:H:192:LEU:HD23	2.36	0.40
2:I:199:VAL:HA	2:I:231:PRO:HB3	2.02	0.40
2:I:17:PRO:O	2:I:19:THR:N	2.55	0.40
2:I:299:LYS:HG3	2:I:300:ASP:N	2.36	0.40
2:I:341:ALA:O	2:I:345:ARG:HG2	2.21	0.40
2:I:609:THR:O	2:I:625:LEU:N	2.54	0.40
2:I:725:ASP:O	2:I:759:THR:HG21	2.21	0.40
3:J:1153:VAL:HB	3:J:1160:LEU:HB3	2.04	0.40
3:J:65:ARG:HA	3:J:65:ARG:HD3	1.93	0.40
3:J:701:LEU:HD21	3:J:763:MET:CG	2.48	0.40
3:J:853:VAL:HA	3:J:858:LEU:HB3	2.04	0.40
5:L:130:LYS:HG2	5:L:188:TYR:CZ	2.56	0.40
7:P:15:DA:OP2	7:P:15:DA:H2'	2.22	0.40
1:B:192:LEU:N	1:B:192:LEU:HD23	2.36	0.40
1:A:35:THR:HG22	1:B:39:PRO:HA	2.02	0.40
2:C:327:HIS:O	2:C:331:ARG:HG3	2.22	0.40
2:C:627:ARG:HD3	2:C:639:GLN:O	2.21	0.40
2:C:878:SER:O	3:D:1034:GLN:NE2	2.51	0.40
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.93	0.40
3:D:364:GLY:HA2	3:D:379:ALA:O	2.21	0.40
3:D:553:ARG:HB3	3:D:570:GLU:OE1	2.20	0.40
3:D:598:ARG:HA	3:D:599:PRO:HD3	1.77	0.40
3:D:711:LEU:HD13	3:D:711:LEU:HA	1.95	0.40
1:G:107:LYS:HE2	1:G:113:ASP:OD2	2.22	0.40
1:H:129:ILE:HG22	1:H:130:ALA:N	2.37	0.40
1:H:75:VAL:O	1:H:79:ILE:HG13	2.21	0.40
2:I:554:ASP:OD2	2:I:556:ASN:HB2	2.22	0.40
2:I:585:GLU:HG2	2:I:665:PHE:CD1	2.56	0.40
3:J:1134:LEU:HD22	3:J:1135:ARG:N	2.37	0.40
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.21	0.40
5:L:145:VAL:HG21	5:L:174:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	20	63
1	B	225/314 (72%)	200 (89%)	20 (9%)	5 (2%)	8	46
1	G	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	20	63
1	H	225/314 (72%)	201 (89%)	18 (8%)	6 (3%)	6	41
2	C	1108/1119 (99%)	958 (86%)	139 (12%)	11 (1%)	18	61
2	I	1108/1119 (99%)	956 (86%)	140 (13%)	12 (1%)	17	60
3	D	1486/1524 (98%)	1315 (88%)	162 (11%)	9 (1%)	28	71
3	J	1361/1524 (89%)	1201 (88%)	150 (11%)	10 (1%)	25	68
4	E	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
4	K	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
5	F	343/347 (99%)	299 (87%)	42 (12%)	2 (1%)	28	71
5	L	343/347 (99%)	302 (88%)	40 (12%)	1 (0%)	44	81
All	All	6831/7434 (92%)	5982 (88%)	789 (12%)	60 (1%)	20	63

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
3	D	1209	LEU
1	G	53	VAL
3	J	1128	VAL
2	C	608	GLY
2	C	972	VAL
3	D	666	PHE
2	I	608	GLY
2	I	972	VAL
3	J	1287	GLU
1	B	161	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	882	LEU
1	H	161	ARG
2	I	882	LEU
3	J	422	ALA
1	A	98	THR
3	J	1130	ARG
1	B	178	ALA
2	C	295	ASP
2	C	365	ASP
2	C	607	ASP
3	D	1075	HIS
1	G	98	THR
1	H	178	ALA
2	I	295	ASP
2	I	365	ASP
2	I	607	ASP
3	J	1075	HIS
3	J	1207	TYR
1	B	202	ASP
3	D	667	ALA
5	F	270	ALA
1	H	51	THR
1	H	202	ASP
2	C	870	ILE
2	C	1016	ILE
3	D	1221	VAL
2	I	870	ILE
2	I	1016	ILE
3	J	667	ALA
3	J	1221	VAL
2	C	989	VAL
3	D	670	VAL
3	D	947	ILE
5	F	407	VAL
3	J	947	ILE
1	H	116	PRO
2	I	989	VAL
3	J	670	VAL
5	L	407	VAL
1	B	48	ILE
1	B	116	PRO
2	C	17	PRO

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Mol	Chain	Res	Type
2	C	852	ILE
3	D	259	VAL
1	H	48	ILE
2	I	17	PRO
2	I	852	ILE
2	I	1060	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	179 (92%)	15 (8%)	15	49
1	B	194/270 (72%)	172 (89%)	22 (11%)	7	31
1	G	194/270 (72%)	178 (92%)	16 (8%)	13	46
1	H	194/270 (72%)	171 (88%)	23 (12%)	6	29
2	C	931/936 (100%)	840 (90%)	91 (10%)	9	37
2	I	931/936 (100%)	840 (90%)	91 (10%)	9	37
3	D	1252/1281 (98%)	1114 (89%)	138 (11%)	7	32
3	J	1150/1281 (90%)	1028 (89%)	122 (11%)	8	34
4	E	83/88 (94%)	79 (95%)	4 (5%)	30	63
4	K	83/88 (94%)	79 (95%)	4 (5%)	30	63
5	F	296/299 (99%)	276 (93%)	20 (7%)	18	53
5	L	296/299 (99%)	276 (93%)	20 (7%)	18	53
All	All	5798/6288 (92%)	5232 (90%)	566 (10%)	9	37

All (566) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	32	PHE
1	A	45	LEU
1	A	51	THR

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Mol	Chain	Res	Type
1	A	63	HIS
1	A	73	GLU
1	A	74	ASP
1	A	113	ASP
1	A	158	ILE
1	A	174	VAL
1	A	176	ARG
1	A	198	ARG
1	A	222	LEU
1	A	227	ASN
1	A	232	LEU
1	B	7	LYS
1	B	23	PHE
1	B	38	ASN
1	B	44	LEU
1	B	51	THR
1	B	58	ILE
1	B	62	LEU
1	B	74	ASP
1	B	75	VAL
1	B	104	GLU
1	B	113	ASP
1	B	114	PHE
1	B	129	ILE
1	B	131	THR
1	B	158	ILE
1	B	177	VAL
1	B	189	ARG
1	B	192	LEU
1	B	201	THR
1	B	215	VAL
1	B	219	LYS
1	B	227	ASN
2	C	10	ARG
2	C	12	VAL
2	C	20	GLU
2	C	30	LEU
2	C	41	ASN
2	C	45	GLN
2	C	55	GLU
2	C	75	ASP
2	C	98	LEU

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Mol	Chain	Res	Type
2	C	101	ILE
2	C	104	ASP
2	C	107	LEU
2	C	134	ARG
2	C	142	ARG
2	C	148	PHE
2	C	174	LEU
2	C	176	VAL
2	C	187	ASN
2	C	194	VAL
2	C	203	ASP
2	C	211	LEU
2	C	221	LEU
2	C	232	GLU
2	C	238	LEU
2	C	242	LEU
2	C	268	ASP
2	C	280	LYS
2	C	283	VAL
2	C	297	GLU
2	C	308	ARG
2	C	323	ASP
2	C	336	VAL
2	C	361	MET
2	C	365	ASP
2	C	383	ARG
2	C	413	LEU
2	C	421	GLU
2	C	425	PHE
2	C	430	VAL
2	C	434	HIS
2	C	438	ILE
2	C	485	TYR
2	C	503	LEU
2	C	506	ASP
2	C	512	ARG
2	C	514	VAL
2	C	516	ARG
2	C	523	ILE
2	C	527	GLU
2	C	530	GLU
2	C	542	LEU

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Mol	Chain	Res	Type
2	C	543	ASN
2	C	571	LEU
2	C	579	VAL
2	C	604	VAL
2	C	653	ASP
2	C	673	LEU
2	C	685	GLU
2	C	707	ARG
2	C	729	LEU
2	C	754	ILE
2	C	761	PHE
2	C	784	ASP
2	C	788	THR
2	C	808	ARG
2	C	823	VAL
2	C	839	LEU
2	C	848	VAL
2	C	857	ASP
2	C	868	ASP
2	C	869	VAL
2	C	892	LEU
2	C	896	PHE
2	C	897	LEU
2	C	899	GLN
2	C	920	GLU
2	C	926	PHE
2	C	934	PHE
2	C	936	VAL
2	C	950	LEU
2	C	952	LEU
2	C	968	ASP
2	C	969	LEU
2	C	972	VAL
2	C	994	ILE
2	C	995	MET
2	C	1001	VAL
2	C	1035	MET
2	C	1061	GLU
2	C	1075	ASP
2	C	1112	PHE
3	D	5	VAL
3	D	26	VAL

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Mol	Chain	Res	Type
3	D	37	LEU
3	D	54	LYS
3	D	62	LYS
3	D	66	GLN
3	D	68	PHE
3	D	80	VAL
3	D	92	HIS
3	D	121	THR
3	D	135	LEU
3	D	152	LEU
3	D	154	THR
3	D	155	ASP
3	D	166	GLN
3	D	168	THR
3	D	171	LEU
3	D	178	LEU
3	D	180	LYS
3	D	214	ASP
3	D	233	LYS
3	D	247	GLU
3	D	251	PHE
3	D	259	VAL
3	D	266	GLU
3	D	277	GLU
3	D	281	ARG
3	D	297	ILE
3	D	306	GLU
3	D	315	ARG
3	D	327	GLU
3	D	332	HIS
3	D	334	THR
3	D	335	LEU
3	D	347	VAL
3	D	350	HIS
3	D	389	GLU
3	D	408	GLU
3	D	414	ARG
3	D	423	ASP
3	D	442	ASN
3	D	450	TYR
3	D	461	ILE
3	D	464	LEU

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Mol	Chain	Res	Type
3	D	475	ARG
3	D	525	ARG
3	D	538	SER
3	D	546	ARG
3	D	548	ILE
3	D	576	GLU
3	D	596	SER
3	D	598	ARG
3	D	619	LEU
3	D	636	GLN
3	D	639	LEU
3	D	658	LEU
3	D	683	ILE
3	D	685	ASP
3	D	688	TRP
3	D	694	VAL
3	D	707	THR
3	D	708	LEU
3	D	709	HIS
3	D	717	GLN
3	D	747	VAL
3	D	748	HIS
3	D	762	GLN
3	D	776	GLU
3	D	787	LEU
3	D	810	GLU
3	D	811	GLU
3	D	832	ARG
3	D	835	SER
3	D	838	ARG
3	D	850	LEU
3	D	861	GLN
3	D	865	THR
3	D	875	THR
3	D	897	GLN
3	D	899	LEU
3	D	903	ASP
3	D	908	LYS
3	D	909	ASN
3	D	930	LEU
3	D	932	ASP
3	D	945	SER

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Mol	Chain	Res	Type
3	D	964	LEU
3	D	976	GLN
3	D	1004	THR
3	D	1015	TYR
3	D	1029	ARG
3	D	1066	THR
3	D	1078	ARG
3	D	1094	LEU
3	D	1100	ASP
3	D	1107	VAL
3	D	1108	ARG
3	D	1112	CYS
3	D	1120	VAL
3	D	1123	PHE
3	D	1130	ARG
3	D	1134	LEU
3	D	1137	ARG
3	D	1139	ASP
3	D	1144	LEU
3	D	1156	LEU
3	D	1160	LEU
3	D	1161	GLU
3	D	1162	GLU
3	D	1170	ASP
3	D	1179	GLU
3	D	1201	CYS
3	D	1203	LYS
3	D	1213	ARG
3	D	1231	GLU
3	D	1256	LEU
3	D	1258	ARG
3	D	1267	ARG
3	D	1278	ASP
3	D	1285	GLU
3	D	1295	GLU
3	D	1297	GLU
3	D	1302	GLU
3	D	1305	LEU
3	D	1310	ARG
3	D	1312	LEU
3	D	1342	GLU
3	D	1380	GLU

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Mol	Chain	Res	Type
3	D	1382	THR
3	D	1386	ASP
3	D	1395	LEU
3	D	1407	LEU
3	D	1413	VAL
3	D	1444	THR
3	D	1448	THR
3	D	1459	LEU
3	D	1462	LEU
3	D	1499	ARG
4	E	14	ASP
4	E	30	LEU
4	E	39	VAL
4	E	56	ASP
5	F	108	LEU
5	F	138	ASP
5	F	139	GLN
5	F	151	LEU
5	F	165	LYS
5	F	175	ASP
5	F	196	GLU
5	F	202	LEU
5	F	224	PHE
5	F	233	GLN
5	F	293	LEU
5	F	328	GLU
5	F	339	GLU
5	F	343	PHE
5	F	371	LYS
5	F	404	TYR
5	F	405	PHE
5	F	409	ARG
5	F	424	LYS
5	F	433	LEU
1	G	20	TYR
1	G	32	PHE
1	G	45	LEU
1	G	51	THR
1	G	63	HIS
1	G	73	GLU
1	G	74	ASP
1	G	80	LEU

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Mol	Chain	Res	Type
1	G	113	ASP
1	G	158	ILE
1	G	174	VAL
1	G	176	ARG
1	G	198	ARG
1	G	222	LEU
1	G	227	ASN
1	G	232	LEU
1	H	7	LYS
1	H	23	PHE
1	H	38	ASN
1	H	44	LEU
1	H	51	THR
1	H	58	ILE
1	H	62	LEU
1	H	74	ASP
1	H	75	VAL
1	H	104	GLU
1	H	113	ASP
1	H	114	PHE
1	H	129	ILE
1	H	131	THR
1	H	140	MET
1	H	158	ILE
1	H	177	VAL
1	H	189	ARG
1	H	192	LEU
1	H	201	THR
1	H	215	VAL
1	H	219	LYS
1	H	227	ASN
2	I	10	ARG
2	I	12	VAL
2	I	20	GLU
2	I	30	LEU
2	I	41	ASN
2	I	45	GLN
2	I	55	GLU
2	I	75	ASP
2	I	98	LEU
2	I	101	ILE
2	I	104	ASP

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Mol	Chain	Res	Type
2	I	107	LEU
2	I	134	ARG
2	I	142	ARG
2	I	148	PHE
2	I	174	LEU
2	I	176	VAL
2	I	187	ASN
2	I	194	VAL
2	I	203	ASP
2	I	211	LEU
2	I	221	LEU
2	I	232	GLU
2	I	238	LEU
2	I	242	LEU
2	I	268	ASP
2	I	280	LYS
2	I	283	VAL
2	I	297	GLU
2	I	308	ARG
2	I	323	ASP
2	I	336	VAL
2	I	361	MET
2	I	365	ASP
2	I	383	ARG
2	I	413	LEU
2	I	421	GLU
2	I	425	PHE
2	I	430	VAL
2	I	434	HIS
2	I	438	ILE
2	I	485	TYR
2	I	487	THR
2	I	503	LEU
2	I	506	ASP
2	I	512	ARG
2	I	514	VAL
2	I	523	ILE
2	I	527	GLU
2	I	530	GLU
2	I	542	LEU
2	I	543	ASN
2	I	571	LEU

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Mol	Chain	Res	Type
2	I	579	VAL
2	I	604	VAL
2	I	653	ASP
2	I	673	LEU
2	I	685	GLU
2	I	707	ARG
2	I	729	LEU
2	I	754	ILE
2	I	761	PHE
2	I	784	ASP
2	I	788	THR
2	I	808	ARG
2	I	823	VAL
2	I	839	LEU
2	I	848	VAL
2	I	857	ASP
2	I	868	ASP
2	I	869	VAL
2	I	892	LEU
2	I	896	PHE
2	I	897	LEU
2	I	899	GLN
2	I	920	GLU
2	I	926	PHE
2	I	934	PHE
2	I	936	VAL
2	I	950	LEU
2	I	952	LEU
2	I	968	ASP
2	I	969	LEU
2	I	972	VAL
2	I	994	ILE
2	I	995	MET
2	I	1001	VAL
2	I	1035	MET
2	I	1061	GLU
2	I	1075	ASP
2	I	1112	PHE
3	J	26	VAL
3	J	37	LEU
3	J	54	LYS
3	J	62	LYS

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Mol	Chain	Res	Type
3	J	66	GLN
3	J	68	PHE
3	J	80	VAL
3	J	121	THR
3	J	135	LEU
3	J	154	THR
3	J	155	ASP
3	J	166	GLN
3	J	168	THR
3	J	171	LEU
3	J	178	LEU
3	J	180	LYS
3	J	210	ARG
3	J	211	VAL
3	J	350	HIS
3	J	375	GLU
3	J	399	ARG
3	J	404	GLU
3	J	410	THR
3	J	411	THR
3	J	414	ARG
3	J	423	ASP
3	J	430	GLU
3	J	450	TYR
3	J	462	GLN
3	J	512	MET
3	J	513	ILE
3	J	523	ASP
3	J	525	ARG
3	J	548	ILE
3	J	574	LEU
3	J	576	GLU
3	J	598	ARG
3	J	600	LEU
3	J	619	LEU
3	J	636	GLN
3	J	639	LEU
3	J	658	LEU
3	J	683	ILE
3	J	685	ASP
3	J	688	TRP
3	J	694	VAL

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Mol	Chain	Res	Type
3	J	707	THR
3	J	708	LEU
3	J	709	HIS
3	J	717	GLN
3	J	747	VAL
3	J	748	HIS
3	J	762	GLN
3	J	776	GLU
3	J	787	LEU
3	J	810	GLU
3	J	811	GLU
3	J	832	ARG
3	J	835	SER
3	J	838	ARG
3	J	850	LEU
3	J	861	GLN
3	J	865	THR
3	J	875	THR
3	J	897	GLN
3	J	899	LEU
3	J	903	ASP
3	J	908	LYS
3	J	909	ASN
3	J	930	LEU
3	J	932	ASP
3	J	945	SER
3	J	958	GLU
3	J	964	LEU
3	J	976	GLN
3	J	1004	THR
3	J	1015	TYR
3	J	1029	ARG
3	J	1066	THR
3	J	1078	ARG
3	J	1094	LEU
3	J	1100	ASP
3	J	1107	VAL
3	J	1112	CYS
3	J	1132	LEU
3	J	1134	LEU
3	J	1137	ARG
3	J	1149	LEU

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Mol	Chain	Res	Type
3	J	1159	ARG
3	J	1160	LEU
3	J	1161	GLU
3	J	1162	GLU
3	J	1170	ASP
3	J	1173	PHE
3	J	1183	VAL
3	J	1201	CYS
3	J	1203	LYS
3	J	1211	MET
3	J	1231	GLU
3	J	1235	GLN
3	J	1238	MET
3	J	1267	ARG
3	J	1285	GLU
3	J	1293	PHE
3	J	1297	GLU
3	J	1305	LEU
3	J	1318	TYR
3	J	1325	LEU
3	J	1326	THR
3	J	1335	LEU
3	J	1342	GLU
3	J	1376	LEU
3	J	1397	LYS
3	J	1407	LEU
3	J	1429	LEU
3	J	1432	LYS
3	J	1433	SER
3	J	1444	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1496	GLU
3	J	1499	ARG
4	K	14	ASP
4	K	30	LEU
4	K	39	VAL
4	K	56	ASP
5	L	108	LEU
5	L	138	ASP
5	L	139	GLN
5	L	151	LEU

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Mol	Chain	Res	Type
5	L	165	LYS
5	L	175	ASP
5	L	196	GLU
5	L	202	LEU
5	L	224	PHE
5	L	233	GLN
5	L	293	LEU
5	L	328	GLU
5	L	339	GLU
5	L	343	PHE
5	L	371	LYS
5	L	404	TYR
5	L	405	PHE
5	L	409	ARG
5	L	424	LYS
5	L	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	212	ASN
1	B	128	HIS
1	B	163	ASN
1	B	213	GLN
2	C	41	ASN
2	C	45	GLN
2	C	393	GLN
2	C	498	GLN
2	C	538	GLN
2	C	567	GLN
2	C	639	GLN
2	C	671	ASN
2	C	765	GLN
2	C	845	ASN
2	C	881	ASN
2	C	962	GLN
2	C	1050	GLN
2	C	1100	GLN
3	D	130	ASN
3	D	274	GLN
3	D	350	HIS

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Mol	Chain	Res	Type
3	D	362	GLN
3	D	549	ASN
3	D	552	ASN
3	D	560	GLN
3	D	569	ASN
3	D	593	ASN
3	D	680	GLN
3	D	703	ASN
3	D	756	GLN
3	D	762	GLN
3	D	768	ASN
3	D	794	GLN
3	D	897	GLN
3	D	991	GLN
3	D	1046	GLN
3	D	1116	ASN
3	D	1235	GLN
3	D	1359	GLN
4	E	37	ASN
4	E	59	ASN
5	F	233	GLN
5	F	294	GLN
5	F	295	GLN
5	F	417	ASN
5	F	426	HIS
1	G	63	HIS
1	G	81	ASN
1	G	212	ASN
1	H	128	HIS
1	H	163	ASN
1	H	213	GLN
2	I	22	GLN
2	I	41	ASN
2	I	45	GLN
2	I	393	GLN
2	I	498	GLN
2	I	538	GLN
2	I	567	GLN
2	I	639	GLN
2	I	671	ASN
2	I	765	GLN
2	I	845	ASN

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Mol	Chain	Res	Type
2	I	881	ASN
2	I	962	GLN
2	I	1050	GLN
2	I	1100	GLN
3	J	130	ASN
3	J	549	ASN
3	J	560	GLN
3	J	703	ASN
3	J	756	GLN
3	J	762	GLN
3	J	794	GLN
3	J	897	GLN
3	J	991	GLN
3	J	1046	GLN
4	K	37	ASN
4	K	59	ASN
5	L	229	GLN
5	L	294	GLN
5	L	295	GLN
5	L	417	ASN
5	L	426	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/314 (72%)	0.08	2 (0%) 84 78	107, 189, 236, 264	0
1	B	227/314 (72%)	-0.23	0 100 100	94, 161, 214, 264	0
1	G	227/314 (72%)	0.39	16 (7%) 17 16	116, 199, 240, 276	0
1	H	227/314 (72%)	-0.13	2 (0%) 84 78	116, 173, 216, 267	0
2	C	1112/1119 (99%)	-0.03	21 (1%) 67 60	90, 179, 243, 314	0
2	I	1112/1119 (99%)	0.01	25 (2%) 62 55	94, 185, 244, 315	0
3	D	1490/1524 (97%)	-0.13	13 (0%) 84 78	64, 149, 204, 259	0
3	J	1367/1524 (89%)	-0.08	18 (1%) 77 69	79, 159, 217, 264	0
4	E	93/99 (93%)	0.05	2 (2%) 62 55	100, 159, 205, 238	0
4	K	93/99 (93%)	0.03	3 (3%) 48 40	112, 168, 216, 253	0
5	F	345/347 (99%)	-0.10	1 (0%) 93 91	115, 185, 255, 300	0
5	L	345/347 (99%)	-0.11	7 (2%) 65 58	121, 188, 252, 300	0
6	O	30/30 (100%)	0.70	4 (13%) 4 6	154, 221, 293, 311	0
6	R	30/30 (100%)	0.22	0 100 100	164, 221, 257, 267	0
7	P	25/26 (96%)	0.81	5 (20%) 1 3	172, 235, 306, 326	0
7	S	26/26 (100%)	0.07	0 100 100	184, 224, 263, 283	0
All	All	6976/7546 (92%)	-0.05	119 (1%) 70 63	64, 171, 235, 326	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	5.1
2	I	175	GLU	4.6
2	C	221	LEU	4.4
1	G	13	ALA	4.1
2	C	175	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	I	176	VAL	3.6
5	L	432	LYS	3.6
3	D	666	PHE	3.5
7	P	22	DT	3.5
3	J	406	ASP	3.5
2	C	190	LYS	3.5
2	I	207	LEU	3.5
2	I	181	VAL	3.4
2	I	221	LEU	3.4
2	I	232	GLU	3.3
3	J	407	VAL	3.2
2	I	182	VAL	3.2
1	G	14	THR	3.2
2	C	174	LEU	3.2
2	C	222	LEU	3.1
3	J	1487	VAL	3.1
2	I	217	LEU	3.0
3	D	444	VAL	3.0
2	C	207	LEU	3.0
2	C	720	GLU	2.9
2	I	649	VAL	2.9
2	C	182	VAL	2.9
7	P	23	DC	2.9
1	G	56	VAL	2.9
2	C	194	VAL	2.9
3	D	256	SER	2.8
2	I	222	LEU	2.8
3	D	1486	VAL	2.8
6	O	3	DT	2.8
1	G	107	LYS	2.8
2	C	232	GLU	2.8
2	C	203	ASP	2.7
2	I	190	LYS	2.7
7	P	26	DG	2.7
3	D	446	VAL	2.6
6	O	2	DT	2.6
1	G	55	SER	2.6
2	I	183	THR	2.6
3	J	421	LEU	2.6
6	O	1	DC	2.6
2	C	231	PRO	2.6
3	J	437	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	250	LYS	2.5
2	I	174	LEU	2.5
2	I	416	GLY	2.5
4	K	74	PHE	2.5
1	G	22	GLU	2.5
1	G	132	LEU	2.5
4	K	84	ARG	2.5
1	G	23	PHE	2.5
3	D	1487	VAL	2.5
1	G	134	GLU	2.4
3	D	324	ALA	2.4
3	J	436	GLU	2.4
3	D	1279	GLY	2.4
1	G	25	LEU	2.4
4	E	88	GLU	2.4
7	P	25	DA	2.4
2	C	292	ARG	2.4
2	I	298	PHE	2.3
2	C	641	PRO	2.3
1	A	134	GLU	2.3
6	O	5	DA	2.3
3	J	1281	VAL	2.3
2	C	183	THR	2.3
3	J	367	ILE	2.3
3	J	1041	MET	2.3
1	G	18	ASP	2.3
3	D	1238	MET	2.3
2	I	296	GLY	2.3
3	J	1283	ILE	2.3
2	C	722	ILE	2.3
1	G	109	VAL	2.2
2	C	250	LYS	2.2
5	L	177	LYS	2.2
5	F	409	ARG	2.2
3	J	216	LEU	2.2
3	J	1486	VAL	2.2
3	D	445	ARG	2.2
2	I	219	GLN	2.2
5	L	135	THR	2.2
5	L	174	VAL	2.2
3	D	255	GLU	2.2
3	J	341	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	101	ILE	2.2
7	P	24	DA	2.2
1	G	15	THR	2.2
2	C	298	PHE	2.2
3	D	257	GLY	2.2
1	H	137	LYS	2.2
2	I	934	PHE	2.1
3	J	444	VAL	2.1
3	J	1040	GLY	2.1
4	K	88	GLU	2.1
1	A	204	SER	2.1
5	L	433	LEU	2.1
2	I	178	ALA	2.1
3	J	427	VAL	2.1
2	C	223	ASP	2.1
2	C	721	ARG	2.1
2	I	310	LEU	2.1
2	I	214	TYR	2.1
1	H	231	SER	2.1
1	G	162	ILE	2.1
3	J	68	PHE	2.1
1	G	102	ARG	2.1
1	G	197	LEU	2.1
5	L	178	LEU	2.1
2	I	508	ILE	2.0
2	I	648	ARG	2.0
4	E	74	PHE	2.0
5	L	409	ARG	2.0
3	D	1313	VAL	2.0
3	J	215	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	ZN	D	2001	1/1	0.99	0.13	-0.59	107,107,107,107	0
8	ZN	J	2001	1/1	0.97	0.12	-1.01	166,166,166,166	0
8	ZN	D	2002	1/1	0.96	0.16	-1.20	182,182,182,182	0
8	ZN	J	2002	1/1	0.93	0.07	-1.44	147,147,147,147	0
9	MG	D	2003	1/1	0.82	0.45	-	286,286,286,286	0
9	MG	J	2003	1/1	0.84	0.41	-	331,331,331,331	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.