



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:18 pm GMT

PDB ID : 4JK2  
Title : X-ray crystal structure of Escherichia coli sigma70 holoenzyme in complex with  
guanosine pentaphosphate (pppGpp)  
Authors : Murakami, K.S.  
Deposited on : 2013-03-09  
Resolution : 4.20 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

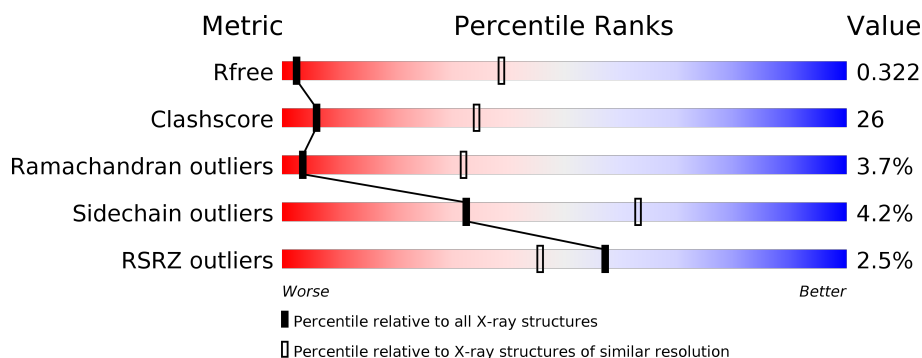
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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))
$R_{free}$	111664	1014 (4.70-3.70)
Clashscore	122126	1082 (4.70-3.70)
Ramachandran outliers	120053	1035 (4.70-3.70)
Sidechain outliers	120020	1021 (4.70-3.70)
RSRZ outliers	108989	1179 (4.80-3.60)

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	329	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>••</div> </div> </div>
1	B	329	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>27%</div> <div>•</div> <div>33%</div> </div> </div>
1	F	329	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>22%</div> <div>•</div> <div>30%</div> </div> </div>
1	G	329	<div> <div>%</div> <div> <div></div> <div>40%</div> <div>24%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> <div>•</div> </div> </div>
2	H	1342	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	
3	I	1407	
4	E	91	
4	J	91	
5	X	613	
5	Y	613	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	0O2	D	1503	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56129 atoms, of which 10 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 Escherichia coli RNA polymerase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called Escherichia coli RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called Escherichia coli RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

- Molecule 4 is a protein called Escherichia coli RNA polymerase omega subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

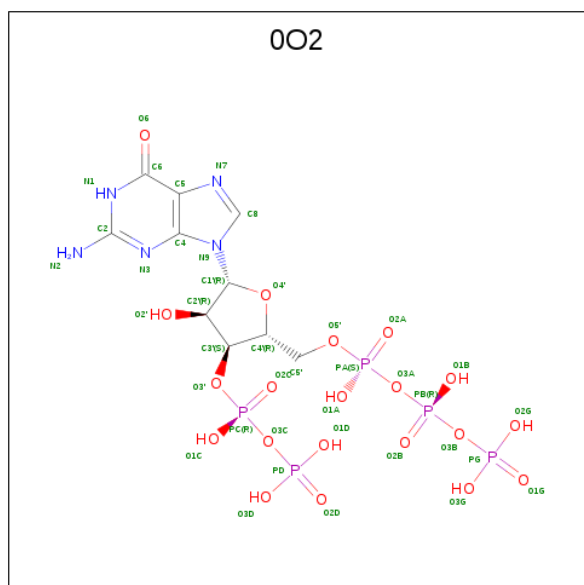
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	Zn	0	0
			2	2		
6	D	2	Total	Zn	0	0
			2	2		

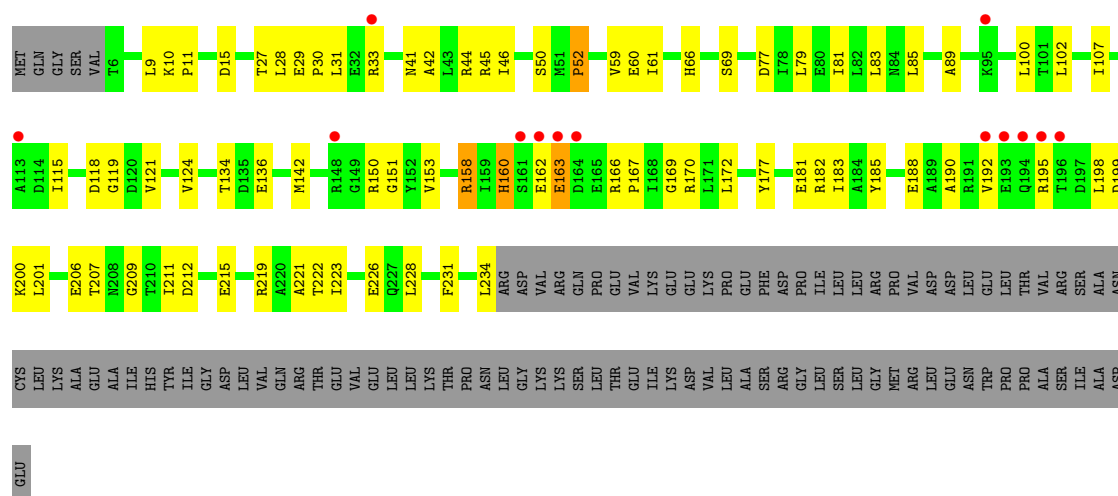
- Molecule 7 is guanosine 5'-(tetrahydrogen triphosphate) 3'-(trihydrogen diphosphate) (three-letter code: OO2) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>5</sub>O<sub>20</sub>P<sub>5</sub>).



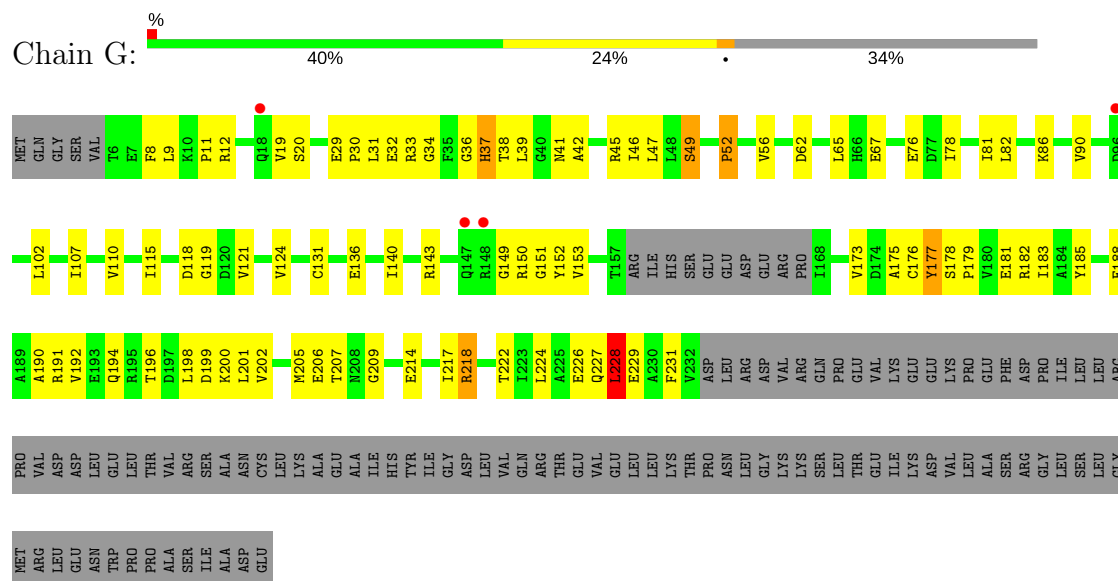


- Molecule 1: Escherichia coli RNA polymerase alpha subunit

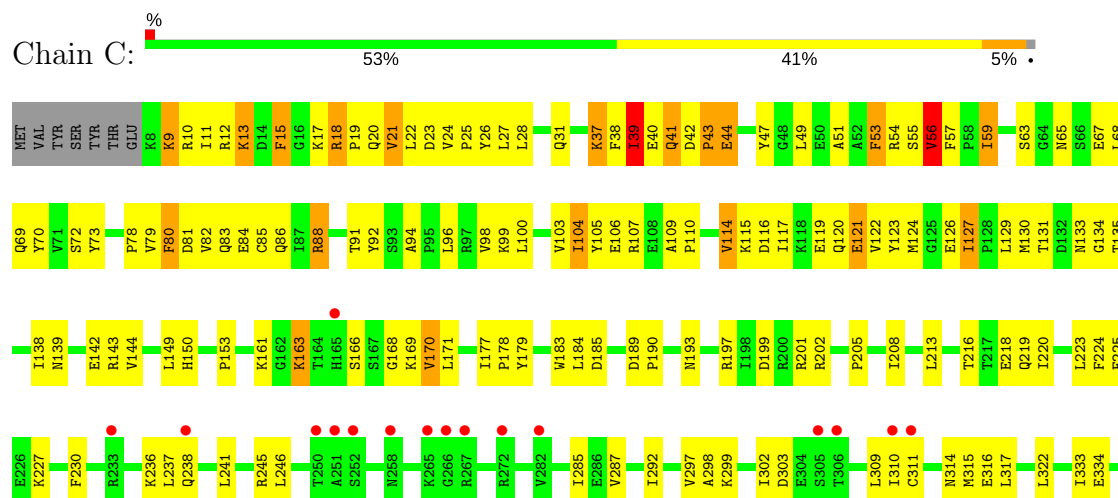


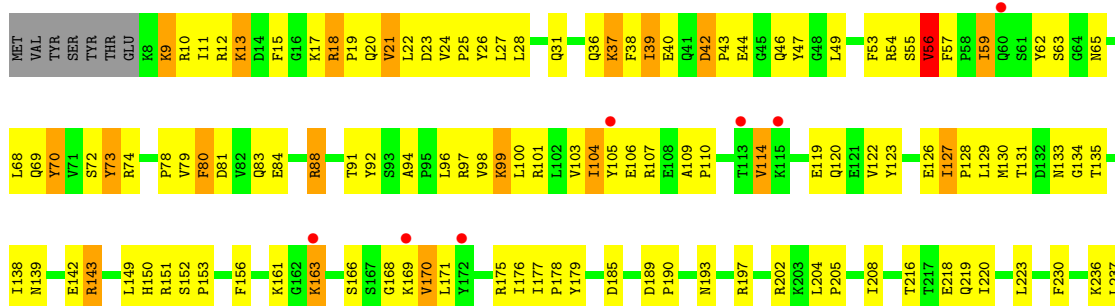


• Molecule 1: Escherichia coli RNA polymerase alpha subunit

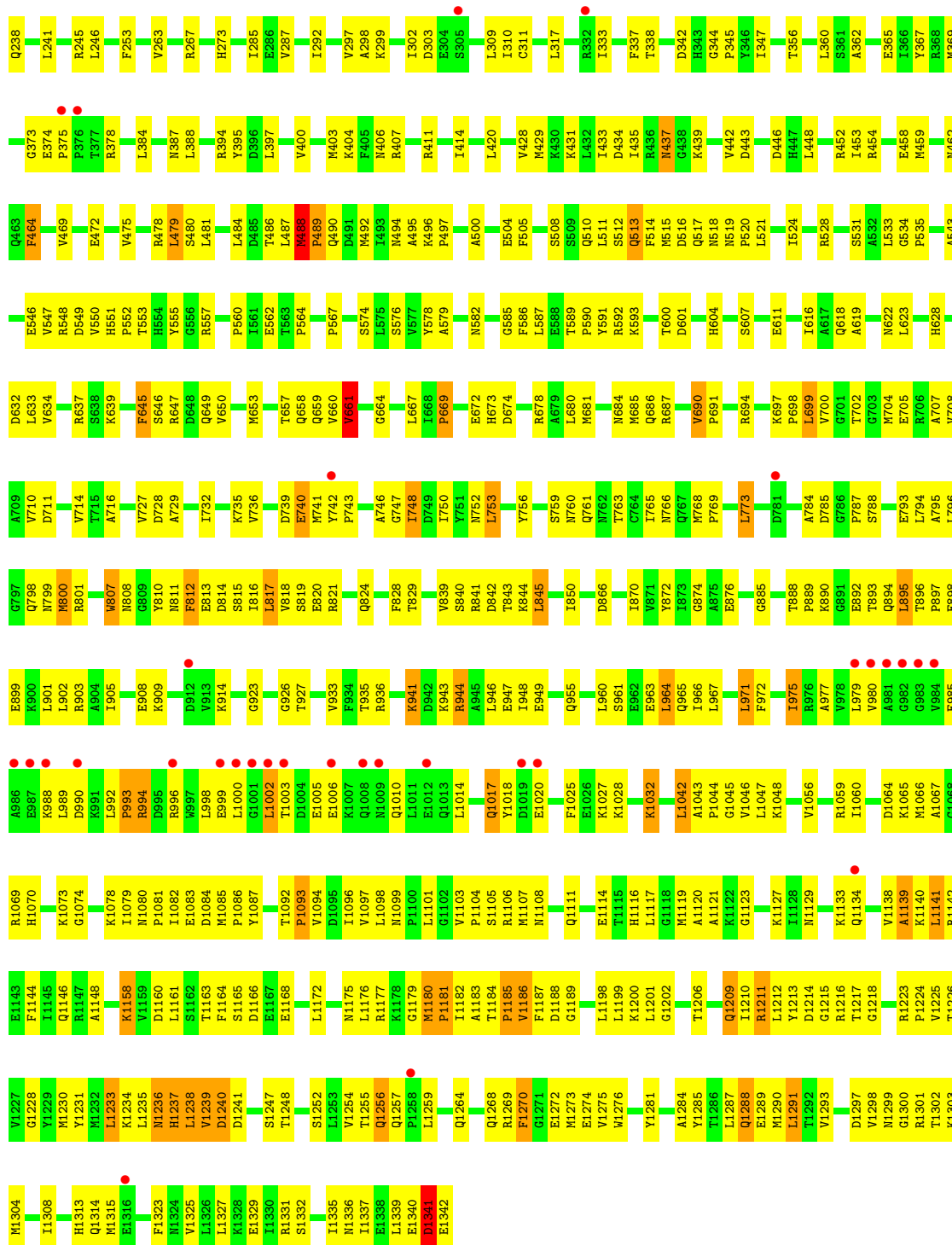


• Molecule 2: Escherichia coli RNA polymerase beta subunit

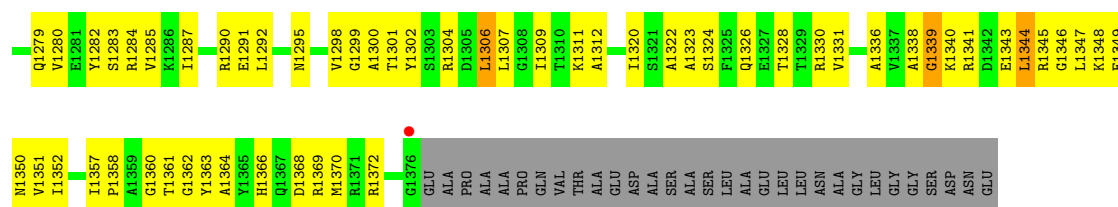




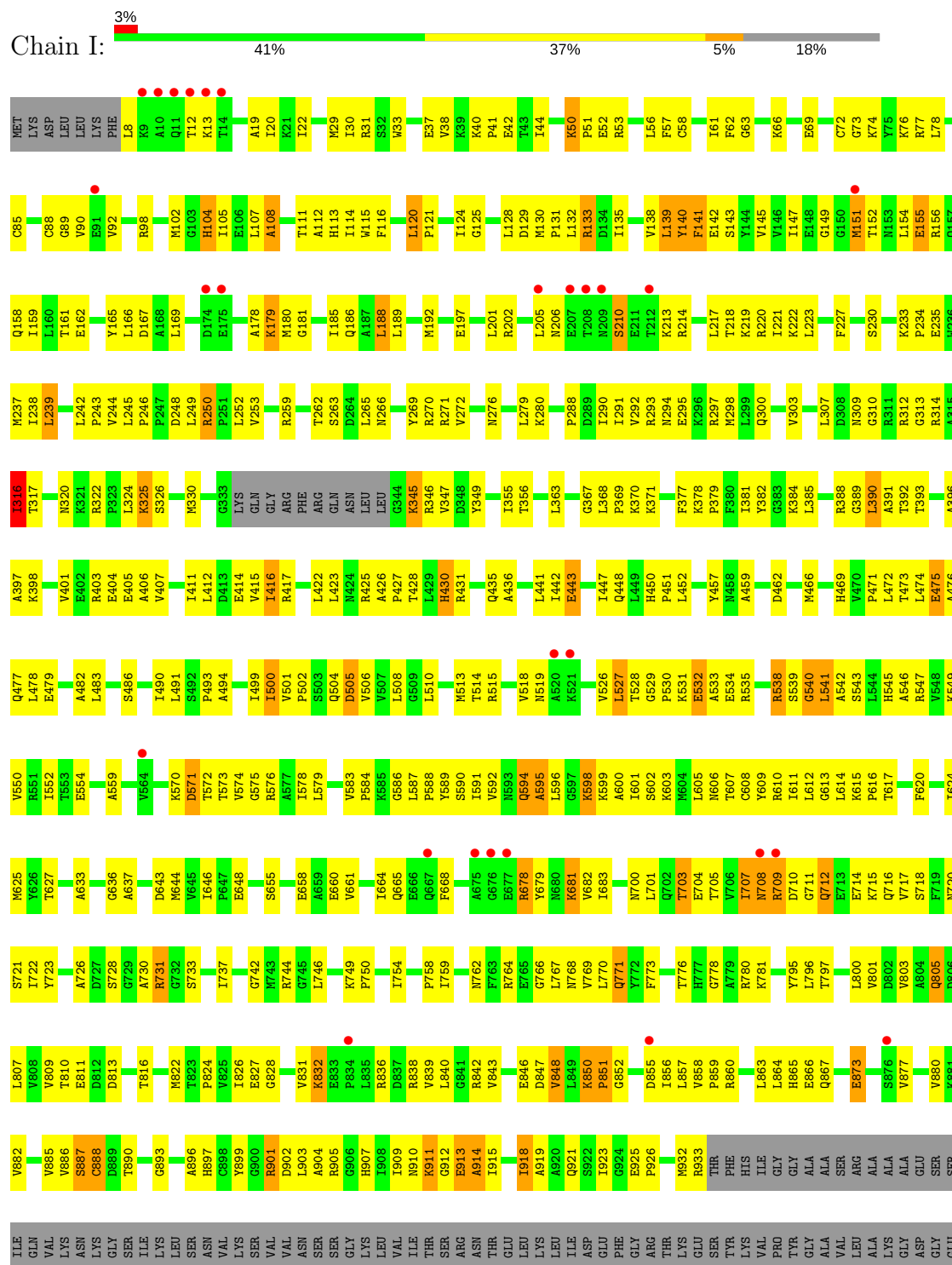




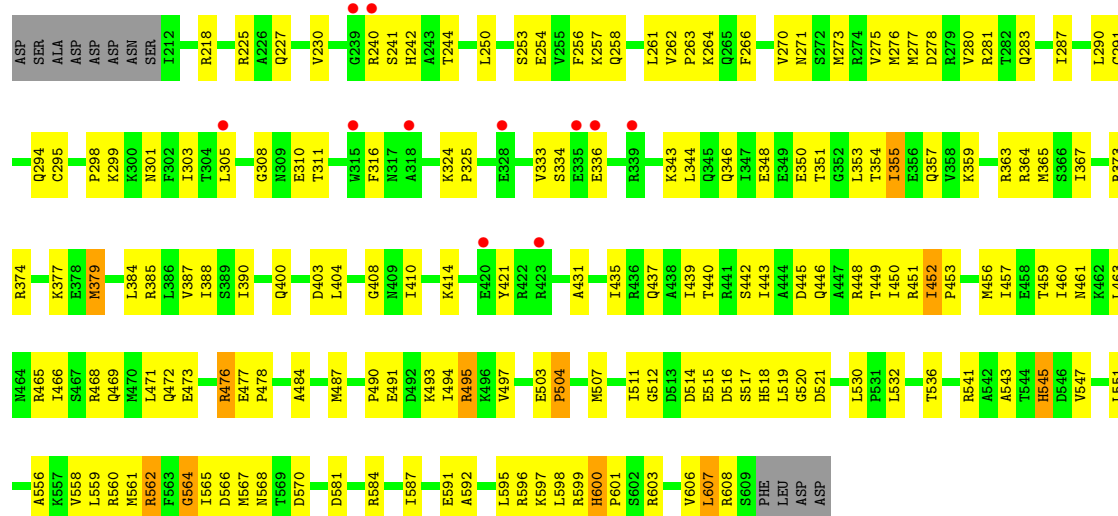
F1199	ALA	ASP	LEU	D806	1722	T627	B554	A476	K395	R311	K219	V146	K79
R1203	ARG	SER	LEU	L807	Y723	G628	Y595	Q477	A396	R312	R220	I147	H80
E1205	ILE	ALA	ALA	V808	M724	A633	D568	L478	A397	G313	K221	E148	R91
D1208	GLN	ALA	GLU	T810	M725	A633	A559	A483	K398	R314	G222	G149	I84
V1209	GLU	ASP	GLU	E811	S728	D643	D571	L482	V401	A315	S230	G150	C85
I1210	THR	THR	GLY	D812	G729	M644	T572	A432	E404	T317	K233	T152	C88
D1212	GLY	GLN	GLN	D813	A730	Y645	T573	T487	E405	N320	P234	H153	G89
D1216	THR	VAL	VAL	T816	R731	P647	V574	M488	A406	E154	V236	L154	V90
A1216	LYS	VAL	VAL	H817	G732	P647	G575	M489	A407	E155	E236	E156	E91
	ASN	GLY	GLY	E818	S733	K649	R576	L491	V408	R322	M237	Q157	V92
	LYS	GLY	GLY	E822	1737		A577		W409	G333	I238	Q158	T93
	LYS	GLY	GLY	T823	A741	I653	I578	P498	L412	LYS	L239	I159	Q94
	THR	THR	THR	T823	G742	S655	L579	I499	D413	GLN	L242	L160	R98
	ALA	VAL	VAL	P824	M743	S655	W580	I500	D413	GLY	P243	T161	R99
	LYS	ASN	ASN	V825	R744	E658	V583	V501	E414	ARG	V244	E162	E100
	TRP	LEU	LEU	I826	G745	A659	P584	P502	V415	PHE	L245	L166	R101
	ASP	SER	SER	E827	L746	E660	K585	Q504	I416	ARG	P246	D187	M102
	PRO	ASN	ASN	G828		V661	K586	Q504	R417	ASN	P247	A168	G103
	VAL	VAL	VAL	V831	K749	A662	P588	V506	L422	LEU	D248	L169	H104
	THR	THR	THR	E833	P750	E663	P588	V507	L423	LEU	L249	L169	I105
	MET	PRO	PRO	E834	1754	I664	Y589	L508	R425	G344	R250	G173	I106
	ASN	VAL	VAL	P835		Q667	S590		R426	K345	P251	D174	L107
	ASP	VAL	VAL	R836	P768	P668	I591	M513	A426	R346	L252	E175	A108
	ILE	ILE	ILE	R837	1759		N593	T514	P427	V347		F176	T111
	GLU	THR	THR	R838	R678	R678	N593	R515	T428	D348	R259	D177	A112
	VAL	GLY	GLY	V839	M762	Y679	A595	M518	L429	LEU	F260	K179	H113
	LYS	LYS	LYS	L840	F763	N680	L596	N519	H430	LEU	A261	K179	H113
	GLY	GLY	GLY	G841	R764	K681	G597	A520	R431	LEU	T262	M180	I114
	PHE	ASP	PHE	R842	S765	V682	K598		A436	LEU	N266	G181	W115
	VAL	VAL	VAL	V843	L767	I683	K599	G522	E443	LEU	Y269	T185	K118
	ARG	THR	THR	V847	L768	W686	A600	E523	G444	LEU	R270	Q186	S119
	ASN	ASN	ASN	L849	W769	M697	S602	N525	K445	LEU	E271	A187	L120
	THR	THR	THR	K850	Q771	L701	M604	L527	I447	LEU	I273	L189	P121
	MET	THR	THR	P851	F773	T702	L605		Q448	LEU	L279	M192	I124
	ASP	LEU	LEU	G852		T703	T607	E532	L449	LEU	L291	D193	G125
	GLY	LYS	LYS	D855	T776	E704	C608	E532	H450	LEU	V292	L127	L127
	ILE	ASP	ILE	I857	H777	T705	Y609	R535	P451	LEU	P288	L128	L128
	THR	THR	THR	L857	G778	V706	R610		L452	LEU	I290	E197	D129
	GLY	PHE	GLY	V858	K781	N708	T611	R538	A459	LEU	L291	L201	M130
	GLY	THR	THR	R860		T707	L612	S539	D462	LEU	V292	R202	P131
	ARG	ARG	ARG	N861	K789	D710	G613	G540	G463	LEU	R293	L194	L132
	LYS	LYS	LYS	T862	Y795	Q711	K615	A542	D464	LEU	N294	L205	D134
	LYS	LYS	LYS	L863	L796	Q712	P616		Q465	LEU	R297	N206	I135
	GLY	GLY	GLY	H865	T797	E714	T617	H545	M466	LEU	M298	S210	E136
	THR	THR	THR	E866		K715	V618	A546	H469	LEU	L299	E211	R137
	LEU	LEU	LEU	Q867	L800	Q716	V618	R547	V470	LEU	Q300	T212	V138
	THR	THR	THR	M868	V801	V717	F620	K549	P471	LEU	L306	R214	L140
	GLY	PRO	PRO	L871	D892	S718	Q623	V550	L472	LEU	L367	K215	E142
	ALA	VAL	VAL	L872	V803	F719	I624	R551	T473	LEU	N309	R216	S143
	ALA	VAL	VAL	E873	Q805	S721	M625	I552	E475	LEU	G310	L217	Y144
							Y626	T553				T218	V145



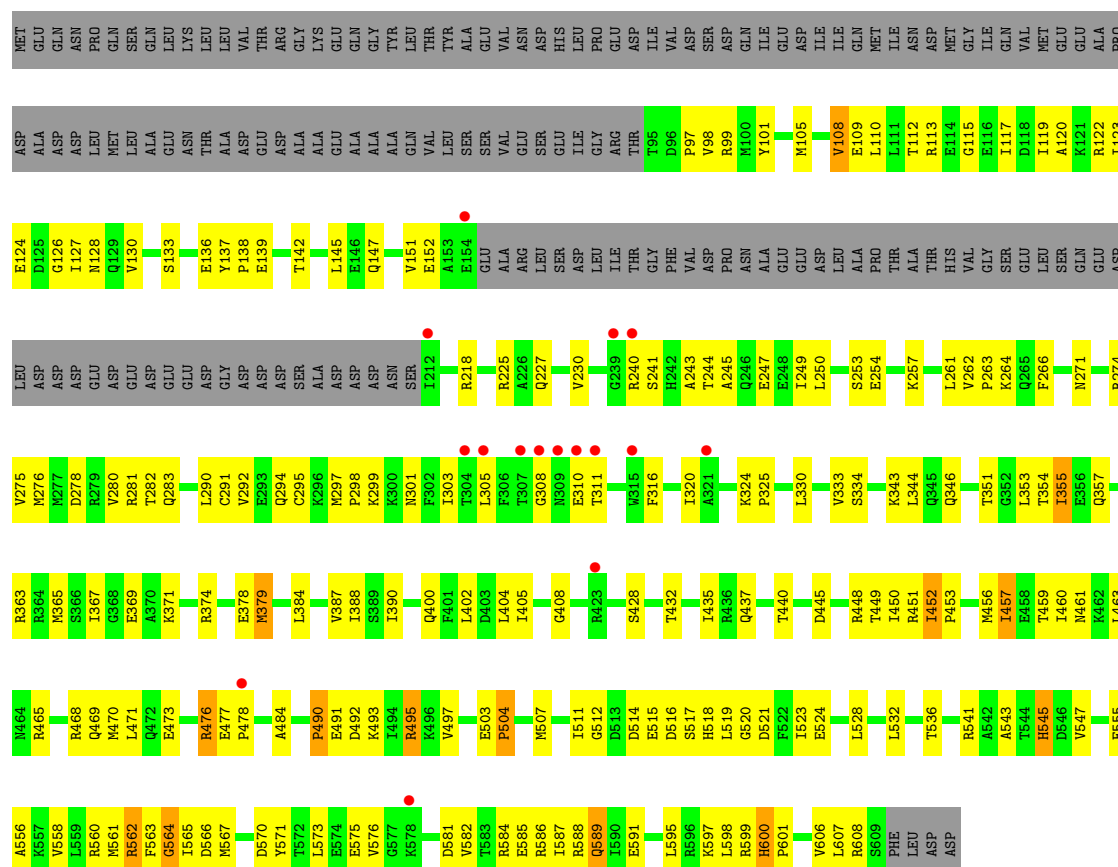
● Molecule 3: Escherichia coli RNA polymerase beta' subunit







• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.32Å 205.41Å 309.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 4.20 30.04 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.4 (29.94-4.20) 70.4 (30.04-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 4.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.244 , 0.322 0.244 , 0.322	Depositor DCC
$R_{free}$ test set	3506 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	155.9	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	56129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OO2

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	0.19	0/2548	0.36	0/3454
1	B	0.19	0/1725	0.39	0/2337
1	F	0.19	0/1797	0.38	0/2436
1	G	0.19	0/1690	0.37	0/2290
2	C	0.20	0/10690	0.38	0/14423
2	H	0.20	0/10690	0.37	0/14423
3	D	0.20	0/9198	0.38	0/12413
3	I	0.20	0/9198	0.38	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.37	0/817
5	X	0.19	0/4253	0.36	0/5719
5	Y	0.20	0/3783	0.36	0/5083
All	All	0.20	0/56889	0.38	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	91	0
1	F	1775	0	1800	79	0
1	G	1671	0	1706	91	0
2	C	10523	0	10546	600	0
2	H	10523	0	10546	574	0
3	D	9060	0	9257	658	0
3	I	9060	0	9257	591	0
4	E	708	0	719	52	0
4	J	605	0	612	33	0
5	X	4198	0	4250	197	0
5	Y	3732	0	3809	157	0
6	D	2	0	0	0	0
6	I	2	0	0	0	0
7	D	40	10	16	9	0
All	All	56119	10	56822	2973	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 26.

All (2973) 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)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.23	1.20
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.24	1.18
2:H:488:MET:HB2	2:H:490:GLN:H	1.07	1.11
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.30	1.09
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.28	1.08
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.21	1.08
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.33	1.07
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.34	1.06
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.38	1.03
2:C:54:ARG:H	2:C:55:SER:HB2	1.21	1.02
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.41	1.01
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.42	1.01
2:H:54:ARG:H	2:H:55:SER:HB2	1.19	1.01
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.42	1.01
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.41	1.01
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.40	1.00
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.38	1.00
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.44	1.00
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.40	0.99
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.44	0.99
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.45	0.99
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.44	0.98
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.41	0.98
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.46	0.98
2:H:487:LEU:HB3	2:H:488:MET:HA	1.47	0.96
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.48	0.95
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.46	0.95
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.47	0.94
1:B:12:ARG:H	1:B:30:PRO:HG2	1.30	0.94
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.47	0.94
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.47	0.94
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.50	0.93
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.50	0.93
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.48	0.93
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.49	0.93
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.50	0.92
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.50	0.92
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.49	0.92
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.51	0.91
2:C:163:LYS:HD3	2:C:163:LYS:H	1.34	0.91
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.53	0.91
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.52	0.91
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.52	0.90
2:H:488:MET:HB2	2:H:490:GLN:N	1.85	0.90
3:D:546:ALA:H	3:D:547:ARG:HA	1.34	0.90
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.54	0.90
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.54	0.89
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.54	0.89
2:C:131:THR:HG21	2:C:135:THR:HG22	1.55	0.89
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.53	0.88
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.55	0.88
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.53	0.88
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.03	0.88
3:I:546:ALA:H	3:I:547:ARG:HA	1.37	0.88
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.38	0.88
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.55	0.87
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.56	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.57	0.87
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.57	0.87
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.57	0.86
2:H:908:GLU:HG2	2:H:909:LYS:H	1.38	0.86
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.39	0.86
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.58	0.86
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.56	0.86
3:D:643:ASP:O	3:D:720:ASN:ND2	2.09	0.85
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.58	0.85
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.57	0.85
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.41	0.85
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.57	0.85
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.85
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.58	0.85
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.57	0.85
3:I:1247:LYS:HD3	3:I:1247:LYS:H	1.41	0.85
5:X:35:ILE:HG13	5:X:36:VAL:H	1.41	0.85
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.84
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.58	0.84
5:Y:448:ARG:HH12	5:Y:457:ILE:HD11	1.42	0.84
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.60	0.84
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.57	0.84
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.59	0.84
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.60	0.84
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.58	0.84
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.60	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.03	0.84
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.58	0.84
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.57	0.83
2:H:487:LEU:CB	2:H:488:MET:HA	2.07	0.83
3:D:1149:ARG:H	3:D:1149:ARG:HD3	1.43	0.83
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.59	0.83
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.59	0.83
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.60	0.83
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.59	0.82
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.04	0.82
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.62	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.61	0.82
2:H:513:GLN:HA	2:H:513:GLN:HE21	1.44	0.82
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.44	0.82
5:X:240:ARG:HD3	5:X:244:THR:HB	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.61	0.82
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.61	0.82
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.60	0.81
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.63	0.81
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.62	0.81
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.62	0.81
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.61	0.81
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.60	0.81
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.63	0.81
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.44	0.81
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.45	0.81
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.46	0.81
2:H:487:LEU:HB3	2:H:488:MET:CA	2.10	0.81
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.61	0.81
4:J:5:THR:HA	4:J:6:VAL:CB	2.11	0.81
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.17	0.80
3:I:230:SER:HB2	3:I:1339:GLY:H	1.46	0.80
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.60	0.80
3:D:541:LEU:H	3:D:541:LEU:HD23	1.46	0.80
3:D:828:GLY:HA2	3:D:832:LYS:H	1.45	0.80
2:H:54:ARG:N	2:H:55:SER:HB2	1.96	0.80
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.64	0.80
3:I:541:LEU:H	3:I:541:LEU:HD23	1.46	0.80
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.64	0.80
4:E:5:THR:HA	4:E:6:VAL:CB	2.11	0.80
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.64	0.80
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.64	0.80
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.63	0.79
2:H:163:LYS:HD3	2:H:163:LYS:H	1.48	0.79
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.64	0.79
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.65	0.79
2:C:54:ARG:N	2:C:55:SER:HB2	1.98	0.78
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.65	0.78
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.49	0.78
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.65	0.78
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.45	0.78
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.66	0.78
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.12	0.78
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.49	0.77
2:C:131:THR:CG2	2:C:135:THR:HG22	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.67	0.77
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.66	0.77
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.49	0.77
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.65	0.77
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.49	0.77
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.50	0.77
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.67	0.77
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.67	0.77
3:I:643:ASP:O	3:I:720:ASN:ND2	2.16	0.76
3:I:828:GLY:HA2	3:I:832:LYS:H	1.48	0.76
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.76
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.67	0.76
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.67	0.76
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.66	0.76
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.16	0.76
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.49	0.76
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
2:C:170:VAL:HG23	2:C:171:LEU:H	1.50	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.66	0.75
1:G:12:ARG:H	1:G:30:PRO:HG2	1.51	0.75
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.68	0.75
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.68	0.75
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.65	0.75
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.68	0.75
3:I:850:LYS:O	3:I:852:GLY:N	2.20	0.75
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.69	0.75
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.67	0.75
2:H:131:THR:CG2	2:H:135:THR:HG22	2.16	0.75
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.68	0.74
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.67	0.74
2:C:800:MET:HE2	2:C:800:MET:HA	1.67	0.74
3:I:20:ILE:HD11	3:I:1320:ILE:CD1	2.15	0.74
2:C:127:ILE:HD13	2:C:127:ILE:H	1.52	0.74
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.68	0.74
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.53	0.74
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.67	0.74
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.69	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.74
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.70	0.74
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.69	0.74
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.68	0.74
3:I:422:LEU:HA	3:I:436:ALA:HA	1.69	0.74
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.53	0.74
2:H:800:MET:HE2	2:H:800:MET:HA	1.69	0.73
4:E:5:THR:HA	4:E:6:VAL:HB	1.68	0.73
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.52	0.73
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.70	0.73
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.71	0.73
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.70	0.73
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.69	0.73
4:J:5:THR:HA	4:J:6:VAL:HB	1.68	0.73
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.70	0.73
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.53	0.73
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.71	0.73
2:C:660:VAL:HG22	2:C:661:VAL:H	1.53	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.53	0.73
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.54	0.73
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.70	0.73
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.71	0.73
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.69	0.73
2:H:600:THR:HG22	2:H:601:ASP:H	1.53	0.73
5:X:511:ILE:HG23	5:X:512:GLY:H	1.53	0.73
3:D:546:ALA:H	3:D:547:ARG:CA	2.02	0.73
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.18	0.73
4:E:5:THR:HB	4:E:7:GLN:HB2	1.71	0.73
2:H:660:VAL:HG22	2:H:661:VAL:H	1.53	0.73
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.70	0.72
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.71	0.72
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.54	0.72
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.71	0.72
2:H:127:ILE:HD13	2:H:127:ILE:H	1.53	0.72
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.71	0.72
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.71	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.05	0.72
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.71	0.72
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.53	0.72
2:C:600:THR:HG22	2:C:601:ASP:H	1.53	0.72
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.71	0.72
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.70	0.72
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.71	0.72
4:J:5:THR:CA	4:J:6:VAL:HB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.70	0.72
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.71	0.72
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.71	0.72
3:D:230:SER:HB2	3:D:1339:GLY:H	1.55	0.72
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.19	0.72
2:C:54:ARG:H	2:C:55:SER:CB	2.01	0.71
3:D:615:LYS:HD2	7:D:1503:OO2:H16	1.55	0.71
2:H:54:ARG:H	2:H:55:SER:CB	1.98	0.71
1:F:11:PRO:HG2	1:G:228:LEU:H	1.55	0.71
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.21	0.71
4:E:5:THR:HB	4:E:7:GLN:H	1.54	0.71
3:I:828:GLY:HA2	3:I:832:LYS:N	2.04	0.71
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.72	0.71
2:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:H:21:VAL:HG13	2:H:22:LEU:H	1.56	0.71
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.23	0.71
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.25	0.71
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.73	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	0.71
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.71
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.56	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.04	0.71
3:I:546:ALA:N	3:I:547:ARG:HA	2.05	0.71
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.72	0.71
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.54	0.71
5:X:112:THR:HG22	5:X:113:ARG:H	1.55	0.71
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.72	0.71
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.25	0.71
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.71	0.71
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.54	0.71
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.71	0.70
2:H:131:THR:HG21	2:H:135:THR:HG22	1.71	0.70
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.73	0.70
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.56	0.70
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.73	0.70
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.74	0.70
1:B:49:SER:HA	1:B:151:GLY:HA2	1.74	0.70
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.56	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.22	0.70
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.72	0.70
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.26	0.70
3:I:412:LEU:O	3:I:416:ILE:HD12	1.92	0.70
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.21	0.70
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.74	0.70
2:H:91:THR:HG22	2:H:139:ASN:H	1.57	0.70
2:H:309:LEU:HD23	2:H:309:LEU:H	1.55	0.70
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.74	0.70
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.74	0.70
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.56	0.70
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.21	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
3:I:546:ALA:H	3:I:547:ARG:CA	2.04	0.70
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.21	0.69
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.73	0.69
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.73	0.69
5:X:457:ILE:O	5:X:461:ASN:ND2	2.25	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.73	0.69
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.27	0.69
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.57	0.69
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.72	0.69
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.72	0.69
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.74	0.69
3:D:316:ILE:HG23	3:D:317:THR:H	1.57	0.69
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.72	0.69
1:G:65:LEU:H	1:G:65:LEU:HD23	1.55	0.69
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.73	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.57	0.69
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.69
2:C:131:THR:HG23	2:C:133:ASN:H	1.57	0.69
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.69
2:H:1239:VAL:O	2:H:1241:ASP:N	2.26	0.69
5:X:139:GLU:HA	5:X:142:THR:HG22	1.74	0.69
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.75	0.69
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.74	0.69
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.74	0.69
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.74	0.69
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.56	0.69
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.56	0.69
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.28	0.69
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.75	0.69
5:X:476:ARG:H	5:X:476:ARG:HD2	1.57	0.69
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.75	0.69
2:C:309:LEU:HD23	2:C:309:LEU:H	1.56	0.68
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.74	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.23	0.68
3:D:932:MET:O	3:D:933:ARG:HG3	1.93	0.68
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.40	0.68
2:C:845:LEU:H	2:C:845:LEU:HD13	1.58	0.68
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.28	0.68
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.73	0.68
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.26	0.68
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.75	0.68
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.68
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.25	0.68
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.68
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.74	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
3:D:905:ARG:HB2	4:E:16:ARG:HH12	1.59	0.68
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.75	0.68
2:H:170:VAL:HG23	2:H:171:LEU:H	1.58	0.68
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.76	0.68
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.58	0.68
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.26	0.68
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.74	0.68
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.74	0.68
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.76	0.68
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.74	0.68
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.74	0.68
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.76	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.24	0.67
2:C:488:MET:N	2:C:489:PRO:HD3	2.09	0.67
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.58	0.67
3:D:609:TYR:HE2	3:D:614:LEU:HD22	1.57	0.67
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.75	0.67
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.76	0.67
2:C:1239:VAL:O	2:C:1241:ASP:N	2.27	0.67
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:CB	2:H:56:VAL:HG22	2.24	0.67
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.77	0.67
2:H:845:LEU:H	2:H:845:LEU:HD13	1.57	0.67
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.74	0.67
2:C:20:GLN:O	2:C:22:LEU:N	2.27	0.67
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.93	0.67
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.59	0.67
3:I:133:ARG:O	3:I:133:ARG:NH2	2.26	0.67
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.76	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.30	0.67
3:D:590:SER:O	3:D:594:GLN:N	2.27	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.76	0.67
1:G:45:ARG:O	3:I:538:ARG:NH2	2.27	0.67
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.77	0.67
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.27	0.67
3:D:362:ARG:HH12	7:D:1503:O2:H7	1.58	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.94	0.67
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.77	0.67
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.27	0.67
2:H:99:LYS:N	2:H:99:LYS:HD3	2.09	0.67
2:C:843:THR:HG22	2:C:844:LYS:H	1.60	0.67
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.28	0.67
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.74	0.67
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.59	0.67
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.77	0.67
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.09	0.67
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.58	0.67
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.27	0.67
2:C:403:MET:HG3	2:C:414:ILE:HB	1.77	0.67
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.76	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.77	0.66
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.60	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	0.66
2:C:533:LEU:HD23	2:C:533:LEU:H	1.60	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.76	0.66
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.76	0.66
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.26	0.66
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.66
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.76	0.66
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.60	0.66
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.77	0.66
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.61	0.66
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.78	0.66
2:C:106:GLU:N	2:C:107:ARG:HA	2.08	0.66
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.77	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.78	0.66
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.10	0.66
2:H:528:ARG:NH2	2:H:576:SER:O	2.29	0.66
2:H:55:SER:CB	2:H:56:VAL:HG13	2.25	0.66
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.77	0.66
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.77	0.66
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.66
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.61	0.66
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.78	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.26	0.66
2:H:923:GLY:HA2	3:I:371:LYS:HE3	1.78	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	0.66
2:C:756:TYR:H	2:C:766:ASN:HB3	1.61	0.66
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.42	0.66
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.61	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.78	0.65
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.76	0.65
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.60	0.65
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.77	0.65
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.77	0.65
2:H:488:MET:CB	2:H:490:GLN:H	1.95	0.65
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.78	0.65
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.29	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.78	0.65
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.79	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.76	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.60	0.65
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.78	0.65
3:I:644:MET:O	3:I:764:ARG:NH1	2.29	0.65
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.77	0.65
4:E:5:THR:CA	4:E:6:VAL:HB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	0.65
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.65
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.10	0.65
3:I:827:GLU:O	3:I:831:VAL:HG12	1.96	0.65
3:I:708:ASN:OD1	3:I:712:GLN:HB2	1.97	0.65
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.78	0.65
2:C:1273:MET:HB3	3:D:428:THR:HB	1.79	0.65
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.78	0.65
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.62	0.65
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.79	0.65
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.27	0.65
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.78	0.65
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.79	0.65
3:I:504:GLN:HA	3:I:730:ALA:HA	1.78	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.78	0.65
2:H:106:GLU:N	2:H:107:ARG:HA	2.10	0.64
2:H:1288:GLN:HE21	2:H:1288:GLN:HA	1.62	0.64
2:H:484:LEU:HD22	2:H:484:LEU:H	1.62	0.64
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.78	0.64
3:I:145:VAL:HG22	3:I:180:MET:SD	2.37	0.64
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	0.64
2:C:189:ASP:OD1	2:C:193:ASN:N	2.24	0.64
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.62	0.64
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.33	0.64
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.12	0.64
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.11	0.64
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.31	0.64
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.13	0.64
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.78	0.64
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.79	0.64
3:I:711:GLY:O	3:I:712:GLN:HG2	1.97	0.64
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.63	0.64
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.63	0.64
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	0.64
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.79	0.64
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.32	0.64
1:B:227:GLN:O	1:B:228:LEU:HG	1.96	0.64
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.80	0.64
2:H:504:GLU:O	2:H:508:SER:HB3	1.98	0.64
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:514:THR:HG23	3:I:576:ARG:HE	1.63	0.64
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.64
3:D:405:GLU:O	3:D:407:VAL:N	2.30	0.64
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.13	0.64
3:I:590:SER:O	3:I:594:GLN:N	2.30	0.64
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.30	0.64
2:C:55:SER:CB	2:C:56:VAL:HG13	2.26	0.64
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.79	0.64
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.62	0.64
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.63	0.64
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.79	0.63
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.77	0.63
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.80	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.80	0.63
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.80	0.63
4:J:15:ASN:HD22	4:J:18:ASP:H	1.44	0.63
3:D:614:LEU:HG	4:E:5:THR:HG21	1.79	0.63
3:I:809:VAL:HG13	3:I:912:GLY:H	1.64	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.63
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.28	0.63
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.78	0.63
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.80	0.63
3:D:932:MET:SD	3:D:932:MET:N	2.67	0.63
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.32	0.63
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.79	0.63
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.81	0.63
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.29	0.63
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.63
3:I:598:LYS:NZ	3:I:726:ALA:O	2.32	0.63
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.80	0.63
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.13	0.63
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.81	0.63
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.30	0.63
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.29	0.63
2:H:1273:MET:HB3	3:I:428:THR:HB	1.81	0.63
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.80	0.63
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.81	0.63
3:D:27:PRO:O	3:D:31:ARG:HD3	1.98	0.63
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.63
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.30	0.63
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.63	0.63
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.33	0.62
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.29	0.62
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.81	0.62
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.63	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.13	0.62
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.80	0.62
2:C:21:VAL:HG13	2:C:22:LEU:H	1.63	0.62
3:D:573:THR:HG22	3:D:576:ARG:CG	2.29	0.62
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.81	0.62
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.19	0.62
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.34	0.62
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.82	0.62
2:C:634:VAL:H	2:C:645:PHE:HE2	1.47	0.62
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.82	0.62
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.65	0.62
2:H:1252:SER:OG	2:H:1255:THR:O	2.17	0.62
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.82	0.62
3:D:107:LEU:HD12	3:D:107:LEU:H	1.64	0.62
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.15	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
2:H:20:GLN:O	2:H:22:LEU:N	2.32	0.62
2:H:562:GLU:HG2	2:H:574:SER:CB	2.29	0.62
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.81	0.62
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.30	0.62
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.65	0.62
3:D:77:ARG:HG3	3:D:78:LEU:H	1.62	0.62
4:E:5:THR:HA	4:E:6:VAL:CG1	2.30	0.62
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.14	0.62
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.64	0.62
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.82	0.62
2:C:901:LEU:O	2:C:905:ILE:HG13	2.00	0.62
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.62
2:H:660:VAL:O	2:H:661:VAL:HG22	2.00	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.32	0.62
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.25	0.62
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.14	0.62
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.64	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.82	0.62
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.82	0.62
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.81	0.61
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.81	0.61
1:B:49:SER:OG	3:D:538:ARG:NH2	2.33	0.61
4:E:5:THR:HA	4:E:6:VAL:HG12	1.82	0.61
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.81	0.61
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.34	0.61
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.29	0.61
3:D:768:ASN:O	3:D:771:GLN:NE2	2.34	0.61
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.65	0.61
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.33	0.61
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.82	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.61
1:B:227:GLN:O	1:B:229:GLU:N	2.30	0.61
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.82	0.61
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.81	0.61
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.01	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.14	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.29	0.61
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.61
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.61
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.31	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.01	0.61
1:F:9:LEU:O	1:G:227:GLN:NE2	2.33	0.61
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.33	0.61
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.23	0.61
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.65	0.61
2:H:152:SER:OG	2:H:404:LYS:NZ	2.25	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.16	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:77:ARG:HG3	3:I:78:LEU:H	1.64	0.61
4:J:5:THR:HA	4:J:6:VAL:CG1	2.30	0.61
2:H:487:LEU:HB3	2:H:488:MET:CG	2.30	0.61
3:I:107:LEU:HD12	3:I:107:LEU:H	1.65	0.61
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.82	0.61
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.82	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.32	0.61
3:D:1362:GLY:O	3:D:1364:ALA:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:422:LEU:HA	3:D:436:ALA:HA	1.83	0.61
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.29	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
1:B:65:LEU:HD23	1:B:65:LEU:H	1.65	0.61
2:C:91:THR:HG22	2:C:139:ASN:H	1.65	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.15	0.61
3:D:827:GLU:O	3:D:831:VAL:HG12	2.00	0.61
2:H:517:GLN:HE21	2:H:760:ASN:H	1.48	0.61
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.83	0.61
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.61
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.61
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.60
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.60
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.83	0.60
3:D:1338:ALA:O	3:D:1340:LYS:N	2.34	0.60
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.36	0.60
2:H:55:SER:HB3	2:H:56:VAL:CB	2.31	0.60
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.33	0.60
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.66	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.32	0.60
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.60
2:C:747:GLY:O	2:C:748:ILE:HG13	2.00	0.60
2:C:752:ASN:O	2:C:753:LEU:HG	2.01	0.60
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.82	0.60
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.17	0.60
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.67	0.60
2:H:892:GLU:O	2:H:893:THR:OG1	2.19	0.60
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.83	0.60
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.83	0.60
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.36	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.49	0.60
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.01	0.60
3:D:202:ARG:O	3:D:206:ASN:ND2	2.34	0.60
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.83	0.60
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.82	0.60
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.82	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
3:I:252:LEU:HD23	3:I:252:LEU:H	1.66	0.60
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.34	0.60
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:584:ARG:O	5:X:587:ILE:HG22	2.01	0.60
5:X:595:LEU:O	5:X:599:ARG:NH1	2.35	0.60
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.35	0.60
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.83	0.60
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.84	0.60
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.67	0.60
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.82	0.60
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.83	0.60
4:J:5:THR:HB	4:J:7:GLN:HB2	1.83	0.60
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.60
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.16	0.60
2:C:963:GLU:O	2:C:966:ILE:HG22	2.02	0.60
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.60
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.66	0.60
5:X:240:ARG:O	5:X:242:HIS:N	2.34	0.60
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.60
2:C:562:GLU:HG2	2:C:574:SER:CB	2.31	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.65	0.60
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.65	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.35	0.60
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.02	0.60
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.82	0.60
3:D:145:VAL:HG22	3:D:180:MET:SD	2.41	0.60
3:D:85:CYS:HB3	3:D:88:CYS:O	2.02	0.60
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.17	0.60
2:H:800:MET:HA	2:H:800:MET:CE	2.32	0.60
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.32	0.60
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.37	0.60
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.17	0.60
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.35	0.60
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.65	0.60
3:D:128:LEU:CD1	3:D:192:MET:HE3	2.28	0.60
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.84	0.60
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.82	0.60
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.60
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.83	0.60
3:D:151:MET:N	3:D:151:MET:SD	2.74	0.60
3:D:252:LEU:HD23	3:D:252:LEU:H	1.67	0.60
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.66	0.60
3:I:1338:ALA:O	3:I:1340:LYS:N	2.35	0.60
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:894:GLN:HE21	3:I:77:ARG:HD3	1.66	0.60
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.83	0.60
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.67	0.59
2:C:660:VAL:O	2:C:661:VAL:HG22	2.01	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.36	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.84	0.59
3:I:681:LYS:NZ	3:I:681:LYS:HB2	2.17	0.59
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.59
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.83	0.59
3:D:473:THR:HB	3:D:476:ALA:HB2	1.83	0.59
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.01	0.59
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.30	0.59
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.31	0.59
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.32	0.59
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.83	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
2:C:619:ALA:HA	2:C:653:MET:HE2	1.84	0.59
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.68	0.59
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.84	0.59
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.85	0.59
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.85	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.84	0.59
3:I:720:ASN:O	3:I:722:ILE:N	2.35	0.59
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.59
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.17	0.59
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.33	0.59
2:C:163:LYS:HD3	2:C:163:LYS:N	2.14	0.59
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.59
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.18	0.59
2:H:130:MET:SD	2:H:134:GLY:HA2	2.42	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.68	0.59
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.85	0.59
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.31	0.59
5:X:442:SER:OG	5:X:446:GLN:NE2	2.34	0.59
3:D:125:GLY:O	3:D:129:ASP:N	2.36	0.59
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.83	0.59
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.59
4:E:45:LYS:O	4:E:49:ILE:HG12	2.03	0.59
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.18	0.59
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.84	0.59
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.83	0.59
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.36	0.59
1:G:176:CYS:O	1:G:178:SER:N	2.33	0.59
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.15	0.59
2:H:94:ALA:N	2:H:126:GLU:OE2	2.27	0.59
2:C:91:THR:HG22	2:C:138:ILE:HA	1.85	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
3:D:389:GLY:O	3:D:391:ALA:N	2.36	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.59
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.50	0.59
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.59
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.33	0.59
3:D:313:GLY:H	5:X:38:SER:HB3	1.67	0.59
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.32	0.59
2:C:1288:GLN:HE21	2:C:1288:GLN:HA	1.68	0.59
4:E:14:GLY:O	4:E:15:ASN:ND2	2.36	0.59
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.59
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.85	0.59
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.85	0.59
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.84	0.59
3:I:704:GLU:HB2	3:I:718:SER:HG	1.67	0.59
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.85	0.59
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.02	0.59
5:X:515:GLU:N	5:X:516:ASP:HA	2.18	0.59
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.84	0.59
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.85	0.58
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.18	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.86	0.58
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.28	0.58
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.67	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.86	0.58
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.58
3:I:85:CYS:HB3	3:I:88:CYS:O	2.02	0.58
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.83	0.58
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.39	0.58
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.39	0.58
2:H:99:LYS:H	2:H:99:LYS:HD3	1.68	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.68	0.58
2:C:42:ASP:O	2:C:44:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.85	0.58
3:D:809:VAL:HG13	3:D:912:GLY:H	1.66	0.58
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.18	0.58
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.04	0.58
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.18	0.58
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.86	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	0.58
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.84	0.58
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.84	0.58
3:I:768:ASN:O	3:I:771:GLN:NE2	2.37	0.58
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.34	0.58
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.84	0.58
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.03	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.02	0.58
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.85	0.58
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.86	0.58
5:X:517:SER:O	5:X:518:HIS:ND1	2.37	0.58
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.68	0.58
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.58
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.86	0.58
3:D:504:GLN:HA	3:D:730:ALA:HA	1.84	0.58
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.34	0.58
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.85	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.86	0.58
1:A:104:LYS:HD3	1:A:105:SER:N	2.19	0.58
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.37	0.58
2:C:1200:LYS:O	2:C:1202:GLY:N	2.34	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.85	0.58
2:C:166:SER:O	2:C:168:GLY:N	2.34	0.58
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.84	0.58
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.86	0.58
3:I:701:LEU:HD23	3:I:723:TYR:HB2	1.86	0.58
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.19	0.58
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.39	0.58
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.68	0.58
3:D:709:ARG:O	3:D:711:GLY:N	2.37	0.58
1:G:49:SER:HA	1:G:151:GLY:HA2	1.86	0.58
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.39	0.58
2:H:1101:LEU:CD1	3:I:504:GLN:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:591:ILE:HA	3:I:594:GLN:HB2	1.86	0.58
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.86	0.58
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.85	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.85	0.58
3:I:125:GLY:O	3:I:129:ASP:N	2.37	0.58
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	0.57
2:C:54:ARG:HG2	2:C:55:SER:CB	2.34	0.57
2:C:898:GLU:N	2:C:898:GLU:OE1	2.34	0.57
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.27	0.57
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.19	0.57
3:I:389:GLY:O	3:I:391:ALA:N	2.37	0.57
1:B:176:CYS:C	1:B:178:SER:H	2.08	0.57
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.33	0.57
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.57
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.57
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.29	0.57
2:H:189:ASP:OD1	2:H:193:ASN:N	2.31	0.57
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.86	0.57
5:Y:457:ILE:HG23	5:Y:461:ASN:HD21	1.69	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.57
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.69	0.57
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.86	0.57
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.19	0.57
2:C:94:ALA:N	2:C:126:GLU:OE2	2.25	0.57
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.85	0.57
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.04	0.57
1:F:181:GLU:OE1	1:F:181:GLU:N	2.38	0.57
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.57
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.34	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.19	0.57
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.34	0.57
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.86	0.57
2:C:24:VAL:HG11	2:C:704:MET:HE1	1.87	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.81	0.57
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.05	0.57
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.87	0.57
3:D:619:ILE:HD13	7:D:1503:OO2:O3D	2.05	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.86	0.57
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.57
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:VAL:O	1:G:20:SER:OG	2.17	0.57
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.86	0.57
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.37	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.33	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.39	0.57
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.86	0.57
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.34	0.57
3:I:704:GLU:HB2	3:I:718:SER:OG	2.05	0.57
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.69	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.57
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.31	0.57
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.86	0.57
2:H:533:LEU:HD23	2:H:533:LEU:H	1.69	0.57
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.87	0.57
3:I:824:PRO:O	3:I:826:ILE:HG13	2.05	0.57
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.86	0.57
2:C:106:GLU:H	2:C:107:ARG:HA	1.70	0.57
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.35	0.57
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.57
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.40	0.57
2:H:753:LEU:HD12	2:H:753:LEU:O	2.05	0.57
3:I:905:ARG:HG2	3:I:907:HIS:H	1.70	0.57
5:X:503:GLU:N	5:X:504:PRO:HA	2.20	0.57
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.70	0.57
4:E:15:ASN:HD21	4:E:18:ASP:HB2	1.70	0.57
3:I:88:CYS:O	3:I:90:VAL:N	2.38	0.57
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.85	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.34	0.56
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.70	0.56
3:D:417:ARG:HH12	4:E:3:ARG:HH22	1.53	0.56
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.05	0.56
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.87	0.56
1:A:227:GLN:HE22	1:B:11:PRO:HD3	1.71	0.56
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.87	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.34	0.56
3:D:141:PHE:O	3:D:297:ARG:HD3	2.04	0.56
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.35	0.56
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:496:LYS:N	2:H:497:PRO:HD2	2.20	0.56
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.05	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.56
2:H:1111:GLN:HG3	2:H:1230:MET:HE2	1.87	0.56
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.38	0.56
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.70	0.56
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.35	0.56
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.31	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.05	0.56
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.88	0.56
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.35	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.39	0.56
3:I:546:ALA:HB3	3:I:547:ARG:O	2.06	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.05	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.87	0.56
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.87	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.56
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.36	0.56
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.86	0.56
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.56
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.56
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.41	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.35	0.56
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.56
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.26	0.56
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.87	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.86	0.56
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.17	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.05	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.56
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.40	0.56
2:H:488:MET:H	2:H:489:PRO:HA	1.70	0.56
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.36	0.56
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.87	0.56
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.85	0.56
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.87	0.56
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.30	0.56
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.37	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.20	0.56
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.40	0.56
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.41	0.56
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.87	0.56
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.21	0.56
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.19	0.56
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.06	0.56
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.19	0.56
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.36	0.56
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.71	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.88	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.88	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
3:D:166:LEU:HD12	3:D:167:ASP:N	2.21	0.56
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.41	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.37	0.56
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.56
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.87	0.56
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.19	0.56
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.36	0.56
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.71	0.56
2:C:487:LEU:HD13	2:C:488:MET:H	1.71	0.55
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.88	0.55
3:I:914:ALA:O	3:I:918:ILE:HG22	2.05	0.55
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.88	0.55
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.35	0.55
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.21	0.55
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.88	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.41	0.55
2:H:505:PHE:O	2:H:512:SER:OG	2.23	0.55
2:H:531:SER:OG	2:H:533:LEU:HD23	2.06	0.55
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.88	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.39	0.55
3:D:919:ALA:O	3:D:923:ILE:HG12	2.06	0.55
1:F:10:LYS:HD2	1:G:226:GLU:O	2.06	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.71	0.55
3:I:166:LEU:HD12	3:I:167:ASP:N	2.20	0.55
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.87	0.55
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.36	0.55
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.06	0.55
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.05	0.55
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.88	0.55
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.89	0.55
3:I:573:THR:HG22	3:I:576:ARG:CG	2.37	0.55
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.36	0.55
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.37	0.55
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.69	0.55
2:C:681:MET:O	2:C:685:MET:HG2	2.06	0.55
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.88	0.55
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.55
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.37	0.55
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.89	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.89	0.55
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.72	0.55
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.89	0.55
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.40	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.87	0.55
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.71	0.55
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.55
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.42	0.55
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.42	0.55
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.55
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.88	0.55
3:D:473:THR:HB	3:D:476:ALA:CB	2.37	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.40	0.55
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.70	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	1.87	0.55
1:G:42:ALA:O	1:G:46:ILE:HG12	2.07	0.55
2:H:664:GLY:O	2:H:686:GLN:NE2	2.39	0.55
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.06	0.55
5:X:379:MET:CE	5:X:379:MET:HA	2.36	0.55
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.55
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.89	0.55
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.42	0.55
2:C:496:LYS:N	2:C:497:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.72	0.55
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.24	0.55
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.88	0.55
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.35	0.55
2:C:142:GLU:HG2	2:C:515:MET:SD	2.47	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.88	0.55
1:G:86:LYS:NZ	3:I:526:VAL:O	2.39	0.55
2:H:106:GLU:HG2	2:H:109:ALA:H	1.71	0.55
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.88	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.35	0.55
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.55
2:C:163:LYS:H	2:C:163:LYS:CD	2.10	0.54
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.72	0.54
3:D:609:TYR:CE2	3:D:614:LEU:HD22	2.41	0.54
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.07	0.54
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.42	0.54
2:H:453:ILE:HG22	2:H:585:GLY:O	2.07	0.54
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.71	0.54
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.42	0.54
2:H:459:MET:SD	2:H:511:LEU:HD22	2.47	0.54
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.88	0.54
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.53	0.54
2:C:639:LYS:HA	2:C:639:LYS:HE2	1.89	0.54
3:D:514:THR:HG21	3:D:595:ALA:O	2.07	0.54
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.54
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.08	0.54
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.88	0.54
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.89	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.89	0.54
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.88	0.54
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.07	0.54
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.32	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.54
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.37	0.54
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.07	0.54
1:A:243:LYS:NZ	1:A:243:LYS:HB2	2.23	0.54
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.88	0.54
2:H:1255:THR:O	2:H:1257:GLN:N	2.38	0.54
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.90	0.54
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.89	0.54
3:I:128:LEU:HD12	3:I:192:MET:CE	2.37	0.54
3:I:589:TYR:O	3:I:591:ILE:N	2.37	0.54
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.89	0.54
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.90	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.90	0.54
3:I:297:ARG:HH22	5:Y:101:TYR:HB2	1.71	0.54
4:J:15:ASN:ND2	4:J:18:ASP:H	2.06	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
2:C:91:THR:HG22	2:C:139:ASN:N	2.23	0.54
1:F:150:ARG:NH1	1:G:8:PHE:HA	2.20	0.54
2:H:660:VAL:HG22	2:H:661:VAL:N	2.22	0.54
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.07	0.54
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.73	0.54
4:E:5:THR:CA	4:E:6:VAL:CB	2.85	0.54
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.08	0.54
2:H:54:ARG:HG2	2:H:55:SER:CB	2.36	0.54
2:H:704:MET:HA	2:H:704:MET:HE2	1.90	0.54
3:I:405:GLU:O	3:I:407:VAL:N	2.41	0.54
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.90	0.54
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.73	0.54
3:I:549:LYS:HE2	3:I:571:ASP:OD2	2.07	0.54
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.34	0.54
3:D:450:HIS:NE2	3:D:625:MET:SD	2.81	0.54
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.90	0.54
3:I:151:MET:N	3:I:151:MET:SD	2.81	0.54
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.90	0.54
1:B:176:CYS:O	1:B:178:SER:N	2.41	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.89	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.90	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.08	0.54
3:I:810:THR:HG22	3:I:893:GLY:HA3	1.90	0.54
5:X:556:ALA:O	5:X:560:ARG:HB2	2.08	0.54
5:X:600:HIS:H	5:X:601:PRO:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:OD1	1:B:119:GLY:N	2.41	0.53
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.20	0.53
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.08	0.53
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.40	0.53
3:D:128:LEU:HA	3:D:192:MET:HE3	1.90	0.53
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.30	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.53
2:H:442:VAL:HG12	2:H:443:ASP:H	1.74	0.53
3:I:571:ASP:N	3:I:571:ASP:OD1	2.39	0.53
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.90	0.53
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.89	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.41	0.53
2:C:134:GLY:O	2:C:527:LYS:NZ	2.40	0.53
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.31	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.89	0.53
2:H:728:ASP:OD2	2:H:729:ALA:N	2.41	0.53
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.34	0.53
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.89	0.53
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.39	0.53
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.43	0.53
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.90	0.53
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.90	0.53
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.90	0.53
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.08	0.53
3:D:393:THR:HG23	3:D:396:ALA:H	1.73	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.38	0.53
5:X:437:GLN:HA	5:X:440:THR:HG22	1.89	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.74	0.53
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.07	0.53
2:C:756:TYR:H	2:C:766:ASN:CB	2.22	0.53
3:D:584:PRO:HG2	3:D:587:LEU:CD1	2.33	0.53
3:D:591:ILE:HD12	3:D:592:VAL:N	2.24	0.53
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.28	0.53
2:H:1332:SER:O	3:I:243:PRO:HG2	2.09	0.53
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.89	0.53
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.90	0.53
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.73	0.53
3:I:363:LEU:O	3:I:486:SER:OG	2.20	0.53
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1119:MET:O	2:C:1123:GLY:N	2.40	0.53
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.44	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.41	0.53
3:D:294:ASN:ND2	3:D:298:MET:SD	2.81	0.53
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.53
2:H:1274:GLU:N	2:H:1274:GLU:OE1	2.41	0.53
2:H:494:ASN:OD1	2:H:495:ALA:N	2.40	0.53
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.91	0.53
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.53
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.19	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
1:B:19:VAL:O	1:B:20:SER:HB3	2.08	0.53
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.91	0.53
2:C:106:GLU:HG2	2:C:109:ALA:H	1.73	0.53
2:C:122:VAL:HG22	5:X:472:GLN:HE21	1.72	0.53
2:C:360:LEU:HD13	2:C:378:ARG:NH1	2.23	0.53
2:C:818:VAL:HG22	2:C:819:SER:H	1.74	0.53
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.91	0.53
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.30	0.53
3:D:41:PRO:HB3	3:D:270:ARG:HG3	1.90	0.53
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.39	0.53
3:D:490:ILE:O	3:D:499:ILE:HG22	2.09	0.53
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.91	0.53
5:X:355:ILE:HD13	5:X:355:ILE:O	2.08	0.53
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.09	0.53
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.90	0.53
1:A:42:ALA:O	1:A:46:ILE:HG12	2.08	0.53
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.39	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.91	0.53
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.43	0.53
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.53
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.44	0.53
1:F:79:LEU:O	1:F:83:LEU:HD13	2.09	0.53
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.43	0.53
3:I:591:ILE:HD12	3:I:592:VAL:N	2.23	0.53
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.08	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.74	0.53
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.74	0.53
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.90	0.53
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.24	0.53
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.91	0.53
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.90	0.53
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.44	0.53
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.44	0.53
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.90	0.53
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.38	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.90	0.53
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.90	0.53
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.90	0.53
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.09	0.53
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.91	0.52
2:C:205:PRO:O	2:C:208:ILE:HG22	2.10	0.52
2:C:402:ARG:NH2	2:C:419:ILE:O	2.43	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.38	0.52
2:H:106:GLU:H	2:H:107:ARG:HA	1.74	0.52
2:H:37:LYS:HE3	2:H:37:LYS:HA	1.91	0.52
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.23	0.52
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.45	0.52
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.52
4:J:45:LYS:O	4:J:49:ILE:HG12	2.09	0.52
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.08	0.52
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.73	0.52
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.52
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.52
3:D:413:ASP:O	3:D:417:ARG:HG2	2.10	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:I:197:GLU:O	3:I:201:LEU:HD23	2.09	0.52
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.74	0.52
5:X:264:LYS:HD2	5:X:264:LYS:H	1.73	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	0.52
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.92	0.52
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.52
4:E:5:THR:HB	4:E:7:GLN:N	2.24	0.52
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.44	0.52
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.10	0.52
3:I:797:THR:O	3:I:801:VAL:HG23	2.09	0.52
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.23	0.52
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.74	0.52
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.09	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.45	0.52
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.52
4:E:77:ALA:O	4:E:80:LEU:HD22	2.10	0.52
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.42	0.52
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.91	0.52
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.09	0.52
3:I:393:THR:HG23	3:I:396:ALA:H	1.73	0.52
3:I:648:GLU:N	3:I:648:GLU:OE2	2.43	0.52
5:X:484:ALA:CB	5:X:494:ILE:HD12	2.39	0.52
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.91	0.52
5:X:493:LYS:O	5:X:497:VAL:HG23	2.09	0.52
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.39	0.52
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.39	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.75	0.52
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.09	0.52
5:X:541:ARG:O	5:X:545:HIS:HB2	2.10	0.52
3:D:615:LYS:HD2	7:D:1503:OO2:N2	2.23	0.52
3:D:655:SER:O	3:D:658:GLU:HG2	2.09	0.52
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.45	0.52
4:E:82:ALA:O	4:E:86:ILE:HG13	2.10	0.52
2:H:131:THR:HG22	2:H:135:THR:HG22	1.91	0.52
2:H:888:THR:O	2:H:914:LYS:N	2.36	0.52
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	0.52
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.91	0.52
2:C:127:ILE:HD13	2:C:127:ILE:N	2.25	0.52
2:C:302:ILE:HG22	2:C:309:LEU:CB	2.39	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.92	0.52
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.91	0.52
2:C:975:ILE:HD13	2:C:975:ILE:O	2.09	0.52
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.91	0.52
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.91	0.52
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.45	0.52
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.91	0.52
3:D:746:LEU:HB3	3:D:754:ILE:HG21	1.91	0.52
4:E:5:THR:CB	4:E:7:GLN:H	2.20	0.52
2:H:18:ARG:HD3	2:H:619:ALA:O	2.09	0.52
2:H:694:ARG:O	2:H:798:GLN:NE2	2.37	0.52
2:H:699:LEU:H	2:H:799:ASN:HD21	1.56	0.52
2:H:741:MET:N	2:H:741:MET:SD	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:598:LEU:O	5:X:599:ARG:HD2	2.08	0.52
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.39	0.52
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.92	0.52
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.90	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.33	0.52
3:D:646:ILE:HG22	3:D:741:ALA:O	2.09	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.52
3:I:504:GLN:HG3	3:I:505:ASP:H	1.75	0.52
5:X:119:ILE:O	5:X:123:ILE:HG13	2.10	0.52
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.58	0.52
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.40	0.52
2:C:755:LYS:HZ1	2:C:756:TYR:HE2	1.58	0.52
2:C:843:THR:HG22	2:C:844:LYS:N	2.24	0.52
2:C:891:GLY:O	2:C:893:THR:HG23	2.10	0.52
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.75	0.52
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.09	0.52
2:C:80:PHE:O	2:C:84:GLU:HB3	2.10	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.91	0.52
3:D:504:GLN:HG3	3:D:505:ASP:H	1.75	0.52
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.91	0.52
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.24	0.52
2:H:403:MET:HG3	2:H:414:ILE:HB	1.91	0.52
2:H:446:ASP:OD1	2:H:547:VAL:N	2.29	0.52
3:I:451:PRO:HG2	3:I:625:MET:SD	2.50	0.52
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
2:C:487:LEU:CD1	2:C:488:MET:H	2.23	0.51
3:D:703:THR:HA	3:D:717:VAL:HA	1.90	0.51
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.24	0.51
2:H:21:VAL:HG13	2:H:22:LEU:N	2.23	0.51
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.10	0.51
3:I:858:VAL:HB	3:I:859:PRO:CD	2.26	0.51
5:X:400:GLN:O	5:X:404:LEU:HD13	2.11	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.51
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.40	0.51
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.93	0.51
2:H:496:LYS:HE2	5:Y:471:LEU:CD2	2.39	0.51
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.92	0.51
5:Y:379:MET:CE	5:Y:379:MET:HA	2.41	0.51
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.91	0.51
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.09	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.45	0.51
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.25	0.51
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.40	0.51
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.51	0.51
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:H:800:MET:HG2	2:H:1096:ILE:HD13	1.91	0.51
2:H:1281:TYR:CZ	3:I:431:ARG:HG2	2.45	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.44	0.51
5:X:484:ALA:HB2	5:X:494:ILE:HD12	1.92	0.51
2:C:1106:ARG:O	2:C:1108:ASN:N	2.40	0.51
2:C:21:VAL:HG13	2:C:22:LEU:N	2.26	0.51
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.41	0.51
3:D:68:TYR:OH	3:D:94:GLN:NE2	2.44	0.51
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.76	0.51
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.75	0.51
2:H:634:VAL:H	2:H:645:PHE:HE2	1.59	0.51
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.40	0.51
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.11	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.51
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.41	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.74	0.51
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.51
2:C:9:LYS:N	2:C:9:LYS:HD3	2.25	0.51
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.92	0.51
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.51
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.92	0.51
3:I:482:ALA:C	3:I:483:LEU:HD12	2.31	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51
1:A:207:THR:OG1	1:A:208:ASN:N	2.44	0.51
1:A:248:GLU:N	1:A:248:GLU:OE1	2.42	0.51
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.39	0.51
4:E:5:THR:HB	4:E:7:GLN:CB	2.38	0.51
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.76	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.76	0.51
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.24	0.51
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.92	0.51
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.30	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.41	0.51
3:I:245:LEU:O	3:I:250:ARG:NH1	2.43	0.51
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.23	0.51
1:B:45:ARG:O	3:D:538:ARG:NH2	2.44	0.51
3:D:648:GLU:N	3:D:648:GLU:OE2	2.42	0.51
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.46	0.51
4:E:4:VAL:O	4:E:5:THR:OG1	2.24	0.51
2:H:1247:SER:O	2:H:1248:THR:HG23	2.11	0.51
5:X:311:THR:HG21	5:X:348:GLU:CD	2.31	0.51
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.44	0.51
5:X:600:HIS:H	5:X:601:PRO:CD	2.23	0.51
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.93	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.20	0.51
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.51
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.92	0.51
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.91	0.51
4:J:5:THR:HB	4:J:7:GLN:H	1.75	0.51
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.93	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.44	0.51
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.93	0.51
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.30	0.51
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.26	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.93	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.51
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.75	0.51
2:H:901:LEU:O	2:H:905:ILE:HG13	2.11	0.51
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.10	0.51
1:A:303:ILE:O	1:A:307:LEU:HD13	2.10	0.51
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.76	0.51
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.93	0.51
2:C:49:LEU:HD21	2:C:464:PHE:HB3	1.93	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.10	0.51
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.92	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.92	0.51
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.92	0.51
2:H:681:MET:O	2:H:685:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.42	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
1:A:256:PRO:HA	1:A:277:TYR:HA	1.92	0.50
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.46	0.50
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.41	0.50
7:D:1503:O2:O2'	7:D:1503:O2:O1C	2.29	0.50
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.41	0.50
1:G:179:PRO:O	1:G:207:THR:OG1	2.25	0.50
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.93	0.50
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.93	0.50
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.10	0.50
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.92	0.50
3:D:262:THR:HG1	3:D:266:ASN:HD22	1.58	0.50
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.41	0.50
3:D:701:LEU:HD23	3:D:723:TYR:HB2	1.93	0.50
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.37	0.50
1:F:42:ALA:O	1:F:46:ILE:HG12	2.11	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.46	0.50
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.12	0.50
1:A:263:THR:HG23	1:A:266:SER:H	1.76	0.50
2:C:149:LEU:HD12	2:C:452:ARG:O	2.11	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.92	0.50
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.92	0.50
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.11	0.50
3:D:910:ASN:HB3	4:E:15:ASN:HA	1.92	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.24	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.10	0.50
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.92	0.50
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.93	0.50
3:D:482:ALA:C	3:D:483:LEU:HD12	2.32	0.50
3:D:840:LEU:O	3:D:840:LEU:HD12	2.11	0.50
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.41	0.50
2:H:707:ALA:O	2:H:710:VAL:HG12	2.11	0.50
3:I:1260:MET:HE2	3:I:1306:LEU:HD11	1.92	0.50
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.32	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:LEU:HB2	2:C:389:PHE:CE1	2.46	0.50
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.26	0.50
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.46	0.50
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.93	0.50
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.50
2:H:38:PHE:O	2:H:39:ILE:HB	2.10	0.50
3:I:513:MET:CE	3:I:579:LEU:HB2	2.41	0.50
5:X:561:MET:HA	5:X:567:MET:SD	2.50	0.50
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
1:A:47:LEU:HD23	1:A:51:MET:SD	2.52	0.50
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.46	0.50
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.77	0.50
3:D:545:HIS:O	3:D:573:THR:OG1	2.18	0.50
3:D:57:PHE:HB3	3:D:98:ARG:HH11	1.76	0.50
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.24	0.50
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.92	0.50
2:H:487:LEU:CB	2:H:488:MET:HG3	2.39	0.50
2:H:946:LEU:O	2:H:949:GLU:HG3	2.11	0.50
3:I:355:ILE:HG21	3:I:466:MET:SD	2.52	0.50
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.77	0.50
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.41	0.50
3:D:245:LEU:O	3:D:250:ARG:NH1	2.44	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.69	0.50
1:F:151:GLY:O	1:F:177:TYR:HB2	2.12	0.50
3:I:1171:GLY:N	3:I:1172:LYS:O	2.44	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.40	0.50
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.94	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.11	0.50
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.93	0.50
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.44	0.50
2:C:131:THR:HG22	2:C:135:THR:N	2.27	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.50
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.93	0.50
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.50
3:D:173:GLY:O	3:D:175:GLU:HG3	2.11	0.50
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.46	0.50
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.93	0.50
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.45	0.50
3:I:316:ILE:N	3:I:316:ILE:HD13	2.27	0.50
3:I:608:CYS:O	3:I:612:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.92	0.50
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.50
3:D:614:LEU:CD1	4:E:5:THR:HG21	2.42	0.50
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.12	0.50
2:H:1335:ILE:HD12	3:I:1336:ALA:HB2	1.94	0.50
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.11	0.50
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.94	0.50
3:I:513:MET:O	3:I:575:GLY:HA3	2.12	0.50
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.45	0.50
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.50
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.26	0.50
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.32	0.50
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.12	0.50
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.50
2:C:1087:TYR:O	2:C:1213:TYR:N	2.28	0.49
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.93	0.49
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.35	0.49
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.12	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.26	0.49
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.47	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.12	0.49
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.94	0.49
3:I:546:ALA:N	3:I:547:ARG:CA	2.70	0.49
3:I:678:ARG:O	3:I:681:LYS:HG3	2.11	0.49
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.26	0.49
5:X:290:LEU:O	5:X:294:GLN:HB3	2.12	0.49
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.93	0.49
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.94	0.49
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.11	0.49
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.49
3:D:57:PHE:CD1	3:D:247:PRO:HB3	2.46	0.49
2:H:794:LEU:HD21	2:H:796:LEU:CG	2.39	0.49
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.12	0.49
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.95	0.49
3:I:579:LEU:HD13	3:I:579:LEU:O	2.12	0.49
3:I:810:THR:OG1	3:I:811:GLU:N	2.42	0.49
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.49
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.49
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.92	0.49
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.49
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.94	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:735:LYS:HA	2:H:748:ILE:HA	1.94	0.49
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.92	0.49
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.49
2:C:1288:GLN:CA	2:C:1288:GLN:HE21	2.26	0.49
2:C:475:VAL:O	2:C:479:LEU:HB2	2.12	0.49
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.13	0.49
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.42	0.49
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.92	0.49
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.93	0.49
3:I:840:LEU:O	3:I:840:LEU:HD12	2.11	0.49
5:X:278:ASP:OD1	5:X:281:ARG:NH2	2.45	0.49
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.95	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
2:H:1119:MET:O	2:H:1123:GLY:N	2.45	0.49
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.42	0.49
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.41	0.49
2:H:998:LEU:O	2:H:998:LEU:HD13	2.12	0.49
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.78	0.49
5:X:108:VAL:HB	5:X:110:LEU:HG	1.94	0.49
5:X:115:GLY:O	5:X:119:ILE:HG12	2.13	0.49
5:X:310:GLU:O	5:X:344:LEU:HD23	2.12	0.49
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
2:C:818:VAL:HG22	2:C:819:SER:N	2.28	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.33	0.49
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.77	0.49
2:H:590:PRO:O	2:H:659:GLN:NE2	2.46	0.49
2:H:975:ILE:HD13	2:H:975:ILE:O	2.12	0.49
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	1.95	0.49
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.47	0.49
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.49
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.48	0.49
2:C:998:LEU:HD13	2:C:998:LEU:O	2.13	0.49
3:D:807:LEU:O	3:D:807:LEU:HD12	2.12	0.49
3:D:614:LEU:CG	4:E:5:THR:HG21	2.42	0.49
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.48	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:SER:O	2:H:98:VAL:HG23	2.12	0.49
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.49
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.32	0.49
5:X:35:ILE:HG23	5:X:36:VAL:N	2.28	0.49
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.78	0.49
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.49
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.43	0.49
2:C:808:ASN:H	3:D:633:ALA:HB2	1.78	0.49
1:G:9:LEU:H	1:G:9:LEU:HD23	1.78	0.49
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.94	0.49
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.95	0.49
2:H:1270:PHE:CE2	2:H:1274:GLU:HB3	2.48	0.49
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.94	0.49
3:I:227:PHE:O	3:I:230:SER:OG	2.24	0.49
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.94	0.49
5:X:379:MET:HE2	5:X:379:MET:HA	1.95	0.49
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.42	0.49
5:X:511:ILE:HG23	5:X:512:GLY:N	2.25	0.49
1:A:158:ARG:HH21	1:A:158:ARG:HB2	1.77	0.49
1:A:79:LEU:O	1:A:83:LEU:HD13	2.13	0.49
2:C:1335:ILE:HD12	3:D:1336:ALA:HB2	1.95	0.49
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.39	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.76	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.53	0.49
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.43	0.49
3:D:531:LYS:HB3	3:D:531:LYS:NZ	2.28	0.49
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.77	0.49
1:F:60:GLU:HG3	1:F:169:GLY:O	2.12	0.49
2:H:119:GLU:HG2	2:H:120:GLN:N	2.26	0.49
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.94	0.49
2:H:843:THR:HG22	2:H:844:LYS:H	1.78	0.49
1:B:227:GLN:C	1:B:229:GLU:H	2.16	0.49
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.27	0.49
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.93	0.49
3:D:644:MET:O	3:D:764:ARG:NH1	2.46	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.94	0.49
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:317:THR:H	3:I:324:LEU:HD21	1.77	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.13	0.49
1:A:310:ARG:HA	1:A:310:ARG:HE	1.77	0.48
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.28	0.48
2:C:740:GLU:HB2	2:C:741:MET:SD	2.53	0.48
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.13	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.78	0.48
2:C:866:ASP:HA	2:C:872:TYR:OH	2.12	0.48
3:D:120:LEU:HA	5:X:46:GLN:OE1	2.13	0.48
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.48
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.48
3:D:914:ALA:O	3:D:918:ILE:HG22	2.13	0.48
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.38	0.48
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.38	0.48
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.94	0.48
3:I:519:ASN:HD21	3:I:707:ILE:HG21	1.78	0.48
5:X:126:GLY:O	5:X:130:VAL:HG23	2.13	0.48
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.95	0.48
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.26	0.48
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.48	0.48
2:C:99:LYS:HG2	2:C:121:GLU:HB3	1.94	0.48
2:C:660:VAL:HG22	2:C:661:VAL:N	2.23	0.48
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.12	0.48
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.78	0.48
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.43	0.48
5:X:123:ILE:O	5:X:127:ILE:HG12	2.13	0.48
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.43	0.48
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.48
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.26	0.48
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.77	0.48
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.40	0.48
3:D:124:ILE:HA	3:D:237:MET:HE2	1.95	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.13	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.12	0.48
3:D:8:LEU:HD23	3:D:8:LEU:N	2.29	0.48
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.96	0.48
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.95	0.48
3:I:221:ILE:HG13	3:I:222:LYS:N	2.28	0.48
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.43	0.48
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.28	0.48
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.95	0.48
2:C:529:ARG:HH22	2:C:687:ARG:NH2	2.12	0.48
2:C:747:GLY:C	2:C:748:ILE:HG13	2.34	0.48
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.48	0.48
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.48
2:H:1339:LEU:N	2:H:1339:LEU:HD12	2.28	0.48
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.13	0.48
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.39	0.48
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.48
1:B:192:VAL:HG12	1:B:194:GLN:H	1.78	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.12	0.48
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.13	0.48
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.95	0.48
3:D:450:HIS:HE2	3:D:625:MET:CE	2.27	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.95	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.29	0.48
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.94	0.48
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.28	0.48
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.37	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.12	0.48
3:I:746:LEU:HB3	3:I:754:ILE:HG21	1.96	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.12	0.48
5:Y:457:ILE:HG23	5:Y:461:ASN:ND2	2.28	0.48
1:A:243:LYS:N	1:A:243:LYS:HD3	2.29	0.48
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.24	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.94	0.48
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.48
3:D:915:ILE:HG22	3:D:1255:VAL:HG11	1.96	0.48
3:D:128:LEU:HD11	3:D:188:LEU:CD2	2.37	0.48
3:D:221:ILE:HG13	3:D:222:LYS:N	2.29	0.48
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.48
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.94	0.48
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.95	0.48
2:H:898:GLU:N	2:H:898:GLU:OE1	2.37	0.48
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.95	0.48
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.48
3:I:703:THR:O	3:I:718:SER:N	2.47	0.48
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.28	0.48
5:X:227:GLN:HA	5:X:230:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:O	1:A:194:GLN:N	2.45	0.48
3:D:579:LEU:O	3:D:579:LEU:HD13	2.14	0.48
2:H:747:GLY:C	2:H:748:ILE:HG13	2.34	0.48
3:I:572:THR:HG22	3:I:594:GLN:OE1	2.14	0.48
3:I:51:PRO:HB3	3:I:57:PHE:O	2.14	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.79	0.48
3:I:888:CYS:SG	3:I:890:THR:HB	2.54	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.53	0.48
3:D:843:VAL:HG11	3:D:897:HIS:HB3	1.96	0.48
3:D:918:ILE:HD13	3:D:919:ALA:N	2.29	0.48
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.46	0.48
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.14	0.48
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.42	0.48
2:H:72:SER:OG	2:H:99:LYS:HE3	2.13	0.48
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.96	0.48
3:I:294:ASN:ND2	3:I:298:MET:SD	2.87	0.48
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.43	0.48
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.78	0.48
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.49	0.48
2:C:59:ILE:HD11	2:C:63:SER:OG	2.14	0.48
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.95	0.48
3:D:363:LEU:HD12	3:D:450:HIS:ND1	2.29	0.48
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.96	0.48
1:G:82:LEU:O	1:G:86:LYS:HG3	2.14	0.48
2:H:127:ILE:HG12	2:H:127:ILE:O	2.14	0.48
2:H:818:VAL:HG22	2:H:819:SER:N	2.28	0.48
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.49	0.48
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.96	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.13	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
2:C:718:ALA:HB2	2:C:783:LEU:HG	1.96	0.48
3:D:120:LEU:HG	5:X:46:GLN:CB	2.42	0.48
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
2:H:356:THR:HG21	2:H:362:ALA:HA	1.95	0.48
3:I:265:LEU:HD11	3:I:330:MET:SD	2.54	0.48
3:I:377:PHE:O	3:I:381:ILE:HG13	2.14	0.48
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.29	0.48
3:I:714:GLU:HG2	3:I:715:LYS:H	1.79	0.48
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.49	0.48
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.48	0.48
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.96	0.47
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.96	0.47
3:D:1347:LEU:HD22	3:D:1357:ILE:CG2	2.44	0.47
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.49	0.47
2:H:759:SER:HB3	2:H:763:THR:H	1.80	0.47
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.13	0.47
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.13	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
1:B:195:ARG:HH21	1:B:198:LEU:HD21	1.79	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.47
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.97	0.47
3:D:269:TYR:CD2	3:D:306:LEU:HD11	2.49	0.47
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.29	0.47
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.29	0.47
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.49	0.47
2:H:750:ILE:HD13	2:H:963:GLU:OE2	2.14	0.47
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.96	0.47
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.14	0.47
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.96	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.95	0.47
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.78	0.47
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.95	0.47
2:C:812:PHE:N	2:C:815:SER:HB2	2.28	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.40	0.47
4:E:18:ASP:O	4:E:22:VAL:HG12	2.14	0.47
1:F:28:LEU:HD22	1:G:231:PHE:CZ	2.49	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.46	0.47
2:H:963:GLU:O	2:H:967:LEU:HD13	2.14	0.47
3:I:161:THR:HG22	3:I:162:GLU:H	1.79	0.47
3:I:288:PRO:O	3:I:292:VAL:HG12	2.14	0.47
3:I:679:TYR:O	3:I:683:ILE:HG13	2.14	0.47
1:A:222:THR:O	1:A:226:GLU:HG3	2.13	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.47
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
3:D:358:GLY:HA3	3:D:361:LEU:HD23	1.96	0.47
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.50	0.47
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.44	0.47
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.97	0.47
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.79	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
2:C:131:THR:HG22	2:C:135:THR:H	1.80	0.47
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.95	0.47
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.47
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.14	0.47
3:D:714:GLU:HG2	3:D:715:LYS:H	1.79	0.47
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.47
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.50	0.47
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.96	0.47
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.96	0.47
3:I:201:LEU:HD12	3:I:205:LEU:HD11	1.97	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.96	0.47
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.15	0.47
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.95	0.47
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.76	0.47
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.79	0.47
3:I:514:THR:HG21	3:I:595:ALA:O	2.15	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.30	0.47
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.43	0.47
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.55	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.28	0.47
1:A:234:LEU:N	1:A:234:LEU:HD12	2.29	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.47
2:C:127:ILE:HG12	2:C:127:ILE:O	2.14	0.47
2:C:237:LEU:HB2	2:C:287:VAL:O	2.14	0.47
3:D:310:GLY:O	3:D:314:ARG:HG2	2.14	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.97	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
2:H:1106:ARG:O	2:H:1108:ASN:N	2.38	0.47
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.14	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.49	0.47
2:H:546:GLU:O	2:H:548:ARG:N	2.43	0.47
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.50	0.47
2:H:908:GLU:CD	2:H:908:GLU:H	2.18	0.47
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.49	0.47
3:I:473:THR:CG2	3:I:475:GLU:HG2	2.44	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.47
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.50	0.47
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.96	0.47
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.47
2:C:941:LYS:HD2	2:C:941:LYS:O	2.14	0.47
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.49	0.47
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47
3:I:12:THR:O	3:I:13:LYS:HD2	2.14	0.47
2:H:1314:GLN:O	3:I:473:THR:HG23	2.15	0.47
5:X:431:ALA:O	5:X:435:ILE:HG13	2.15	0.47
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.80	0.47
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.97	0.47
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.47
3:D:856:ILE:HG13	3:D:857:LEU:O	2.14	0.47
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.15	0.47
2:H:59:ILE:HB	2:H:480:SER:OG	2.15	0.47
2:H:876:GLU:N	2:H:876:GLU:OE2	2.48	0.47
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.80	0.47
5:Y:291:CYS:O	5:Y:295:CYS:HB2	2.14	0.47
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.96	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.15	0.47
2:C:538:LEU:HD12	2:C:538:LEU:N	2.29	0.47
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.77	0.47
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.32	0.47
3:D:154:LEU:HD22	3:D:176:PHE:CE1	2.49	0.47
3:I:720:ASN:ND2	3:I:720:ASN:O	2.48	0.47
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.15	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.29	0.47
3:D:356:THR:O	3:D:448:GLN:HA	2.15	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.48	0.47
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.97	0.47
2:H:845:LEU:CD2	2:H:889:PRO:HG2	2.41	0.47
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.47
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.30	0.47
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.96	0.47
1:B:232:VAL:O	1:B:233:ASP:HB2	2.15	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
2:C:41:GLN:CD	2:C:42:ASP:H	2.17	0.46
2:C:28:LEU:HD22	2:C:527:LYS:HD2	1.96	0.46
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.50	0.46
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.46
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.96	0.46
3:D:607:THR:O	3:D:611:ILE:HG12	2.15	0.46
1:G:190:ALA:N	1:G:198:LEU:O	2.37	0.46
2:H:1017:GLN:HA	2:H:1020:GLU:HB3	1.97	0.46
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.46
3:I:210:SER:O	3:I:214:ARG:HG3	2.15	0.46
3:I:72:CYS:SG	3:I:73:GLY:N	2.88	0.46
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.15	0.46
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.96	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
1:B:179:PRO:O	1:B:207:THR:OG1	2.29	0.46
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.46
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.46
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.96	0.46
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.50	0.46
3:D:545:HIS:HA	3:D:546:ALA:HA	1.80	0.46
1:G:36:GLY:O	1:G:201:LEU:HD13	2.14	0.46
1:F:221:ALA:CB	1:G:228:LEU:HD12	2.37	0.46
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.48	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.49	0.46
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.29	0.46
2:H:697:LYS:HE2	2:H:793:GLU:HB3	1.97	0.46
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.45	0.46
3:I:605:LEU:HD13	3:I:605:LEU:O	2.15	0.46
5:X:291:CYS:O	5:X:295:CYS:HB2	2.15	0.46
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
3:D:260:PHE:O	5:X:504:PRO:HG2	2.15	0.46
5:Y:124:GLU:HG2	5:Y:128:ASN:ND2	2.31	0.46
5:Y:101:TYR:HE2	5:Y:388:ILE:HD11	1.79	0.46
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.80	0.46
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.45	0.46
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	1.96	0.46
1:F:45:ARG:NH1	2:H:1216:ARG:HA	2.26	0.46
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.51	0.46
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.46
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.97	0.46
3:D:394:ILE:HG21	5:X:536:THR:HA	1.97	0.46
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.48	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.15	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.50	0.46
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	1.98	0.46
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.50	0.46
2:C:908:GLU:CG	2:C:909:LYS:H	2.27	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.27	0.46
3:D:233:LYS:HB3	3:D:236:TRP:CE2	2.50	0.46
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.37	0.46
1:G:185:TYR:HA	1:G:202:VAL:O	2.15	0.46
2:H:1006:GLU:CD	2:H:1006:GLU:H	2.19	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.15	0.46
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.96	0.46
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.49	0.46
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.16	0.46
3:I:911:LYS:O	3:I:911:LYS:HD2	2.15	0.46
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.97	0.46
2:C:843:THR:HB	2:C:845:LEU:CD2	2.46	0.46
3:D:33:TRP:O	3:D:102:MET:HB2	2.15	0.46
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.98	0.46
3:D:868:TRP:HA	3:D:871:LEU:HD23	1.96	0.46
1:F:207:THR:HG23	1:F:209:GLY:H	1.81	0.46
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.97	0.46
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.96	0.46
3:I:356:THR:O	3:I:448:GLN:HA	2.16	0.46
3:I:773:PHE:O	3:I:776:THR:HG22	2.15	0.46
2:C:372:PRO:HB3	5:X:34:ASP:HB3	1.98	0.46
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.45	0.46
3:D:12:THR:C	3:D:13:LYS:HD2	2.36	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.34	0.46
3:D:73:GLY:O	3:D:76:LYS:HE3	2.15	0.46
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.46
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.47	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.50	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:138:VAL:O	3:I:143:SER:HB3	2.15	0.46
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.80	0.46
5:X:139:GLU:HG3	5:X:351:THR:HA	1.97	0.46
2:C:1255:THR:O	2:C:1257:GLN:N	2.42	0.46
2:C:505:PHE:HA	2:C:509:SER:CB	2.46	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:369:PRO:HB2	3:D:372:MET:CB	2.46	0.46
2:H:1032:LYS:NZ	2:H:1032:LYS:HB2	2.30	0.46
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.36	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.46	0.46
2:H:1290:MET:SD	3:I:347:VAL:HG11	2.55	0.46
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.46
5:X:276:MET:O	5:X:280:VAL:HG23	2.16	0.46
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.46
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.51	0.46
2:C:408:SER:O	2:C:431:LYS:NZ	2.31	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.16	0.46
3:D:1195:GLN:N	3:D:1195:GLN:OE1	2.48	0.46
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.46
3:D:586:GLY:O	3:D:587:LEU:HB2	2.16	0.46
3:D:72:CYS:SG	3:D:73:GLY:N	2.87	0.46
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.30	0.46
3:I:217:LEU:O	3:I:221:ILE:HG12	2.15	0.46
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.51	0.46
5:X:264:LYS:HD2	5:X:264:LYS:N	2.30	0.46
5:Y:585:GLU:O	5:Y:589:GLN:N	2.43	0.46
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.56	0.46
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.45	0.46
2:C:944:ARG:HD3	2:C:944:ARG:O	2.15	0.46
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.81	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.16	0.46
3:D:720:ASN:ND2	3:D:720:ASN:O	2.48	0.46
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.16	0.46
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.31	0.46
2:H:205:PRO:O	2:H:208:ILE:HG22	2.16	0.46
2:H:453:ILE:HG23	2:H:453:ILE:O	2.16	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.98	0.46
2:H:895:LEU:HD21	2:H:903:ARG:NH2	2.30	0.46
3:I:129:ASP:HB2	3:I:220:ARG:CZ	2.45	0.46
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:539:SER:O	3:I:541:LEU:N	2.49	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.16	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.16	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.98	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.49	0.46
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.51	0.46
2:C:475:VAL:HG23	2:C:492:MET:SD	2.56	0.46
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.46
3:D:1287:ILE:O	3:D:1290:ARG:HG2	2.16	0.46
3:D:573:THR:HG23	3:D:576:ARG:H	1.80	0.46
2:H:40:GLU:O	2:H:73:TYR:OH	2.33	0.46
2:H:500:ALA:O	2:H:504:GLU:HB2	2.16	0.46
3:I:613:GLY:O	3:I:617:THR:OG1	2.22	0.46
5:Y:562:ARG:HG3	5:Y:591:GLU:CD	2.36	0.46
2:C:515:MET:HE2	2:C:523:GLU:HB3	1.97	0.45
2:C:800:MET:HG2	2:C:1096:ILE:HD13	1.98	0.45
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.31	0.45
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	1.98	0.45
3:D:111:THR:HG23	3:D:300:GLN:NE2	2.30	0.45
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.45
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.80	0.45
1:G:218:ARG:HH12	1:G:222:THR:HB	1.81	0.45
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.98	0.45
2:H:337:PHE:O	2:H:338:THR:OG1	2.26	0.45
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.30	0.45
2:H:600:THR:HG22	2:H:601:ASP:N	2.28	0.45
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.97	0.45
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.98	0.45
3:I:390:LEU:N	3:I:390:LEU:HD12	2.31	0.45
3:I:596:LEU:HD23	3:I:596:LEU:N	2.31	0.45
3:I:620:PHE:O	3:I:624:ILE:HG23	2.16	0.45
3:I:800:LEU:O	3:I:803:VAL:HG12	2.16	0.45
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.16	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	1.97	0.45
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.45	0.45
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.45
1:A:318:LEU:HD13	1:A:318:LEU:N	2.32	0.45
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.19	0.45
2:C:314:ASN:HD21	2:C:348:SER:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.98	0.45
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.47	0.45
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.99	0.45
3:D:1347:LEU:HD23	3:D:1358:PRO:CG	2.30	0.45
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.98	0.45
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.16	0.45
2:H:1117:LEU:HD11	2:H:1182:ILE:CD1	2.47	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.51	0.45
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.81	0.45
2:H:521:LEU:HD22	2:H:667:LEU:HD12	1.99	0.45
3:I:238:ILE:HG13	3:I:238:ILE:O	2.16	0.45
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.81	0.45
3:I:589:TYR:O	3:I:591:ILE:HG13	2.16	0.45
5:X:112:THR:HG22	5:X:113:ARG:N	2.27	0.45
3:D:120:LEU:HG	5:X:46:GLN:CD	2.36	0.45
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.31	0.45
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.15	0.45
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.45
1:A:317:ARG:C	1:A:318:LEU:HD13	2.36	0.45
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.98	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.48	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.30	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:H	1.81	0.45
3:D:290:ILE:O	3:D:293:ARG:HG3	2.15	0.45
3:D:605:LEU:O	3:D:605:LEU:HD13	2.17	0.45
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.31	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.97	0.45
3:D:909:ILE:O	3:D:909:ILE:HD12	2.16	0.45
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.52	0.45
3:I:214:ARG:O	3:I:218:THR:HG22	2.16	0.45
3:I:29:MET:HE3	3:I:29:MET:HA	1.98	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.98	0.45
1:B:129:VAL:HG11	1:B:132:HIS:CE1	2.51	0.45
2:C:1141:LEU:HD22	2:C:1141:LEU:O	2.16	0.45
2:C:131:THR:HG23	2:C:133:ASN:N	2.30	0.45
2:C:620:ASN:HD21	3:D:769:VAL:HG12	1.80	0.45
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:362:ARG:HH22	7:D:1503:O02:H7	1.82	0.45
3:D:514:THR:HG23	3:D:576:ARG:HE	1.80	0.45
4:E:15:ASN:ND2	4:E:18:ASP:HB2	2.31	0.45
1:F:45:ARG:HD3	1:G:34:GLY:HA3	1.97	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.98	0.45
2:H:1103:VAL:H	2:H:1104:PRO:HD2	1.80	0.45
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.31	0.45
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.46	0.45
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.99	0.45
3:I:586:GLY:O	3:I:587:LEU:HB2	2.17	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.97	0.45
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.16	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:N	2.31	0.45
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.47	0.45
2:C:22:LEU:HD13	2:C:23:ASP:O	2.17	0.45
2:C:845:LEU:N	2:C:845:LEU:HD13	2.27	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.81	0.45
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.45
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.16	0.45
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.99	0.45
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.45
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.30	0.45
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.45
3:I:846:GLU:HA	3:I:858:VAL:HA	1.98	0.45
5:X:445:ASP:N	5:X:445:ASP:OD1	2.38	0.45
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.39	0.45
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.98	0.45
1:B:48:LEU:HB3	3:D:538:ARG:HD3	1.99	0.45
2:C:446:ASP:OD1	2:C:546:GLU:HB3	2.17	0.45
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.80	0.45
2:C:699:LEU:HD11	2:C:1179:GLY:CA	2.43	0.45
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.98	0.45
3:D:513:MET:O	3:D:575:GLY:HA3	2.17	0.45
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.76	0.45
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.46	0.45
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.98	0.45
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.98	0.45
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.38	0.45
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.81	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.45
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.17	0.45
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.99	0.45
2:C:49:LEU:CD1	2:C:461:GLU:HA	2.47	0.45
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.52	0.45
2:C:958:LYS:O	2:C:962:GLU:HG2	2.17	0.45
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.32	0.45
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.97	0.45
3:D:1357:ILE:N	3:D:1357:ILE:HD12	2.32	0.45
3:D:238:ILE:HG13	3:D:238:ILE:O	2.15	0.45
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.31	0.45
3:I:1297:LYS:HE2	3:I:1297:LYS:HA	1.97	0.45
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.98	0.45
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.82	0.45
4:J:60:ASN:H	4:J:63:ILE:HB	1.82	0.45
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.45
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.51	0.45
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.51	0.45
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.16	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.98	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
3:D:619:ILE:HD11	3:D:623:GLN:HE21	1.82	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.16	0.45
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.98	0.45
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.52	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.80	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
5:X:240:ARG:HD3	5:X:244:THR:CB	2.40	0.45
5:X:451:ARG:O	5:X:452:ILE:HG13	2.17	0.45
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.16	0.45
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.17	0.45
2:C:1017:GLN:HA	2:C:1020:GLU:HB3	1.98	0.45
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.45
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.47	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.32	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.99	0.45
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.45
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.82	0.45
2:H:149:LEU:HD12	2:H:452:ARG:O	2.17	0.45
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.45
3:I:704:GLU:O	3:I:705:THR:OG1	2.28	0.45
5:Y:354:THR:HG23	5:Y:357:GLN:HB3	1.97	0.45
1:A:181:GLU:OE2	1:A:181:GLU:N	2.50	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.17	0.45
3:D:210:SER:O	3:D:214:ARG:HG3	2.17	0.45
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.47	0.45
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.82	0.45
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.45
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.51	0.45
2:H:1081:PRO:O	2:H:1085:MET:HG3	2.17	0.45
2:H:475:VAL:O	2:H:479:LEU:HB2	2.16	0.45
2:H:756:TYR:H	2:H:766:ASN:HB3	1.82	0.45
3:I:120:LEU:HD22	3:I:1330:ARG:HD2	1.99	0.45
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.22	0.45
3:I:527:LEU:HD12	3:I:535:ARG:NE	2.32	0.45
3:I:856:ILE:HG13	3:I:857:LEU:O	2.16	0.45
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.99	0.45
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.17	0.45
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.45	0.44
3:D:596:LEU:HD23	3:D:596:LEU:N	2.32	0.44
3:D:663:GLU:O	3:D:667:GLN:HG3	2.17	0.44
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.99	0.44
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.99	0.44
3:D:915:ILE:O	3:D:918:ILE:HG23	2.16	0.44
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.31	0.44
2:H:489:PRO:HB2	2:H:492:MET:CB	2.37	0.44
2:H:961:SER:O	2:H:965:GLN:HG3	2.17	0.44
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.32	0.44
3:I:515:ARG:HH22	3:I:717:VAL:C	2.19	0.44
3:I:74:LYS:HB3	3:I:74:LYS:NZ	2.32	0.44
5:X:113:ARG:O	5:X:117:ILE:HD13	2.18	0.44
5:Y:119:ILE:CG2	5:Y:379:MET:HG2	2.45	0.44
5:Y:555:GLU:OE2	5:Y:597:LYS:NZ	2.33	0.44
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.18	0.44
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.44
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.47	0.44
3:D:239:LEU:HD12	3:D:239:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.82	0.44
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.98	0.44
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.32	0.44
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.32	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.88	0.44
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.44
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.98	0.44
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.44
2:C:1027:LYS:NZ	2:C:1027:LYS:HB2	2.33	0.44
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	1.99	0.44
2:C:88:ARG:HB3	2:C:88:ARG:NH1	2.33	0.44
3:D:316:ILE:CG2	3:D:317:THR:H	2.25	0.44
3:D:526:VAL:HG12	3:D:549:LYS:O	2.17	0.44
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.44	0.44
4:E:30:MET:O	4:E:35:LYS:HG2	2.17	0.44
1:G:178:SER:HA	1:G:179:PRO:HD3	1.87	0.44
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.99	0.44
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.99	0.44
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.65	0.44
2:H:1111:GLN:CG	2:H:1230:MET:HE2	2.48	0.44
2:H:484:LEU:HD22	2:H:484:LEU:N	2.31	0.44
2:H:820:GLU:O	2:H:824:GLN:HG3	2.18	0.44
3:I:161:THR:HG22	3:I:162:GLU:N	2.33	0.44
3:I:490:ILE:O	3:I:499:ILE:HG22	2.18	0.44
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.98	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.17	0.44
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.98	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.53	0.44
3:D:825:VAL:HG23	3:D:835:LEU:HB2	1.99	0.44
7:D:1503:O2:O2G	4:E:3:ARG:NH2	2.50	0.44
1:F:185:TYR:HB2	1:F:201:LEU:HD11	1.98	0.44
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.32	0.44
2:H:429:MET:O	2:H:433:ILE:HG13	2.17	0.44
2:H:702:THR:HA	2:H:1184:THR:O	2.16	0.44
2:H:943:LYS:O	2:H:947:GLU:HG2	2.17	0.44
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.16	0.44
3:I:909:ILE:O	3:I:909:ILE:HD12	2.18	0.44
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.83	0.44
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.29	0.44
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.44
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.48	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.80	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.44
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.83	0.44
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.35	0.44
1:G:65:LEU:HD23	1:G:65:LEU:N	2.30	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.30	0.44
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.33	0.44
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.33	0.44
2:H:839:VAL:HG11	2:H:841:ARG:HE	1.83	0.44
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	0.44
3:I:700:ASN:O	3:I:704:GLU:HG2	2.17	0.44
2:H:1276:TRP:CD2	3:I:801:VAL:HG11	2.53	0.44
5:X:61:ASP:HA	5:X:64:ASP:OD2	2.17	0.44
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.00	0.44
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.51	0.44
2:C:177:ILE:HD12	2:C:177:ILE:N	2.33	0.44
2:C:892:GLU:O	2:C:893:THR:OG1	2.22	0.44
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.00	0.44
3:D:704:GLU:HB2	3:D:718:SER:OG	2.18	0.44
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.51	0.44
4:E:5:THR:CA	4:E:7:GLN:H	2.30	0.44
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.58	0.44
1:F:234:LEU:HD21	1:G:217:ILE:HD11	1.98	0.44
1:G:67:GLU:O	1:G:78:ILE:HB	2.18	0.44
1:G:33:ARG:HD3	2:H:1081:PRO:HG3	1.98	0.44
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.64	0.44
2:H:736:VAL:HG11	2:H:740:GLU:HA	1.98	0.44
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.48	0.44
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.46	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.18	0.44
3:I:899:TYR:CE1	3:I:915:ILE:HG23	2.53	0.44
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.51	0.44
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.53	0.44
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.83	0.44
3:D:161:THR:HG22	3:D:162:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.44
3:D:382:TYR:HE1	3:D:401:VAL:CG2	2.31	0.44
2:H:1086:PRO:HA	2:H:1213:TYR:O	2.18	0.44
2:H:1103:VAL:HB	2:H:1104:PRO:HD3	2.00	0.44
2:H:202:ARG:NE	2:H:369:MET:HG2	2.33	0.44
2:H:845:LEU:HD13	2:H:845:LEU:N	2.30	0.44
3:I:664:ILE:HG21	3:I:681:LYS:HD2	2.00	0.44
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.47	0.44
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.99	0.44
1:A:45:ARG:NE	1:B:38:THR:OG1	2.46	0.44
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.32	0.44
2:C:11:ILE:HG21	2:C:697:LYS:HZ1	1.80	0.44
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.18	0.44
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.82	0.44
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.18	0.44
3:D:888:CYS:SG	3:D:890:THR:HB	2.58	0.44
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.18	0.44
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.82	0.44
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.46	0.44
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.53	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.21	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.99	0.44
3:I:12:THR:C	3:I:13:LYS:HD2	2.39	0.44
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.99	0.44
3:I:873:GLU:OE2	3:I:877:VAL:HB	2.18	0.44
5:X:469:GLN:O	5:X:473:GLU:HB2	2.18	0.44
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.26	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.75	0.44
1:B:22:THR:HG22	1:B:208:ASN:O	2.18	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.33	0.44
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.99	0.44
2:C:1081:PRO:O	2:C:1085:MET:HG3	2.17	0.44
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.30	0.44
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.00	0.44
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.44
2:C:697:LYS:NZ	2:C:791:LEU:HD11	2.32	0.44
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.43	0.44
3:D:490:ILE:HG23	3:D:500:ILE:CD1	2.48	0.44
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.32	0.44
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.44
3:D:801:VAL:O	3:D:805:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.99	0.44
1:F:11:PRO:HD2	1:G:227:GLN:HA	1.99	0.44
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	2.00	0.44
2:H:106:GLU:CG	2:H:109:ALA:H	2.31	0.44
2:H:632:ASP:O	2:H:633:LEU:HD23	2.18	0.44
2:H:850:ILE:HG23	2:H:885:GLY:O	2.17	0.44
2:H:890:LYS:NZ	2:H:890:LYS:HB3	2.32	0.44
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.44
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.53	0.44
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.51	0.44
3:I:801:VAL:O	3:I:805:GLN:HG2	2.17	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44
5:X:532:LEU:O	5:X:536:THR:HG23	2.18	0.44
5:Y:123:ILE:O	5:Y:127:ILE:HG12	2.18	0.44
1:B:180:VAL:HG11	1:B:183:ILE:HG12	2.00	0.43
1:B:190:ALA:N	1:B:198:LEU:O	2.37	0.43
2:C:19:PRO:HA	2:C:1157:GLN:HE21	1.83	0.43
2:C:1247:SER:O	2:C:1248:THR:HG23	2.18	0.43
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.86	0.43
2:C:384:LEU:O	2:C:388:LEU:HG	2.17	0.43
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.51	0.43
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.53	0.43
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.98	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.83	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.43
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.46	0.43
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.18	0.43
1:B:46:ILE:HG23	1:B:50:SER:HB2	2.00	0.43
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.69	0.43
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.49	0.43
2:C:515:MET:HE2	2:C:523:GLU:CG	2.48	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.00	0.43
3:D:62:PHE:O	3:D:101:ARG:HG3	2.18	0.43
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.48	0.43
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.00	0.43
1:F:31:LEU:HB2	1:F:199:ASP:O	2.17	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
3:I:1257:VAL:HA	3:I:1260:MET:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.82	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:H	1.82	0.43
3:I:843:VAL:HG21	3:I:897:HIS:HA	2.00	0.43
5:X:299:LYS:O	5:X:303:ILE:HG12	2.18	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.17	0.43
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.47	0.43
2:C:1166:ASP:C	2:C:1168:GLU:H	2.22	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.44	0.43
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.50	0.43
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.01	0.43
2:H:1067:ALA:HB3	2:H:1235:LEU:HD11	2.00	0.43
2:H:216:THR:O	2:H:220:ILE:HG13	2.18	0.43
2:H:73:TYR:N	2:H:73:TYR:CD2	2.86	0.43
3:I:508:LEU:HD23	3:I:508:LEU:O	2.19	0.43
3:I:52:GLU:OE1	5:Y:451:ARG:HD2	2.17	0.43
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.26	0.43
3:I:905:ARG:NH2	4:J:10:VAL:HG11	2.30	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.50	0.43
5:X:456:MET:O	5:X:460:ILE:HG13	2.18	0.43
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.48	0.43
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.99	0.43
1:A:179:PRO:O	1:A:207:THR:OG1	2.25	0.43
1:A:246:LYS:N	1:A:246:LYS:HD3	2.33	0.43
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.99	0.43
2:C:1158:LYS:O	2:C:1158:LYS:HD2	2.19	0.43
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.34	0.43
2:C:219:GLN:O	2:C:223:LEU:HG	2.17	0.43
2:C:590:PRO:O	2:C:659:GLN:NE2	2.50	0.43
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.18	0.43
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.43
3:D:390:LEU:HD12	3:D:390:LEU:N	2.32	0.43
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.84	0.43
1:F:77:ASP:O	1:F:81:ILE:HG13	2.18	0.43
2:H:177:ILE:N	2:H:177:ILE:HD12	2.33	0.43
2:H:944:ARG:HD3	2:H:944:ARG:O	2.17	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	0.43
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.33	0.43
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.43
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:LEU:N	2:C:533:LEU:HD23	2.31	0.43
3:D:1159:ILE:HD12	3:D:1186:TYR:CE2	2.53	0.43
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	2.00	0.43
3:D:215:LYS:O	3:D:219:LYS:HG3	2.19	0.43
3:D:500:ILE:H	3:D:500:ILE:CD1	2.31	0.43
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.33	0.43
3:D:79:LYS:HE3	5:X:568:ASN:C	2.38	0.43
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.00	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.00	0.43
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.18	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.17	0.43
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	2.00	0.43
3:I:179:LYS:N	3:I:179:LYS:HD3	2.33	0.43
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.51	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.83	0.43
1:G:227:GLN:O	1:G:228:LEU:HD23	2.19	0.43
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.54	0.43
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.43
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.84	0.43
2:H:748:ILE:HD12	2:H:748:ILE:C	2.39	0.43
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.89	0.43
3:I:1284:ARG:HA	3:I:1287:ILE:CD1	2.49	0.43
1:G:191:ARG:NH2	3:I:441:LEU:O	2.52	0.43
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.43
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.54	0.43
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
3:I:796:LEU:HG	3:I:800:LEU:HD23	2.01	0.43
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	2.01	0.43
2:C:51:ALA:HB3	2:C:465:ARG:HH11	1.83	0.43
2:C:500:ALA:O	2:C:504:GLU:HB2	2.18	0.43
2:C:611:GLU:HG2	2:C:616:ILE:HD11	2.00	0.43
2:C:622:ASN:OD1	2:C:623:LEU:N	2.51	0.43
2:C:617:ALA:HB2	2:C:650:VAL:HG21	2.01	0.43
2:C:811:ASN:HA	2:C:815:SER:HB2	2.00	0.43
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.99	0.43
3:D:619:ILE:HD13	7:D:1503:O2:H2	1.83	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.19	0.43
1:F:11:PRO:HA	1:F:30:PRO:O	2.19	0.43
1:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.52	0.43
2:H:582:ASN:HB3	2:H:586:PHE:C	2.39	0.43
2:H:816:ILE:HD13	2:H:1074:GLY:CA	2.43	0.43
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.33	0.43
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
3:I:37:GLU:HB2	3:I:104:HIS:HE1	1.83	0.43
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.53	0.43
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.43
5:X:469:GLN:O	5:X:473:GLU:N	2.47	0.43
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.18	0.43
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.43
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.00	0.43
3:D:259:ARG:HH21	5:X:504:PRO:CB	2.26	0.43
3:D:573:THR:HG22	3:D:576:ARG:CD	2.48	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.66	0.43
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.19	0.43
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.34	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:H:622:ASN:OD1	2:H:623:LEU:N	2.52	0.43
1:F:66:HIS:HB3	2:H:874:GLY:HA2	2.00	0.43
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.19	0.43
3:I:159:ILE:N	3:I:159:ILE:HD12	2.33	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
3:I:733:SER:O	3:I:737:ILE:HG12	2.19	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.53	0.43
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.43
2:C:17:LYS:N	2:C:17:LYS:HD2	2.34	0.43
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.47	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CD1	2.48	0.43
3:D:393:THR:H	3:D:396:ALA:HB3	1.83	0.43
3:D:591:ILE:HA	3:D:594:GLN:HB2	2.01	0.43
3:D:491:LEU:HB2	3:D:904:ALA:HA	2.00	0.43
1:F:219:ARG:O	1:F:223:ILE:HG13	2.18	0.43
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.99	0.43
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.01	0.43
2:H:768:MET:O	2:H:785:ASP:N	2.50	0.43
2:H:894:GLN:O	2:H:895:LEU:HB2	2.18	0.43
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.43
5:X:283:GLN:O	5:X:287:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
1:A:257:VAL:HG13	1:A:276:HIS:O	2.19	0.43
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.00	0.43
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.19	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.34	0.43
2:C:453:ILE:HG22	2:C:585:GLY:O	2.19	0.43
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.43
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.43
3:D:416:ILE:O	3:D:416:ILE:HD12	2.19	0.43
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.01	0.43
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.82	0.43
2:H:971:LEU:HG	2:H:1018:TYR:HD1	1.84	0.43
2:H:1276:TRP:CE2	3:I:801:VAL:HG11	2.54	0.43
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.18	0.43
2:H:935:THR:HA	2:H:1048:LYS:HB3	2.00	0.43
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.97	0.43
3:I:1287:ILE:O	3:I:1290:ARG:HG2	2.18	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.34	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.43
3:I:431:ARG:HH21	3:I:493:PRO:HG3	1.83	0.43
3:I:655:SER:O	3:I:658:GLU:HG2	2.19	0.43
3:I:809:VAL:CG1	3:I:913:GLU:H	2.32	0.43
2:C:1329:GLU:O	2:C:1332:SER:HB3	2.19	0.42
2:C:515:MET:HA	2:C:526:HIS:CE1	2.54	0.42
2:C:794:LEU:HD21	2:C:796:LEU:CG	2.46	0.42
3:D:1284:ARG:HA	3:D:1287:ILE:CD1	2.49	0.42
3:D:377:PHE:O	3:D:381:ILE:HG13	2.18	0.42
3:D:508:LEU:HD22	3:D:508:LEU:O	2.18	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.19	0.42
3:D:704:GLU:O	3:D:705:THR:OG1	2.27	0.42
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.83	0.42
2:H:130:MET:CG	2:H:134:GLY:HA2	2.48	0.42
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.42
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.01	0.42
3:I:252:LEU:N	3:I:252:LEU:HD23	2.33	0.42
5:X:250:LEU:O	5:X:254:GLU:HG2	2.18	0.42
5:Y:460:ILE:HG12	5:Y:497:VAL:HG13	2.01	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.18	0.42
2:C:1252:SER:HB3	2:C:1259:LEU:HD23	2.01	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.00	0.42
2:C:542:ARG:HG2	2:C:543:ALA:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:556:GLY:O	2:C:579:ALA:HB2	2.18	0.42
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.01	0.42
2:C:994:ARG:N	2:C:994:ARG:HD3	2.34	0.42
3:D:506:VAL:HG23	3:D:628:GLY:HA3	2.00	0.42
3:D:800:LEU:O	3:D:803:VAL:HG12	2.18	0.42
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.00	0.42
1:G:222:THR:O	1:G:226:GLU:HG2	2.19	0.42
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.01	0.42
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.52	0.42
2:H:557:ARG:NH2	2:H:607:SER:O	2.51	0.42
1:F:134:THR:HG21	2:H:727:VAL:O	2.18	0.42
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.49	0.42
2:H:972:PHE:HA	2:H:975:ILE:HG22	2.01	0.42
3:I:124:ILE:HA	3:I:237:MET:HE2	2.00	0.42
3:I:595:ALA:HB1	3:I:596:LEU:HD23	2.01	0.42
1:A:152:TYR:CE1	1:A:154:PRO:HD3	2.53	0.42
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.32	0.42
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.00	0.42
1:B:19:VAL:HG12	1:B:19:VAL:O	2.20	0.42
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.49	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.33	0.42
2:C:645:PHE:CD1	2:C:650:VAL:HB	2.54	0.42
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.01	0.42
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.19	0.42
3:D:362:ARG:NH1	7:D:1503:O2:H7	2.32	0.42
3:D:288:PRO:O	3:D:292:VAL:HG12	2.19	0.42
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.50	0.42
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.54	0.42
3:D:746:LEU:HB3	3:D:754:ILE:CG2	2.49	0.42
3:D:843:VAL:HA	3:D:861:ASN:HA	2.01	0.42
3:D:789:LYS:HD2	3:D:932:MET:SD	2.59	0.42
3:D:614:LEU:HD12	4:E:5:THR:HG21	2.01	0.42
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.49	0.42
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.83	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:941:LYS:O	2:H:941:LYS:HD2	2.19	0.42
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.50	0.42
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.01	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.42
3:I:805:GLN:HE21	3:I:805:GLN:HB2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:448:ARG:HH11	5:X:452:ILE:HD12	1.85	0.42
1:A:152:TYR:CD1	1:A:154:PRO:HD3	2.54	0.42
2:C:51:ALA:C	2:C:53:PHE:H	2.22	0.42
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.90	0.42
2:C:890:LYS:NZ	2:C:890:LYS:HB3	2.33	0.42
3:D:201:LEU:HD12	3:D:205:LEU:HD11	2.02	0.42
3:D:114:ILE:CG2	3:D:308:ASP:HB3	2.50	0.42
3:D:355:ILE:HG12	3:D:464:ASP:O	2.19	0.42
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.42
3:D:909:ILE:HG13	3:D:909:ILE:H	1.56	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.01	0.42
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.42
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.49	0.42
2:H:302:ILE:HA	2:H:309:LEU:HA	2.01	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
2:H:81:ASP:OD1	2:H:83:GLN:HG2	2.19	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
3:I:1282:TYR:HA	3:I:1285:VAL:CG2	2.49	0.42
3:I:403:ARG:O	3:I:405:GLU:N	2.53	0.42
3:I:58:CYS:SG	3:I:61:ILE:HG13	2.60	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
5:Y:469:GLN:O	5:Y:473:GLU:HB2	2.19	0.42
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.42
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.42
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.54	0.42
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.30	0.42
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.42
3:D:425:ARG:CZ	3:D:459:ALA:HA	2.49	0.42
2:H:94:ALA:O	2:H:126:GLU:HG2	2.19	0.42
2:H:27:LEU:O	2:H:528:ARG:NH1	2.49	0.42
2:H:896:THR:O	2:H:899:GLU:N	2.48	0.42
3:I:313:GLY:O	3:I:314:ARG:HB2	2.20	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.02	0.42
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	2.00	0.42
5:Y:532:LEU:O	5:Y:536:THR:HG23	2.19	0.42
1:B:153:VAL:O	1:B:175:ALA:N	2.52	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.42
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:487:LEU:H	2:C:487:LEU:HD12	1.84	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.39	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.42
3:D:558:ASP:OD1	3:D:559:ALA:N	2.52	0.42
3:D:77:ARG:CG	3:D:78:LEU:H	2.31	0.42
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.42
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.83	0.42
2:H:22:LEU:HD13	2:H:23:ASP:O	2.19	0.42
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.52	0.42
3:I:1324:SER:CB	3:I:1348:LYS:HD3	2.48	0.42
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.54	0.42
3:I:607:THR:O	3:I:611:ILE:HG12	2.19	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
5:X:139:GLU:HA	5:X:142:THR:CG2	2.48	0.42
5:Y:278:ASP:O	5:Y:282:THR:OG1	2.24	0.42
2:C:104:ILE:HD11	2:C:115:LYS:HB2	2.02	0.42
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.55	0.42
2:C:836:LEU:HB3	2:C:918:LEU:HD21	2.02	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.42
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.01	0.42
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.84	0.42
2:H:17:LYS:HD2	2:H:17:LYS:N	2.35	0.42
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.42
2:H:553:THR:O	2:H:557:ARG:HD3	2.19	0.42
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.50	0.42
3:I:1297:LYS:NZ	3:I:1297:LYS:CA	2.82	0.42
3:I:147:ILE:HG13	3:I:149:GLY:H	1.84	0.42
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.42
2:H:1268:GLN:O	3:I:346:ARG:HA	2.20	0.42
3:I:397:ALA:O	3:I:401:VAL:HG13	2.20	0.42
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.42
3:I:66:LYS:HB3	3:I:66:LYS:NZ	2.34	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.85	0.42
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.42
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.67	0.42
2:C:348:SER:O	2:C:352:ARG:HG3	2.20	0.42
2:C:632:ASP:O	2:C:633:LEU:HD23	2.20	0.42
2:C:99:LYS:HZ3	2:C:99:LYS:HB3	1.83	0.42
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.55	0.42
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.48	0.42
3:D:619:ILE:O	3:D:623:GLN:HG2	2.19	0.42
2:H:1073:LYS:HD3	3:I:462:ASP:CB	2.21	0.42
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.40	0.42
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.34	0.42
2:H:766:ASN:H	2:H:787:PRO:HG3	1.85	0.42
3:I:105:ILE:HG13	3:I:244:VAL:CG2	2.50	0.42
5:X:316:PHE:CZ	5:X:334:SER:HA	2.55	0.42
5:Y:119:ILE:CD1	5:Y:122:ARG:HH21	2.33	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.42
2:C:768:MET:O	2:C:785:ASP:N	2.48	0.42
3:D:154:LEU:HD22	3:D:176:PHE:HE1	1.83	0.42
3:D:466:MET:HE2	3:D:466:MET:HB3	1.88	0.42
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.20	0.42
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.01	0.42
3:D:843:VAL:HG21	3:D:897:HIS:HA	2.02	0.42
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.84	0.42
2:H:80:PHE:O	2:H:84:GLU:HB3	2.19	0.42
3:I:1148:ARG:HB2	3:I:1148:ARG:NH2	2.35	0.42
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.35	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.19	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.00	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
5:X:608:ARG:HB3	5:X:608:ARG:NH1	2.35	0.42
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.84	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.20	0.42
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.59	0.42
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.54	0.42
3:D:574:VAL:O	3:D:578:ILE:HG22	2.20	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.50	0.42
1:F:234:LEU:HD12	1:F:234:LEU:N	2.35	0.42
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.42
2:H:1161:LEU:HD21	2:H:1172:LEU:HD11	2.02	0.42
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.50	0.42
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.55	0.42
2:H:549:ASP:OD1	2:H:550:VAL:N	2.53	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.42
5:X:477:GLU:H	5:X:477:GLU:CD	2.23	0.42
5:X:52:GLY:O	5:X:53:ILE:HB	2.20	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.79	0.41
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.41
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.41
2:C:72:SER:O	2:C:98:VAL:HG23	2.20	0.41
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	2.02	0.41
3:D:141:PHE:HD2	3:D:141:PHE:HA	1.71	0.41
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.84	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.20	0.41
2:H:122:VAL:HG22	2:H:123:TYR:N	2.34	0.41
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.19	0.41
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.41
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.46	0.41
2:H:469:VAL:O	2:H:472:GLU:HB3	2.20	0.41
2:H:481:LEU:C	2:H:481:LEU:HD13	2.40	0.41
2:H:54:ARG:N	2:H:55:SER:C	2.74	0.41
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	2.01	0.41
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	2.02	0.41
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.46	0.41
3:I:326:SER:O	3:I:330:MET:HG3	2.19	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
3:I:532:GLU:OE1	3:I:578:ILE:HB	2.20	0.41
3:I:746:LEU:HD22	3:I:746:LEU:H	1.85	0.41
5:Y:363:ARG:HE	5:Y:363:ARG:HA	1.84	0.41
1:B:228:LEU:HD12	1:B:228:LEU:C	2.41	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.85	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.41
2:H:103:VAL:HG22	2:H:104:ILE:N	2.34	0.41
2:H:1323:PHE:O	2:H:1327:LEU:HG	2.20	0.41
2:H:170:VAL:HG23	2:H:171:LEU:N	2.31	0.41
2:H:985:GLU:HG2	2:H:989:LEU:HD13	2.01	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.36	0.41
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.49	0.41
3:I:290:ILE:O	3:I:293:ARG:HG3	2.20	0.41
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.33	0.41
3:I:500:ILE:H	3:I:500:ILE:CD1	2.33	0.41
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.35	0.41
3:I:73:GLY:O	3:I:76:LYS:HE3	2.19	0.41
3:I:843:VAL:HG11	3:I:897:HIS:HB3	2.02	0.41
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.20	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.54	0.41
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.41
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.20	0.41
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
2:C:135:THR:OG1	2:C:142:GLU:HG3	2.20	0.41
2:C:230:PHE:HB2	2:C:333:ILE:HB	2.01	0.41
2:C:82:VAL:HG13	2:C:83:GLN:N	2.36	0.41
2:C:81:ASP:OD1	2:C:83:GLN:HG2	2.21	0.41
2:C:943:LYS:O	2:C:947:GLU:HG2	2.20	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.47	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
2:H:513:GLN:NE2	2:H:513:GLN:HA	2.24	0.41
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.02	0.41
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.55	0.41
3:I:120:LEU:HD12	3:I:120:LEU:N	2.35	0.41
3:I:141:PHE:O	3:I:297:ARG:HD3	2.21	0.41
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.55	0.41
1:A:22:THR:O	1:A:207:THR:N	2.50	0.41
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.36	0.41
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.41
2:C:27:LEU:O	2:C:528:ARG:NH1	2.52	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB2	1.89	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.21	0.41
3:D:369:PRO:HB2	3:D:372:MET:HB2	2.01	0.41
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.55	0.41
1:B:86:LYS:NZ	3:D:526:VAL:O	2.48	0.41
3:D:805:GLN:HB2	3:D:805:GLN:HE21	1.72	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.20	0.41
2:H:1199:LEU:HD13	2:H:1206:THR:HA	2.02	0.41
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.34	0.41
2:H:142:GLU:O	2:H:143:ARG:HB2	2.21	0.41
2:H:619:ALA:HA	2:H:653:MET:CE	2.51	0.41
2:H:518:ASN:ND2	2:H:761:GLN:HG2	2.35	0.41
2:H:843:THR:HB	2:H:845:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:219:LYS:O	3:I:223:LEU:HG	2.20	0.41
1:A:166:ARG:HG3	1:A:166:ARG:O	2.21	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.41
1:B:47:LEU:HD13	1:B:205:MET:HE2	2.03	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.41
2:C:546:GLU:O	2:C:548:ARG:N	2.48	0.41
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.55	0.41
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.90	0.41
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.36	0.41
3:D:678:ARG:HD2	3:D:678:ARG:C	2.41	0.41
1:F:190:ALA:N	1:F:198:LEU:O	2.48	0.41
1:F:46:ILE:O	1:F:50:SER:HB2	2.20	0.41
3:I:1193:TRP:CD1	3:I:1194:ARG:HD2	2.55	0.41
3:I:135:ILE:O	3:I:139:LEU:HD12	2.20	0.41
3:I:217:LEU:O	3:I:221:ILE:HG23	2.21	0.41
3:I:279:LEU:HD23	3:I:295:GLU:HB3	2.02	0.41
3:I:303:VAL:O	3:I:307:LEU:HG	2.20	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
5:X:133:SER:OG	5:X:365:MET:HB2	2.21	0.41
5:Y:528:LEU:O	5:Y:528:LEU:HD12	2.20	0.41
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.50	0.41
1:A:45:ARG:HH12	2:C:1216:ARG:HA	1.86	0.41
2:C:397:LEU:O	2:C:398:SER:OG	2.33	0.41
3:D:128:LEU:HA	3:D:192:MET:CE	2.49	0.41
3:D:214:ARG:HA	3:D:217:LEU:HD12	2.02	0.41
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.54	0.41
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.56	0.41
3:D:649:LYS:O	3:D:653:ILE:HG12	2.21	0.41
4:E:16:ARG:O	4:E:19:LEU:HB3	2.20	0.41
2:H:1165:SER:O	2:H:1168:GLU:HB3	2.21	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.20	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.96	0.41
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.19	0.41
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.50	0.41
3:I:392:THR:HG22	5:Y:606:VAL:HG11	2.01	0.41
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.41
2:C:99:LYS:HA	2:C:121:GLU:HA	2.02	0.41
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.84	0.41
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.41
2:C:901:LEU:HD13	5:X:559:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.54	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.21	0.41
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.69	0.41
1:F:89:ALA:HB3	1:F:124:VAL:HB	2.03	0.41
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.03	0.41
2:H:680:LEU:O	2:H:680:LEU:HD23	2.21	0.41
2:H:843:THR:HB	2:H:845:LEU:CD2	2.51	0.41
3:I:1322:ALA:O	3:I:1326:GLN:HG3	2.21	0.41
3:I:382:TYR:CE1	3:I:398:LYS:HA	2.56	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
3:I:494:ALA:HA	3:I:1252:HIS:CE1	2.53	0.41
5:X:363:ARG:HE	5:X:363:ARG:HA	1.85	0.41
5:Y:453:PRO:CD	5:Y:456:MET:HB2	2.42	0.41
5:Y:476:ARG:HB2	5:Y:477:GLU:OE1	2.20	0.41
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.02	0.41
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.03	0.41
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.56	0.41
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
2:C:975:ILE:O	2:C:978:VAL:HG12	2.21	0.41
3:D:1149:ARG:H	3:D:1149:ARG:CD	2.23	0.41
3:D:27:PRO:HD3	3:D:236:TRP:CE3	2.56	0.41
3:D:53:ARG:HA	3:D:53:ARG:HD2	1.96	0.41
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.41
3:D:746:LEU:H	3:D:746:LEU:HD22	1.85	0.41
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.20	0.41
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.41
2:H:1285:TYR:HA	2:H:1288:GLN:HB3	2.02	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
2:H:977:ALA:O	2:H:980:VAL:HG12	2.20	0.41
3:I:422:LEU:O	3:I:422:LEU:HD12	2.20	0.41
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.41
3:I:873:GLU:H	3:I:873:GLU:HG3	1.64	0.41
5:X:261:LEU:HD12	5:X:261:LEU:N	2.36	0.41
5:X:270:VAL:HA	5:X:273:MET:HE3	2.01	0.41
5:X:35:ILE:HG13	5:X:36:VAL:N	2.21	0.41
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.30	0.41
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.01	0.41
5:Y:261:LEU:N	5:Y:261:LEU:HD12	2.36	0.41
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.35	0.41
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.41
2:C:688:GLN:O	2:C:1236:ASN:N	2.54	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
2:C:752:ASN:C	2:C:753:LEU:HG	2.40	0.41
2:C:82:VAL:O	2:C:86:GLN:HG3	2.20	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB2	2.01	0.41
3:D:128:LEU:HD12	3:D:192:MET:CE	2.35	0.41
2:H:374:GLU:HA	2:H:375:PRO:HD3	1.93	0.41
2:H:690:VAL:HA	2:H:691:PRO:HD3	1.91	0.41
3:I:1173:ARG:CA	3:I:1174:ARG:CB	2.86	0.41
3:I:155:GLU:H	3:I:155:GLU:CD	2.24	0.41
3:I:552:ILE:HD13	3:I:570:LYS:HB2	2.03	0.41
2:C:122:VAL:CG2	5:X:472:GLN:HE21	2.34	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.20	0.41
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.55	0.41
2:C:442:VAL:HG12	2:C:443:ASP:N	2.36	0.41
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.41
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.41	0.41
3:D:647:PRO:HG3	3:D:697:MET:HA	2.03	0.41
2:H:1138:VAL:O	2:H:1139:ALA:HB3	2.20	0.41
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.89	0.41
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.21	0.41
2:H:618:GLN:HG2	2:H:637:ARG:NH2	2.36	0.41
3:I:116:PHE:HB3	3:I:237:MET:HE3	2.03	0.41
3:I:526:VAL:HG12	3:I:549:LYS:O	2.20	0.41
3:I:746:LEU:HD22	3:I:746:LEU:N	2.36	0.41
5:X:262:VAL:HG13	5:X:263:PRO:CD	2.48	0.41
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.20	0.41
5:Y:374:ARG:O	5:Y:378:GLU:HG3	2.21	0.41
1:B:176:CYS:C	1:B:178:SER:N	2.74	0.41
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.21	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.21	0.41
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.54	0.41
2:C:661:VAL:HG23	2:C:662:SER:O	2.22	0.41
2:C:84:GLU:HG3	2:C:88:ARG:HD3	2.03	0.41
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.41
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:361:LEU:HD22	3:D:361:LEU:N	2.36	0.41
3:D:409:TRP:O	3:D:412:LEU:HB3	2.21	0.41
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.61	0.41
3:D:681:LYS:HD3	3:D:682:VAL:N	2.36	0.41
4:E:15:ASN:HD21	4:E:18:ASP:CB	2.32	0.41
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.20	0.41
2:H:698:PRO:HB3	2:H:1231:TYR:CE1	2.56	0.41
2:H:31:GLN:HG3	2:H:130:MET:HE1	2.03	0.41
2:H:691:PRO:HA	2:H:788:SER:OG	2.21	0.41
2:H:812:PHE:H	2:H:815:SER:HB2	1.86	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
3:I:128:LEU:HD12	3:I:192:MET:HE1	2.02	0.41
3:I:527:LEU:HB3	3:I:528:THR:H	1.72	0.41
3:I:856:ILE:HD12	3:I:857:LEU:H	1.86	0.41
3:I:903:LEU:HD11	3:I:909:ILE:CG2	2.45	0.41
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.50	0.41
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.02	0.40
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.86	0.40
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.21	0.40
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.56	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.40
2:C:73:TYR:HA	2:C:98:VAL:HA	2.02	0.40
2:C:854:ILE:HB	2:C:857:VAL:HG11	2.03	0.40
3:D:1274:PHE:CD2	3:D:1275:LEU:HG	2.50	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.20	0.40
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
1:F:59:VAL:HG21	1:F:85:LEU:HD13	2.03	0.40
2:H:130:MET:HG3	2:H:134:GLY:HA2	2.03	0.40
2:H:740:GLU:CD	2:H:740:GLU:H	2.24	0.40
2:H:892:GLU:C	2:H:894:GLN:H	2.24	0.40
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.51	0.40
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	2.02	0.40
5:Y:591:GLU:O	5:Y:595:LEU:HG	2.21	0.40
1:A:102:LEU:HD12	1:A:115:ILE:HG12	2.03	0.40
1:A:323:PRO:HA	1:A:324:ALA:HA	1.77	0.40
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.40
1:A:67:GLU:HA	1:A:78:ILE:HG21	2.03	0.40
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.86	0.40
2:C:1269:ARG:HD2	3:D:344:GLY:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:538:LEU:HD12	2:C:538:LEU:H	1.86	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.86	0.40
2:C:848:GLU:HG2	2:C:888:THR:HA	2.02	0.40
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.52	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.86	0.40
3:D:697:MET:SD	3:D:741:ALA:HB3	2.62	0.40
3:D:836:ARG:HA	3:D:836:ARG:HD2	1.88	0.40
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.03	0.40
2:H:219:GLN:O	2:H:223:LEU:HG	2.21	0.40
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	2.03	0.40
2:H:821:ARG:HB2	2:H:1082:ILE:HD13	2.04	0.40
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.86	0.40
2:H:870:ILE:HD12	2:H:870:ILE:N	2.36	0.40
3:I:385:LEU:HD23	3:I:411:ILE:HG13	2.03	0.40
3:I:519:ASN:HD21	3:I:707:ILE:CG2	2.33	0.40
5:X:253:SER:O	5:X:257:LYS:HG3	2.21	0.40
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.02	0.40
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.21	0.40
1:A:313:SER:OG	1:A:314:LEU:N	2.53	0.40
2:C:1004:ASP:N	2:C:1004:ASP:OD1	2.55	0.40
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.51	0.40
2:C:1259:LEU:HD12	2:C:1259:LEU:C	2.40	0.40
2:C:18:ARG:HG3	2:C:19:PRO:HD2	2.03	0.40
2:C:517:GLN:HG3	2:C:759:SER:OG	2.21	0.40
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.50	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.22	0.40
3:D:1341:ARG:HD3	3:D:1343:GLU:CD	2.42	0.40
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.49	0.40
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.55	0.40
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.86	0.40
3:I:1243:LEU:O	3:I:1243:LEU:HD23	2.22	0.40
3:I:510:LEU:HD12	3:I:601:ILE:HD11	2.03	0.40
3:I:545:HIS:HA	3:I:546:ALA:HA	1.80	0.40
5:X:283:GLN:CD	5:X:343:LYS:HD2	2.41	0.40
3:D:395:LYS:NZ	5:X:607:LEU:O	2.50	0.40
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.21	0.40
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.03	0.40
1:B:61:ILE:HB	1:B:64:VAL:HB	2.03	0.40
2:C:115:LYS:O	2:C:116:ASP:HB2	2.21	0.40
2:C:409:LEU:HD11	2:C:428:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:505:PHE:HA	2:C:509:SER:HB3	2.04	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
3:D:205:LEU:HB3	3:D:217:LEU:HD22	2.04	0.40
3:D:588:PRO:O	3:D:589:TYR:HB2	2.21	0.40
3:D:679:TYR:O	3:D:683:ILE:HG13	2.21	0.40
3:D:746:LEU:N	3:D:746:LEU:HD22	2.36	0.40
3:D:483:LEU:HD11	4:E:20:VAL:HG21	2.03	0.40
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.03	0.40
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.85	0.40
2:H:623:LEU:HD12	2:H:623:LEU:N	2.36	0.40
3:I:310:GLY:HA2	3:I:314:ARG:HG2	2.04	0.40
3:I:325:LYS:NZ	3:I:325:LYS:HB3	2.36	0.40
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.91	0.40
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.52	0.40
5:X:410:ILE:O	5:X:414:LYS:HG3	2.22	0.40
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.87	0.40
5:X:559:LEU:HD23	5:X:559:LEU:HA	1.90	0.40
1:A:50:SER:HA	1:A:150:ARG:HD2	2.02	0.40
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.56	0.40
2:C:1195:ILE:O	2:C:1199:LEU:HG	2.22	0.40
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.46	0.40
2:C:465:ARG:O	2:C:469:VAL:HG23	2.21	0.40
2:C:59:ILE:HG12	2:C:65:ASN:O	2.20	0.40
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.04	0.40
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.40
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.86	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.04	0.40
3:D:355:ILE:HG21	3:D:466:MET:SD	2.61	0.40
3:D:678:ARG:O	3:D:682:VAL:HG13	2.21	0.40
3:D:709:ARG:O	3:D:712:GLN:N	2.53	0.40
3:D:84:ILE:HG13	3:D:84:ILE:H	1.76	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.52	0.40
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.37	0.40
3:I:609:TYR:HE2	3:I:614:LEU:HD13	1.86	0.40
2:H:894:GLN:NE2	3:I:77:ARG:HD3	2.32	0.40
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.40
3:I:915:ILE:O	3:I:918:ILE:HG23	2.22	0.40
3:I:417:ARG:NH1	4:J:43:ASN:O	2.55	0.40
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.87	0.40
5:X:400:GLN:HE21	5:X:403:ASP:CG	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:530:LEU:H	5:X:530:LEU:HD12	1.86	0.40
5:X:558:VAL:O	5:X:562:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	2	27
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	4	32
1	F	227/329 (69%)	193 (85%)	28 (12%)	6 (3%)	6	39
1	G	213/329 (65%)	186 (87%)	22 (10%)	5 (2%)	7	42
2	C	1333/1342 (99%)	1073 (80%)	208 (16%)	52 (4%)	3	31
2	H	1333/1342 (99%)	1078 (81%)	206 (16%)	49 (4%)	4	32
3	D	1154/1407 (82%)	926 (80%)	182 (16%)	46 (4%)	3	30
3	I	1154/1407 (82%)	925 (80%)	184 (16%)	45 (4%)	3	31
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	2	23
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	2	24
5	X	511/613 (83%)	450 (88%)	46 (9%)	15 (3%)	5	37
5	Y	454/613 (74%)	409 (90%)	34 (8%)	11 (2%)	6	41
All	All	7079/8222 (86%)	5834 (82%)	984 (14%)	261 (4%)	4	32

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	B	20	SER

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Mol	Chain	Res	Type
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	686	GLN
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1339	GLY
3	D	1344	LEU
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
1	G	177	TYR
2	H	21	VAL
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	669	PRO
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP

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Mol	Chain	Res	Type
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	710	ASP
3	I	847	ASP
3	I	1339	GLY
5	Y	241	SER
1	A	52	PRO
1	A	160	HIS
1	A	187	VAL
1	A	193	GLU
1	B	19	VAL
1	B	177	TYR
2	C	56	VAL
2	C	78	PRO
2	C	79	VAL
2	C	753	LEU
2	C	1236	ASN
2	C	1239	VAL
2	C	1240	ASP
3	D	89	GLY
3	D	155	GLU
3	D	316	ILE
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	887	SER
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
4	E	6	VAL
4	E	35	LYS
5	X	20	GLY
2	H	56	VAL
2	H	78	PRO
2	H	170	VAL
2	H	298	ALA
2	H	535	PRO
2	H	753	LEU
2	H	1186	VAL
2	H	1239	VAL
2	H	1240	ASP

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Mol	Chain	Res	Type
2	H	1256	GLN
3	I	89	GLY
3	I	155	GLU
3	I	345	LYS
3	I	406	ALA
3	I	540	GLY
3	I	542	ALA
3	I	707	ILE
3	I	708	ASN
3	I	731	ARG
3	I	851	PRO
3	I	901	ARG
3	I	913	GLU
3	I	914	ALA
3	I	1268	ASN
3	I	1344	LEU
4	J	6	VAL
4	J	35	LYS
5	Y	490	PRO
5	Y	564	GLY
1	A	14	VAL
1	B	235	ARG
2	C	44	GLU
2	C	53	PHE
2	C	143	ARG
2	C	437	ASN
2	C	699	LEU
2	C	740	GLU
2	C	812	PHE
2	C	1107	MET
2	C	1256	GLN
3	D	559	ALA
3	D	703	THR
3	D	707	ILE
3	D	731	ARG
3	D	848	VAL
3	D	851	PRO
3	D	902	ASP
5	X	23	THR
5	X	308	GLY
5	X	514	ASP
5	X	581	ASP

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Mol	Chain	Res	Type
1	F	160	HIS
1	F	188	GLU
1	G	188	GLU
1	G	228	LEU
2	H	13	LYS
2	H	44	GLU
2	H	53	PHE
2	H	437	ASN
2	H	740	GLU
2	H	812	PHE
2	H	1107	MET
2	H	1236	ASN
3	I	53	ARG
3	I	132	LEU
3	I	559	ALA
3	I	595	ALA
3	I	703	THR
3	I	721	SER
3	I	887	SER
3	I	1195	GLN
5	Y	108	VAL
5	Y	308	GLY
5	Y	491	GLU
5	Y	581	ASP
1	A	166	ARG
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	298	ALA
2	C	1080	ASN
2	C	1139	ALA
3	D	53	ARG
3	D	132	LEU
3	D	598	LYS
3	D	728	SER
3	D	855	ASP
3	D	888	CYS
3	D	1195	GLN
3	D	1363	TYR
4	E	5	THR
5	X	50	ASP
5	X	108	VAL

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Mol	Chain	Res	Type
5	X	504	PRO
1	F	153	VAL
1	F	166	ARG
2	H	43	PRO
2	H	143	ARG
2	H	699	LEU
2	H	739	ASP
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1270	PHE
3	I	598	LYS
3	I	728	SER
3	I	848	VAL
3	I	855	ASP
3	I	888	CYS
5	Y	504	PRO
5	Y	514	ASP
1	A	93	GLN
1	A	163	GLU
1	A	195	ARG
2	C	13	LYS
2	C	487	LEU
2	C	543	ALA
2	C	746	ALA
2	C	895	LEU
2	C	1093	PRO
2	C	1237	HIS
2	C	1238	LEU
2	C	1270	PHE
3	D	62	PHE
3	D	210	SER
3	D	540	GLY
3	D	1167	LYS
5	X	25	ALA
5	X	491	GLU
5	X	564	GLY
5	X	600	HIS
1	F	33	ARG
2	H	488	MET
2	H	746	ALA

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Mol	Chain	Res	Type
2	H	1045	GLY
2	H	1237	HIS
3	I	62	PHE
3	I	210	SER
3	I	902	ASP
4	J	5	THR
5	Y	600	HIS
1	A	153	VAL
1	B	49	SER
1	B	228	LEU
2	C	59	ILE
2	C	69	GLN
2	C	739	ASP
2	C	1003	THR
2	C	1315	MET
3	D	417	ARG
3	D	742	GLY
3	D	1173	ARG
4	E	15	ASN
4	E	59	ILE
1	G	49	SER
2	H	1139	ALA
2	H	1238	LEU
3	I	108	ALA
3	I	443	GLU
3	I	712	GLN
3	I	742	GLY
3	I	1167	LYS
4	J	59	ILE
1	A	232	VAL
2	C	104	ILE
2	H	59	ILE
2	H	104	ILE
2	C	1045	GLY
3	I	850	LYS
1	A	322	PRO
2	C	373	GLY
3	D	850	LYS
2	H	373	GLY
5	X	35	ILE
3	I	316	ILE
5	Y	97	PRO

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Mol	Chain	Res	Type
2	C	117	ILE
3	D	471	PRO
3	D	1184	ASP
3	I	471	PRO
2	H	489	PRO
2	H	1181	PRO
2	C	1181	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	273 (97%)	8 (3%)	47	71
1	B	189/286 (66%)	186 (98%)	3 (2%)	65	83
1	F	197/286 (69%)	194 (98%)	3 (2%)	67	84
1	G	185/286 (65%)	182 (98%)	3 (2%)	65	83
2	C	1150/1157 (99%)	1094 (95%)	56 (5%)	27	59
2	H	1150/1157 (99%)	1097 (95%)	53 (5%)	29	61
3	D	971/1168 (83%)	921 (95%)	50 (5%)	26	59
3	I	971/1168 (83%)	918 (94%)	53 (6%)	24	57
4	E	74/75 (99%)	72 (97%)	2 (3%)	48	72
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	447 (97%)	13 (3%)	47	71
5	Y	407/540 (75%)	392 (96%)	15 (4%)	37	66
All	All	6100/7024 (87%)	5841 (96%)	259 (4%)	32	63

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	LEU
1	A	117	HIS

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	182	ARG
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	80	PHE
2	C	88	ARG
2	C	121	GLU
2	C	127	ILE
2	C	150	HIS
2	C	163	LYS
2	C	479	LEU
2	C	487	LEU
2	C	514	PHE
2	C	603	ILE
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU
2	C	908	GLU
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE

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Mol	Chain	Res	Type
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1241	ASP
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	20	ILE
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	104	HIS
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	179	LYS
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	430	HIS

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Mol	Chain	Res	Type
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	614	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	805	GLN
3	D	816	THR
3	D	832	LYS
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1306	LEU
4	E	8	ASP
4	E	15	ASN
5	X	21	TYR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	452	ILE
5	X	476	ARG
5	X	495	ARG

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Mol	Chain	Res	Type
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	G	37	HIS
1	G	218	ARG
1	G	228	LEU
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	955	GLN

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Mol	Chain	Res	Type
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1042	LEU
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	104	HIS
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	179	LYS
3	I	188	LEU
3	I	235	GLU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	309	ASN
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS

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Mol	Chain	Res	Type
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	805	GLN
3	I	816	THR
3	I	832	LYS
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1369	ARG
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	495	ARG
5	Y	545	HIS

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Mol	Chain	Res	Type
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	227	GLN
1	A	239	GLN
1	B	66	HIS
1	B	84	ASN
2	C	41	GLN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	462	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	554	HIS
2	C	673	HIS
2	C	799	ASN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1264	GLN
2	C	1288	GLN
3	D	94	GLN
3	D	419	HIS
3	D	477	GLN
3	D	488	ASN
3	D	504	GLN
3	D	519	ASN
3	D	623	GLN

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Mol	Chain	Res	Type
3	D	875	ASN
3	D	907	HIS
3	D	1197	ASN
3	D	1268	ASN
3	D	1350	ASN
4	E	31	GLN
5	X	30	HIS
5	X	54	GLN
5	X	258	GLN
5	X	301	ASN
5	X	400	GLN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	461	ASN
5	X	469	GLN
1	G	37	HIS
1	G	41	ASN
1	G	66	HIS
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	673	HIS
2	H	799	ASN
2	H	894	GLN
2	H	955	GLN
2	H	1010	GLN
2	H	1017	GLN
2	H	1108	ASN
2	H	1111	GLN
2	H	1134	GLN
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
3	I	94	GLN
3	I	274	ASN
3	I	300	GLN

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Mol	Chain	Res	Type
3	I	419	HIS
3	I	477	GLN
3	I	504	GLN
3	I	519	ASN
3	I	1227	HIS
3	I	1350	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	301	ASN
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
5	Y	461	ASN
5	Y	469	GLN
5	Y	589	GLN

### 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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	002	D	1503	-	34,42,42	2.24	11 (32%)	40,68,68	2.51	11 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	002	D	1503	-	-	0/29/49/49	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	002	PD-O3C	-5.59	1.51	1.60
7	D	1503	002	O2'-C2'	-4.24	1.32	1.43
7	D	1503	002	C6-C5	-3.54	1.35	1.41
7	D	1503	002	C2'-C3'	-2.69	1.47	1.53
7	D	1503	002	O4'-C4'	-2.61	1.39	1.45
7	D	1503	002	O4'-C1'	-2.50	1.37	1.41
7	D	1503	002	PC-O3'	-2.49	1.54	1.60
7	D	1503	002	C8-N9	2.39	1.39	1.36
7	D	1503	002	C8-N7	3.49	1.41	1.34
7	D	1503	002	C2-N2	4.50	1.43	1.33
7	D	1503	002	O6-C6	4.80	1.36	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	002	C4'-O4'-C1'	-10.07	99.33	109.83
7	D	1503	002	PB-O3A-PA	-5.80	113.14	132.63
7	D	1503	002	PC-O3C-PD	-5.46	114.28	132.63
7	D	1503	002	N3-C2-N1	-3.16	122.77	127.41
7	D	1503	002	PB-O3B-PG	-2.41	124.52	132.63
7	D	1503	002	PC-O3'-C3'	2.19	127.36	119.41
7	D	1503	002	C1'-N9-C4	2.19	130.43	126.64
7	D	1503	002	O3C-PC-O3'	2.37	107.36	102.53
7	D	1503	002	O4'-C4'-C3'	2.40	110.06	104.85
7	D	1503	002	O3'-C3'-C2'	2.72	121.55	111.62
7	D	1503	002	C2-N3-C4	3.21	118.91	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1503	0O2	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/329 (98%)	-0.19	4 (1%) 79 70	0, 55, 172, 230	0
1	B	221/329 (67%)	-0.04	7 (3%) 47 35	0, 86, 193, 260	0
1	F	229/329 (69%)	-0.01	13 (5%) 24 18	2, 123, 212, 293	0
1	G	217/329 (65%)	0.04	4 (1%) 68 58	5, 113, 204, 271	0
2	C	1335/1342 (99%)	-0.29	20 (1%) 73 63	0, 38, 168, 304	0
2	H	1335/1342 (99%)	-0.13	39 (2%) 51 39	0, 78, 206, 346	0
3	D	1160/1407 (82%)	-0.21	16 (1%) 75 65	0, 28, 152, 297	0
3	I	1160/1407 (82%)	-0.10	40 (3%) 45 34	0, 54, 183, 316	0
4	E	90/91 (98%)	-0.22	0 100 100	0, 33, 116, 167	0
4	J	76/91 (83%)	0.08	1 (1%) 77 67	12, 83, 181, 230	0
5	X	517/613 (84%)	-0.11	20 (3%) 39 29	0, 98, 238, 341	0
5	Y	458/613 (74%)	-0.09	16 (3%) 44 33	1, 100, 216, 296	0
All	All	7121/8222 (86%)	-0.15	180 (2%) 57 46	0, 63, 198, 346	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	9.3
2	H	982	GLY	9.3
3	I	521	LYS	8.7
2	H	981	ALA	8.0
2	H	983	GLY	7.7
3	I	9	LYS	7.0
3	I	1376	GLY	6.2
3	I	208	THR	5.6
1	F	162	GLU	5.1
5	Y	309	ASN	5.0
3	I	1294	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
5	Y	311	THR	4.6
1	F	193	GLU	4.5
3	I	12	THR	4.5
2	H	1009	ASN	4.5
3	I	207	GLU	4.4
3	D	1171	GLY	4.3
2	H	1020	GLU	4.3
2	C	251	ALA	4.2
2	H	1008	GLN	4.2
1	F	148	ARG	4.2
3	D	1133	ASP	4.1
5	X	35	ILE	4.1
5	X	34	ASP	4.0
3	I	1295	ASN	4.0
3	I	11	GLN	3.9
5	Y	239	GLY	3.9
3	I	13	LYS	3.9
2	C	252	SER	3.8
2	C	266	GLY	3.8
1	A	196	THR	3.8
1	F	195	ARG	3.8
3	D	1170	LYS	3.7
3	I	1375	ALA	3.7
5	X	328	GLU	3.5
3	I	1167	LYS	3.5
5	Y	305	LEU	3.4
2	C	1166	ASP	3.4
2	H	172	TYR	3.4
3	D	1199	PHE	3.4
5	X	240	ARG	3.4
2	H	1019	ASP	3.3
3	I	1203	ARG	3.3
2	C	165	HIS	3.3
2	H	305	SER	3.2
2	H	987	GLU	3.2
2	H	113	THR	3.2
2	H	376	PRO	3.2
5	X	16	GLY	3.1
5	Y	478	PRO	3.1
2	C	282	VAL	3.1
2	H	988	LYS	3.0
2	C	272	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	212	THR	3.0
1	F	194	GLN	3.0
3	I	1133	ASP	3.0
2	C	265	LYS	3.0
3	I	676	GLY	3.0
5	Y	315	TRP	3.0
1	F	161	SER	3.0
1	F	164	ASP	2.9
2	H	1012	GLU	2.9
1	A	191	ARG	2.9
3	I	1161	GLY	2.9
2	C	306	THR	2.8
1	B	169	GLY	2.8
2	H	60	GLN	2.8
3	D	1168	GLU	2.8
5	Y	212	ILE	2.8
1	B	75	GLN	2.8
3	I	667	GLN	2.8
2	C	311	CYS	2.8
2	H	375	PRO	2.8
1	F	192	VAL	2.7
3	I	855	ASP	2.7
2	C	305	SER	2.7
2	H	332	ARG	2.7
5	X	36	VAL	2.7
1	G	96	ASP	2.7
2	H	1000	LEU	2.7
5	X	423	ARG	2.7
3	I	175	GLU	2.7
1	B	73	GLY	2.7
2	C	310	ILE	2.7
2	H	980	VAL	2.7
5	X	64	ASP	2.7
2	H	115	LYS	2.7
5	X	20	GLY	2.6
3	D	81	ARG	2.6
5	Y	240	ARG	2.6
5	X	420	GLU	2.6
5	X	339	ARG	2.6
2	C	250	THR	2.6
2	H	1001	GLY	2.6
5	Y	307	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.6
3	I	677	GLU	2.6
2	C	233	ARG	2.5
3	I	709	ARG	2.5
1	B	147	GLN	2.5
2	H	1316	GLU	2.5
2	H	1003	THR	2.5
5	Y	310	GLU	2.5
1	F	163	GLU	2.5
3	I	1172	LYS	2.5
2	H	996	ARG	2.5
3	I	708	ASN	2.5
5	X	318	ALA	2.5
5	Y	304	THR	2.5
2	C	267	ARG	2.5
1	G	18	GLN	2.5
2	H	742	TYR	2.5
5	X	239	GLY	2.5
2	C	238	GLN	2.5
3	D	834	PRO	2.5
1	F	196	THR	2.4
5	X	56	MET	2.4
3	D	1376	GLY	2.4
2	H	169	LYS	2.4
3	D	1172	LYS	2.4
2	H	105	TYR	2.4
1	B	136	GLU	2.4
5	X	153	ALA	2.4
5	Y	308	GLY	2.4
3	I	675	ALA	2.4
2	H	979	LEU	2.4
2	H	999	GLU	2.4
3	I	564	VAL	2.4
1	F	113	ALA	2.3
3	I	876	SER	2.3
3	I	1213	GLY	2.3
3	I	151	MET	2.3
3	D	1134	ILE	2.3
3	I	1204	VAL	2.3
5	Y	154	GLU	2.3
3	D	212	THR	2.3
3	I	209	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	163	LYS	2.3
2	H	986	ALA	2.3
5	Y	578	LYS	2.3
3	I	205	LEU	2.3
1	G	148	ARG	2.3
5	Y	321	ALA	2.3
1	A	4	SER	2.3
2	H	990	ASP	2.3
5	X	57	GLU	2.2
2	C	258	ASN	2.2
3	I	174	ASP	2.2
2	H	1002	LEU	2.2
3	I	14	THR	2.2
2	H	781	ASP	2.2
4	J	35	LYS	2.2
3	D	211	GLU	2.2
2	H	984	VAL	2.2
1	F	95	LYS	2.2
2	C	375	PRO	2.2
3	I	1170	LYS	2.1
5	X	305	LEU	2.1
2	H	1134	GLN	2.1
2	H	1006	GLU	2.1
1	A	190	ALA	2.1
1	G	147	GLN	2.1
2	C	1002	LEU	2.1
3	I	520	ALA	2.1
2	H	1258	PRO	2.1
3	D	80	HIS	2.1
3	I	834	PRO	2.1
3	I	1160	SER	2.1
2	H	912	ASP	2.1
5	X	315	TRP	2.1
1	B	105	SER	2.1
1	F	33	ARG	2.0
3	D	89	GLY	2.0
3	D	831	VAL	2.0
5	X	336	GLU	2.0
2	C	1001	GLY	2.0
5	X	335	GLU	2.0
3	D	333	GLY	2.0
3	I	91	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	Y	423	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
7	0O2	D	1503	40/40	0.90	0.17	20,20,20,20	0
6	ZN	I	1501	1/1	0.97	0.04	60,60,60,60	0
6	ZN	D	1502	1/1	0.97	0.18	8,8,8,8	0
6	ZN	D	1501	1/1	0.98	0.06	54,54,54,54	0
6	ZN	I	1502	1/1	0.99	0.17	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.