



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:16 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

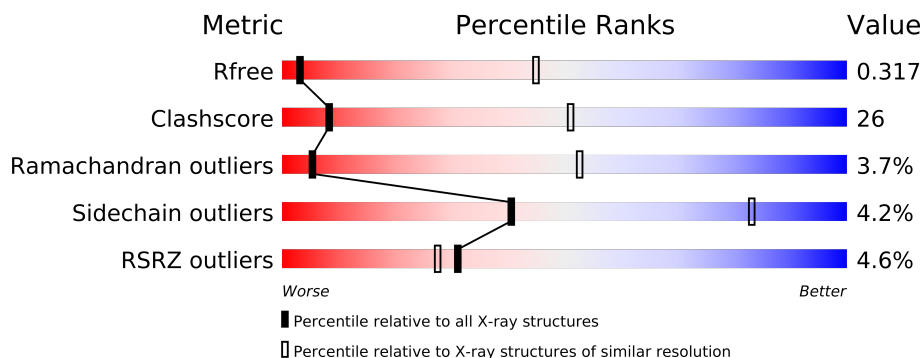
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1001 (4.84-3.50)
Clashscore	79885	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)
RSRZ outliers	66119	1001 (4.84-3.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	
2	H	1342	
3	D	1407	
3	I	1407	
4	E	91	
4	J	91	
5	X	613	
5	Y	613	

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 deuterium.

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			

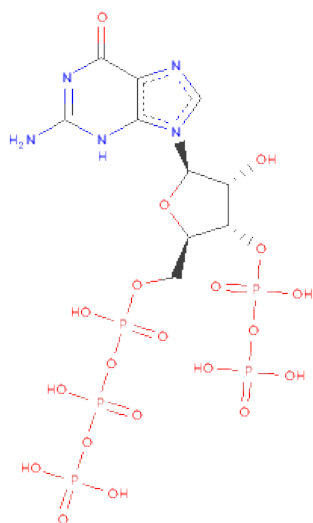
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

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			

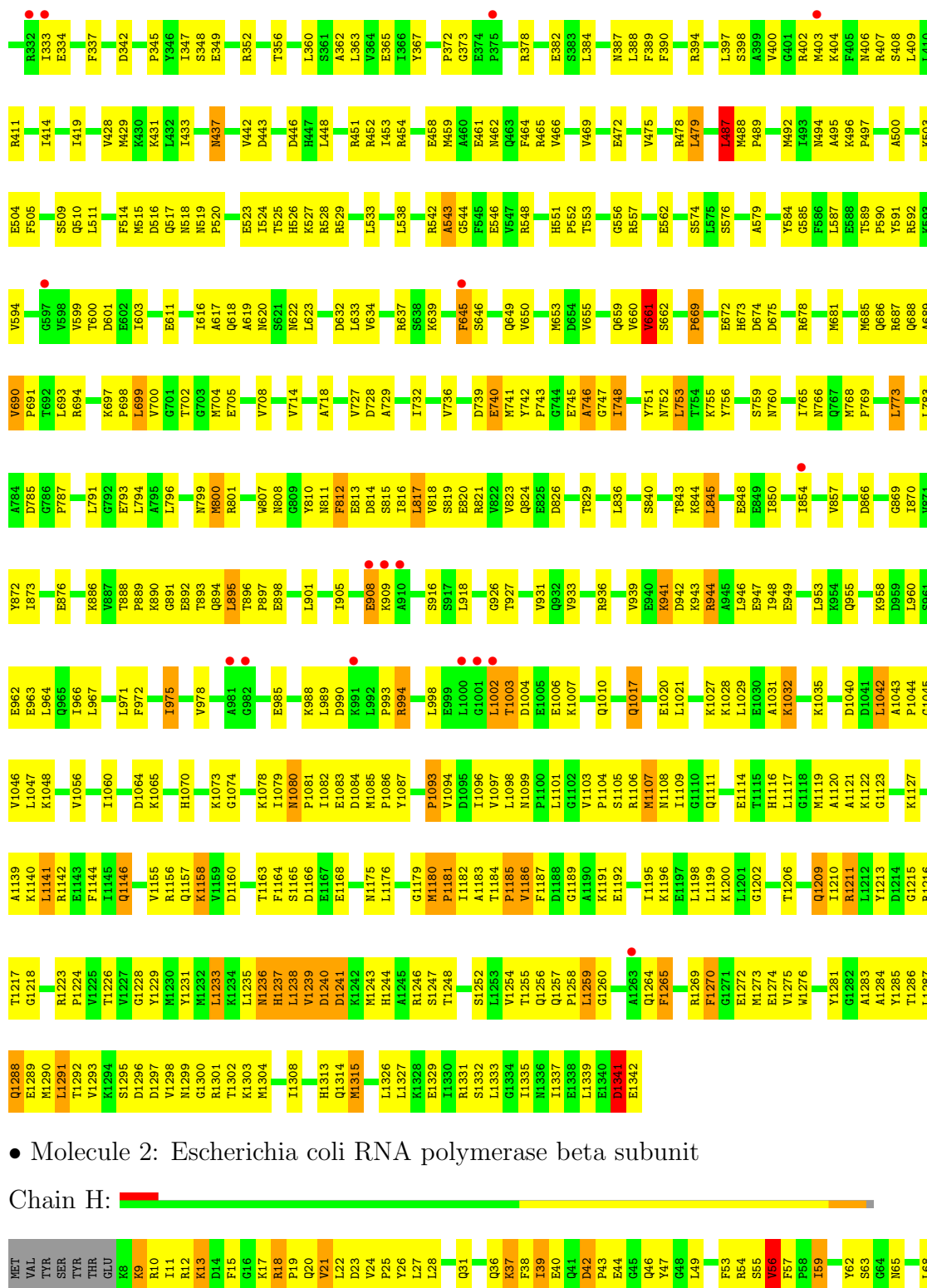
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

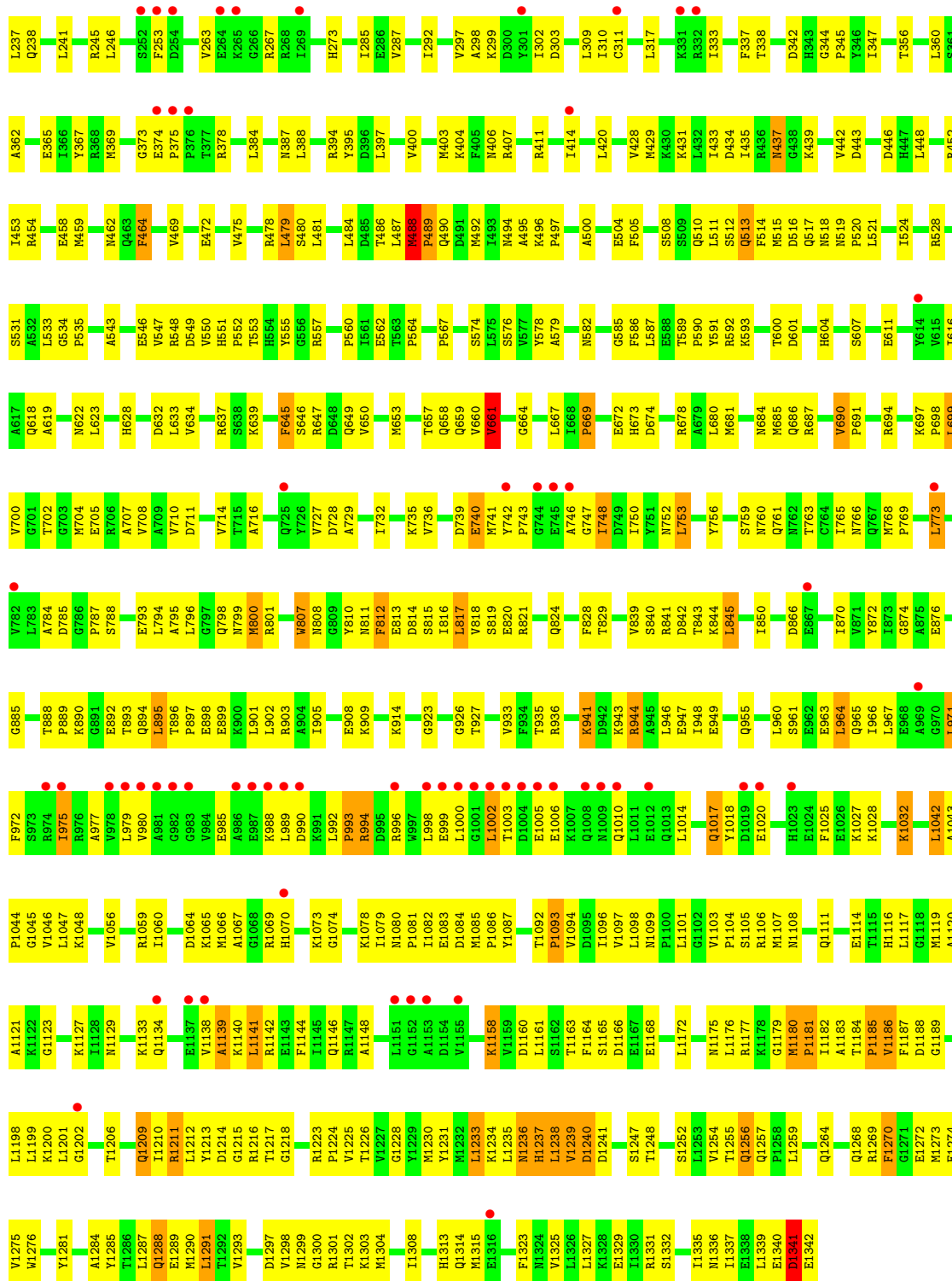
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	Zn	0	0
			2	2		
6	D	2	Total	Zn	0	0
			2	2		

- Molecule 7 is GUANOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE) 3'-(TRIHYDROGEN DIPHOSPHATE) (three-letter code: 002) (formula: C₁₀H₁₈N₅O₂₀P₅).

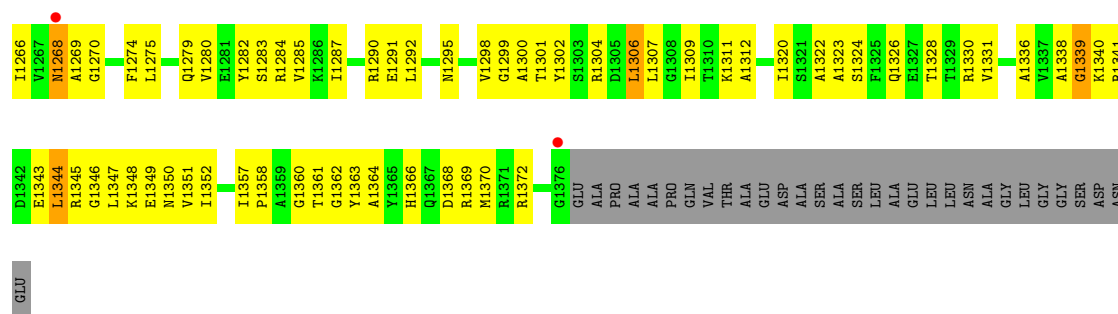


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	0	0
			50	10	10	5	20		



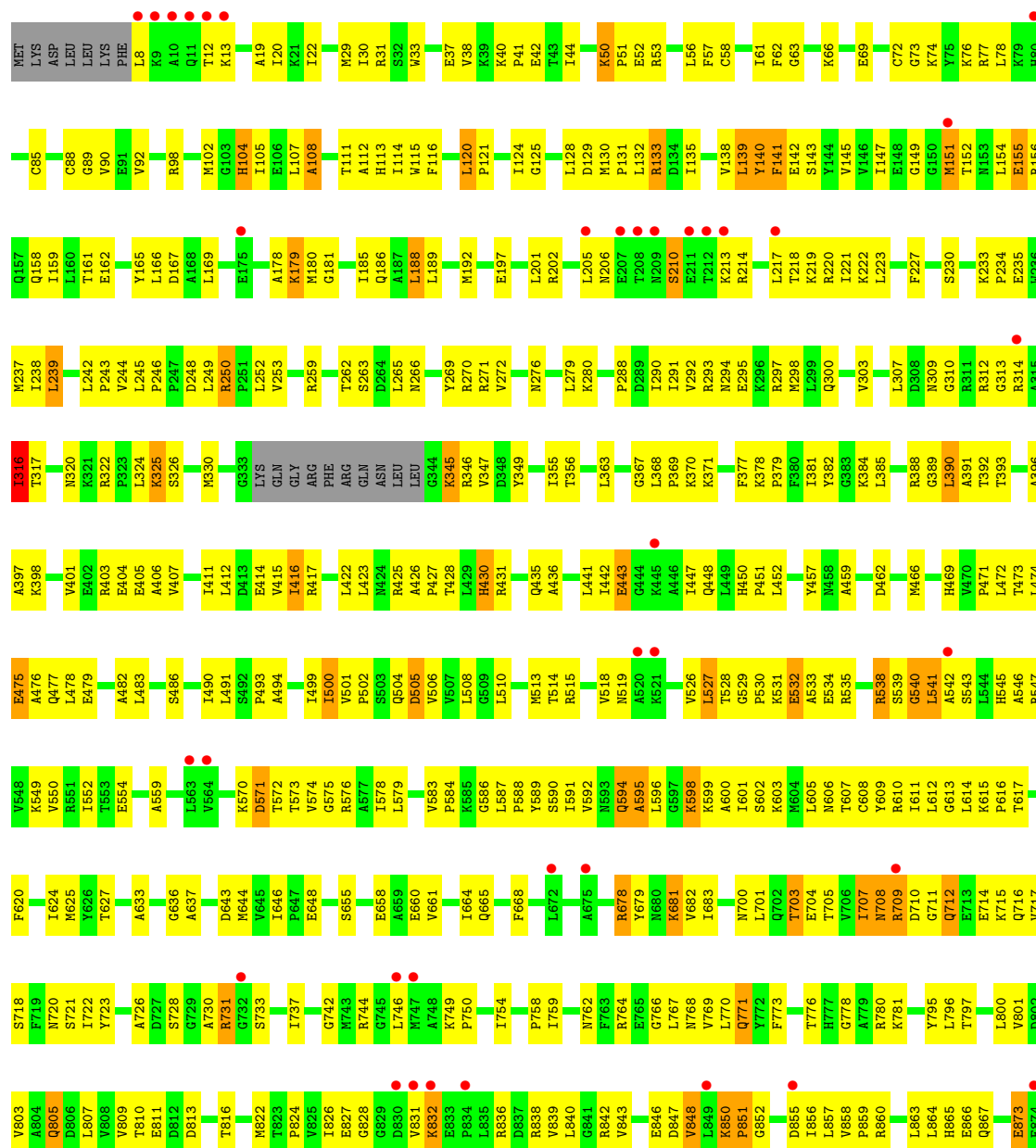


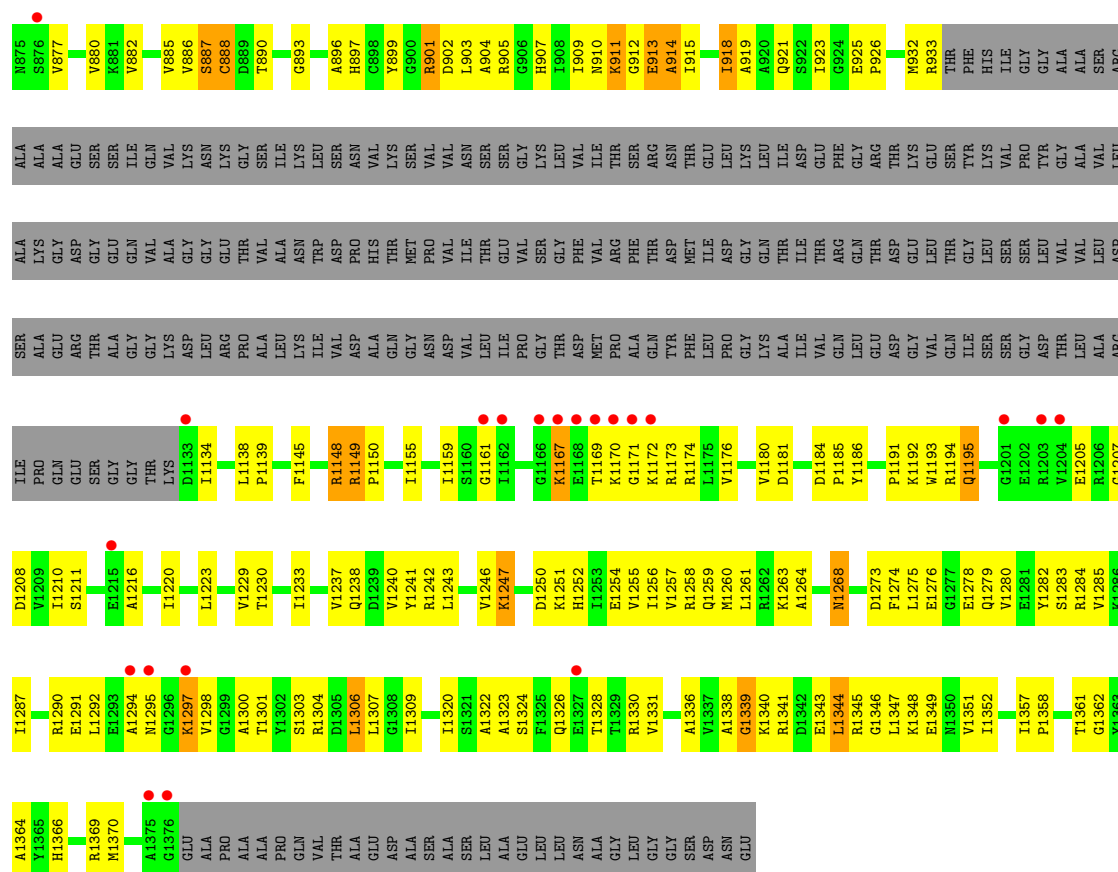
V1193	SER	LEU	LYS	HIS	Q867	V801	W717	Q823	T553	E475	I394	G310	T218	V146	K79
R1194	SER	SER	VAL	ILE	W868	D802	S718	Q823	E584	A476	K395	R311	K219	I147	H80
Q1195	GLY	SER	PRO	GLY	L871	V803	F719	M625	Y555	L478	A396	R312	R220	E148	R91
L1196	ASP	LEU	THR	GLY	L872	Q805	N720	M625	D558		K398	R313	K222	G150	I84
N1197	THR	VAL	ALA	ALA	E873	D806	S721	T627	A559	A482	V401	R316	S230	M151	C85
V1198	LEU	VAL	ALA	SER	V877	L807	W723	G628	L563	L483	E404	T317		T152	C88
F1199	ARG	ASP	LEU	ARG	V880	V809	M725	A633	Y564	T487	E405	N320	K233	H153	G89
E1200	ALA	SER	ALA	ALA	V881	T810	S728	D643	A585	M488	A406	K321	E235	E155	G99
G1201	PRO	ALA	LYS	ALA	V882	E811	G729	M644	D571	M489	V407	R322	E236	E156	V90
L1202	GLN	GLU	GLY	ALA	V883	D812	A730	V645	D572	I490	W408		Q157	V92	E91
R1203	ASP	ARG	ASP	GLU	V884	D813	W731	I646	T573	L491	W409	G333	M237	Q158	T93
V1204	THR	THR	GLY	SER	S884	E813	G732	I647	W574				I238	Q159	Q94
E1205	GLY	ALA	GLU	ILE	V885	T816	S733	P647	G575	P498	L412	LYS	L239	T160	R98
D1208	THR	ALA	GLN	GLY	V886	H817	G732	E648	A576	I499	D413	GLY	E162	T161	R99
V1209	GLY	VAL	VAL	VAL	V887	E818	S733	K649	A577	V500	E414	ARG	L242	E162	E100
I1210	LYS	LYS	ALA	LYS	C888		I737		L578	I501	PHE	ARG	P243	E166	R101
S1211	ASP	LEU	GLY	ASN	V889	M822	A741	I653	L579	S502	V415	ARG	L245	D167	M102
D1212	GLY	ARG	GLU	LYS	T690	T823	G742	S655	W590	S503	I416	ASN	P247	L169	G103
A1216	THR	THR	GLY	LYS	C893	V825	W743			D505	R417	LEU	D248	I105	H104
I1220	ALA	ALA	ALA	ILE	A896	I826	R744	E658	V583	V506	L422	LEU	L249	E106	I107
L1221	LYS	LYS	LYS	LYS	H897	E827	G745	E660	P584	V507	M424	LEU	G173	D174	L107
R1222	ILE	ILE	TRP	TRP	C898	G829	L746	V661	K585	L508	R425	G344	R250	P251	A108
L1223	VAL	VAL	ASP	SER	C899	D830	K749	A662	G586		A426	K345	P251	E175	
R1224	ASP	ASN	PRO	ASN	G900	V831	P750	E663	L587	M613	P427	V347	L252	F176	T111
G1225	ALA	ALA	HIS	VAL	C901	K832	S754	I664	P588	T514	T428	D348	D259	A178	A112
V1226	GLN	GLY	THR	LYS	D902	E833	I754		V589	R515	L429	V349	F260	K179	H113
	GLY	GLY	MET	SER	R901	K833			S590		L429	V349	A261	M180	I114
V1229	ASN	ASN	PRO	VAL	L903	R834		Q667	I591	V518	H430		T262	G181	W115
T1230	ASP	VAL	VAL	VAL	A904	L835	P758	F668	V592	M519	R431		N266	T185	K118
I1233	ASN	VAL	ASN	ASN	R905	R836	I759		H592	A520	A436		N266	T185	S119
V1234	LEU	THR	THR	SER	G906	D837	N762	R678	Q594	K521	A436		Y269	A187	L120
	ILE	GLY	GLY	SER	V907	R838	F763	K680	L596	E523	E443		R270	L188	P121
V1237	GLY	GLY	LYS	LYS	N909	V839	R764	K681	G524	G524	K445		E271	L189	
Q1238	THR	THR	GLY	LEU	N910	G841	E785	V682	K598	V525	K445		I272	M192	I124
D1239	ASP	PHE	PHE	VAL	K911	R842	G766	I683	K599	V526	A446		I272	M192	G125
V1240	MET	VAL	VAL	ILE	G912	V843	L767		A600	L527	I447		D193	L194	L126
V1241	PRO	ARG	ARG	THR	E913	N768	N769	W686	L601	K531	Q448		L279	L194	L127
R1242	ALA	PHE	PHE	SER	A914	D847	W769		S602	E532	H450		L279	L194	L128
	ALA	THR	THR	THR	L915	L849	L770	M697	K603		P451		P288	E197	D129
V1246	GLN	THR	ASP	ASN		K850	Q771		W604	R535	L452		D289	M130	
K1247	PHE	PHE	MET	THR	T918	R851	T772	L701	L605		A459		I290	P131	
K1251	LEU	LEU	ILE	GLU	A919	G852	F773	Q702	N606	R538	A373		I290	P131	L132
H1252	PRO	ASP	ASP	LEU	Q921	G852		T703	T607	S539	A373		I292	R202	L133
V1253	GLY	GLY	GLY	LYS	S922	D855	T776	T704	C608	G540	F377		R293	L205	D134
V1255	ALA	THR	THR	LEU	I923	L856	G778	W706	Y609	L541	K378		N294	L206	I135
V1256	ILE	ILE	ILE	ASP	G924	L857	G778	I707	L611	A542	P379		E207	E136	E137
I1257	VAL	THR	THR	GLY	E925	V858	K781	N708	L612		F380		R297	T208	
R1258	GLN	ARG	ARG	PHE	P926	R860	K789	R709	L614	A546	I381		M298	T208	
Q1259	LEU	GLN	GLN	GLY	N861	R860	K789	D710	G613	R547	Y382		Q300	S210	L139
M1260	GLY	THR	THR	THR	T931	T862	Y786	I707	G711	H469	W470		E207	E136	F141
L1261	ASP	ASP	LYS	LYS	N932	L863	L786	I713	K615	V548	P471		L306	R214	E142
K1262	VAL	LEU	GLY	GLY	R933	L864	T797	E714	P616	K549	L472		L307	R215	S143
	GLN	THR	THR	SER	THR	H865		K715	T617	V550	T473		L216	K216	Y144
	ILE	ILE	THR	TYR	PHE	E866	L800	Q716	F620	I552	L474		N309	L217	V145



• Molecule 3: Escherichia coli RNA polymerase beta' subunit

Chain I:





• Molecule 4: Escherichia coli RNA polymerase omega subunit

Chain E:



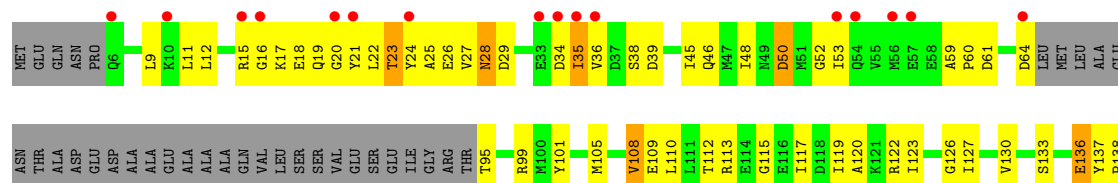
• Molecule 4: Escherichia coli RNA polymerase omega subunit

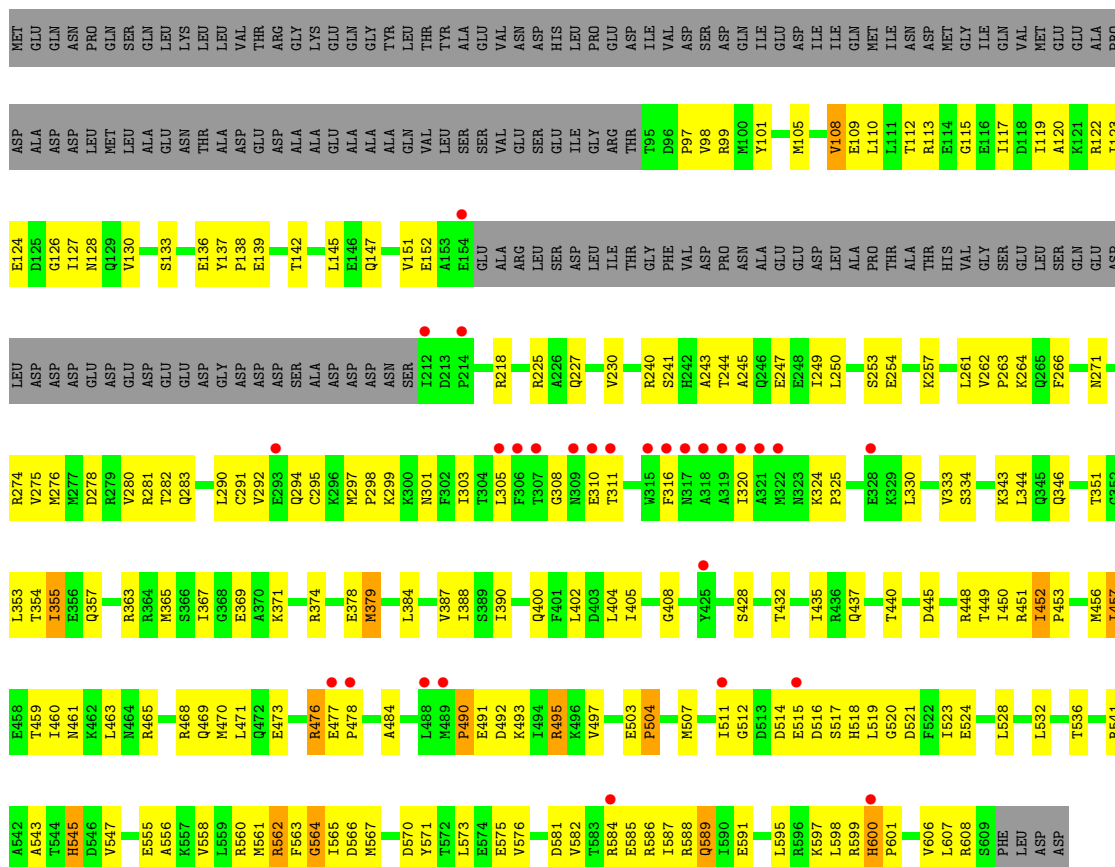
Chain J:



• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

Chain X:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 4.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.244 , 0.322 0.239 , 0.317	Depositor DCC
R_{free} test set	3075 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	159.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69537 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56129	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	110	0
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	657	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	6	9	0
All	All	56119	10	56812	2973	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (2973) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:858:VAL:HB	3:D:859:PRO:HD3	1.41	1.01
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.42	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H	2:C:163:LYS:HD3	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
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.57	0.87
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H:38:PHE:HE2	2:H:49:LEU:HD12	1.41	0.85
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.57	0.85
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.85
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.57	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:H	3:I:1247:LYS:HD3	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:876:GLU:HG3	2:C:927:THR:HG22	1.60	0.84
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.59	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:HD3	3:D:1149:ARG:H	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
2:H:513:GLN:HA	2:H:513:GLN:HE21	1.44	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.62	0.82
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.61	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.62	0.81
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.61	0.81
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.62	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
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.45	0.81
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.44	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
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.60	0.80
3:I:230:SER:HB2	3:I:1339:GLY:H	1.46	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:H:487:LEU:HB3	2:H:488:MET:HG3	1.64	0.80
4:E:5:THR:HA	4:E:6:VAL:CB	2.11	0.80
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.64	0.80
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	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
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.45	0.78
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.12	0.78
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.66	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
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:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.50	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.49	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:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.49	0.76
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.16	0.76
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.66	0.75
2:C:170:VAL:HG23	2:C:171:LEU:H	1.50	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:I:850:LYS:O	3:I:852:GLY:N	2.20	0.75
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.68	0.75
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.68	0.75
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.65	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:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.67	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:C:127:ILE:HD13	2:C:127:ILE:H	1.52	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:H:478:ARG:HD3	2:H:492:MET:HG3	1.68	0.74
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.53	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
3:I:422:LEU:HA	3:I:436:ALA:HA	1.69	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.70	0.73
4:J:5:THR:HA	4:J:6:VAL:HB	1.68	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
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: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
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.71	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:B:41:ASN:HD21	2:C:1217:THR:HG22	1.54	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
2:H:660:VAL:HG22	2:H:661:VAL:H	1.53	0.73
4:E:5:THR:HB	4:E:7:GLN:HB2	1.71	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
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.71	0.72
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.70	0.72
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.54	0.72
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.71	0.72
2:H:127:ILE:HD13	2:H:127:ILE:H	1.53	0.72
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.71	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.05	0.72
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.71	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
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.71	0.72
2:C:600:THR:HG22	2:C:601:ASP:H	1.53	0.72
4:J:5:THR:CA	4:J:6:VAL:HB	2.20	0.72
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.71	0.72
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.70	0.72
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
2:H:54:ARG:H	2:H:55:SER:CB	1.98	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.21	0.71
1:F:11:PRO:HG2	1:G:228:LEU:H	1.55	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:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.72	0.71
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.23	0.71
2:H:21:VAL:HG13	2:H:22:LEU:H	1.56	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
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	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:262:VAL:HG13	5:X:263:PRO:HD2	1.72	0.71
5:X:112:THR:HG22	5:X:113:ARG:H	1.55	0.71
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.71
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.25	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:185:ASP:HB2	2:C:197:ARG:HB2	1.73	0.70
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.56	0.70
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.74	0.70
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.22	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.31	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:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.72	0.70
3:I:412:LEU:O	3:I:416:ILE:HD12	1.92	0.70
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.26	0.70
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.21	0.70
2:H:309:LEU:H	2:H:309:LEU:HD23	1.55	0.70
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.74	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.56	0.70
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.74	0.70
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.21	0.70
3:I:546:ALA:H	3:I:547:ARG:CA	2.04	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.21	0.69
5:X:457:ILE:O	5:X:461:ASN:ND2	2.25	0.69
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.73	0.69
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.73	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
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: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
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.72	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
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.69
2:C:131:THR:HG23	2:C:133:ASN:H	1.57	0.69
5:X:139:GLU:HA	5:X:142:THR:HG22	1.74	0.69
2:H:1239:VAL:O	2:H:1241:ASP:N	2.26	0.69
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.74	0.69
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.75	0.69
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.56	0.69
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.74	0.69
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.74	0.69
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.73	0.69
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.56	0.69
5:X:476:ARG:H	5:X:476:ARG:HD2	1.57	0.69
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.28	0.69
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.75	0.69
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.75	0.69
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
2:C:309:LEU:HD23	2:C:309:LEU:H	1.56	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.28	0.68
2:C:845:LEU:H	2:C:845:LEU:HD13	1.58	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:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.68
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.68
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.25	0.68
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.75	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:368:LEU:HD12	3:D:369:PRO:HD2	1.74	0.68
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.74	0.68
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.74	0.68
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.26	0.68
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.76	0.68
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.74	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.76	0.68
3:D:609:TYR:HE2	3:D:614:LEU:HD22	1.57	0.67
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
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.75	0.67
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.58	0.67
2:H:55:SER:CB	2:H:56:VAL:HG22	2.24	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
2:H:845:LEU:H	2:H:845:LEU:HD13	1.57	0.67
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.77	0.67
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.74	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
2:C:20:GLN:O	2:C:22:LEU:N	2.27	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
3:D:590:SER:O	3:D:594:GLN:N	2.27	0.67
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.30	0.67
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.77	0.67
1:G:45:ARG:O	3:I:538:ARG:NH2	2.27	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.76	0.67
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.27	0.67
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.77	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.94	0.67
3:D:615:LYS:HD2	7:D:1503:OO2:H16	1.60	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:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.74	0.67
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.77	0.67
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.28	0.67
2:C:843:THR:HG22	2:C:844:LYS:H	1.60	0.67
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.59	0.67
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.58	0.67
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.09	0.67
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.27	0.67
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.76	0.67
2:C:403:MET:HG3	2:C:414:ILE:HB	1.77	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.77	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.60	0.66
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	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: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
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.66
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.76	0.66
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.78	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
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.78	0.66
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.61	0.66
2:H:55:SER:CB	2:H:56:VAL:HG13	2.25	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
2:C:106:GLU:N	2:C:107:ARG:HA	2.08	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
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.78	0.66
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.66
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.78	0.66
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.61	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:519:ASN:HB2	2:C:520:PRO:HD2	1.78	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
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.77	0.65
2:C:400:VAL:HG12	2:C:404:LYS:HE2	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:202:ARG:HD3	5:X:35:ILE:HB	1.77	0.65
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.60	0.65
3:I:644:MET:O	3:I:764:ARG:NH1	2.29	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.76	0.65
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.78	0.65
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.79	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.78	0.65
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.65
4:E:5:THR:CA	4:E:6:VAL:HB	2.25	0.65
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	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
3:D:362:ARG:HH12	7:D:1503:OO2:H8	1.59	0.65
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.78	0.65
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.78	0.65
2:C:1273:MET:HB3	3:D:428:THR:HB	1.79	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
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.78	0.65
3:I:504:GLN:HA	3:I:730:ALA:HA	1.78	0.65
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.79	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.78	0.65
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.62	0.64
2:H:106:GLU:N	2:H:107:ARG:HA	2.10	0.64
2:H:484:LEU:H	2:H:484:LEU:HD22	1.62	0.64
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	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: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
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.11	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:I:325:LYS:NZ	3:I:330:MET:HG2	2.13	0.64
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.31	0.64
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.78	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
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.79	0.64
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.63	0.64
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.79	0.64
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	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
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:I:590:SER:O	3:I:594:GLN:N	2.30	0.64
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.13	0.64
3:D:405:GLU:O	3:D:407:VAL: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
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.62	0.64
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.79	0.64
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.63	0.64
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.77	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.80	0.63
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.80	0.63
4:J:15:ASN:HD22	4:J:18:ASP:H	1.44	0.63
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.80	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
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.28	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.63
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.78	0.63
3:D:932:MET:SD	3:D:932:MET:N	2.67	0.63
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.81	0.63
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.79	0.63
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.80	0.63
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.32	0.63
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.80	0.63
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.29	0.63
3:I:598:LYS:NZ	3:I:726:ALA:O	2.32	0.63
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.63
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.13	0.63
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.29	0.63
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.30	0.63
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.81	0.63
2:H:1273:MET:HB3	3:I:428:THR:HB	1.81	0.63
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.63
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.80	0.63
3:D:27:PRO:O	3:D:31:ARG:HD3	1.98	0.63
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.30	0.63
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.63	0.63
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.79	0.63
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.81	0.63
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.29	0.62
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.63	0.62
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.33	0.62
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.81	0.62
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.13	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
3:D:573:THR:HG22	3:D:576:ARG:CG	2.29	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.82	0.62
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.82	0.62
2:C:634:VAL:H	2:C:645:PHE:HE2	1.47	0.62
2:H:1252:SER:OG	2:H:1255:THR:O	2.17	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:C:197:ARG:NH1	5:X:29:ASP:OD1	2.30	0.62
2:H:20:GLN:O	2:H:22:LEU:N	2.32	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.15	0.62
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.81	0.62
3:D:107:LEU:HD12	3:D:107:LEU:H	1.64	0.62
2:H:562:GLU:HG2	2:H:574:SER:CB	2.29	0.62
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.65	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
3:D:77:ARG:HG3	3:D:78:LEU:H	1.62	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
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
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.64	0.62
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.64	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
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62
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
4:E:5:THR:HA	4:E:6:VAL:HG12	1.82	0.61
1:B:49:SER:OG	3:D:538:ARG:NH2	2.33	0.61
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.81	0.61
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.81	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:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.61
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.82	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
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:908:GLU:HG2	2:H:909:LYS:N	2.14	0.61
1:B:227:GLN:O	1:B:229:GLU:N	2.30	0.61
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.81	0.61
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.82	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.29	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
1:F:9:LEU:O	1:G:227:GLN:NE2	2.33	0.61
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.31	0.61
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.01	0.61
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.61
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.33	0.61
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.61
4:J:5:THR:HA	4:J:6:VAL:CG1	2.30	0.61
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.23	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.65	0.61
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.16	0.61
2:H:152:SER:OG	2:H:404:LYS:NZ	2.25	0.61
3:I:77:ARG:HG3	3:I:78:LEU:H	1.64	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
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.29	0.61
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.82	0.61
3:D:422:LEU:HA	3:D:436:ALA:HA	1.83	0.61
3:D:1362:GLY:O	3:D:1364:ALA:N	2.32	0.61
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.82	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.32	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.15	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
3:D:827:GLU:O	3:D:831:VAL:HG12	2.00	0.61
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	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
2:C:91:THR:HG22	2:C:139:ASN:H	1.65	0.61
1:B:65:LEU:HD23	1:B:65:LEU:H	1.65	0.61
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.61
2:H:55:SER:HB3	2:H:56:VAL:CB	2.31	0.60
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.36	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.32	0.60
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.60
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.60
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.66	0.60
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	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
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
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.83	0.60
2:H:892:GLU:O	2:H:893:THR:OG1	2.19	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
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.83	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.36	0.60
3:I:252:LEU:HD23	3:I:252:LEU:H	1.66	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.49	0.60
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.83	0.60
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.84	0.60
3:D:202:ARG:O	3:D:206:ASN:ND2	2.34	0.60
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.82	0.60
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.82	0.60
5:X:584:ARG:O	5:X:587:ILE:HG22	2.01	0.60
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.01	0.60
5:X:595:LEU:O	5:X:599:ARG:NH1	2.35	0.60
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.34	0.60
4:J:5:THR:HB	4:J:7:GLN:HB2	1.83	0.60
1:G:181:GLU:HG2	3:I:531:LYS:HD3	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:C:1254:VAL:O	3:D:99:ARG:NH1	2.35	0.60
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.82	0.60
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.83	0.60
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.60
5:X:240:ARG:O	5:X:242:HIS:N	2.34	0.60
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.66	0.60
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.16	0.60
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.60
2:C:963:GLU:O	2:C:966:ILE:HG22	2.02	0.60
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.60
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.02	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.35	0.60
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.65	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:I:19:ALA:CB	3:I:1343:GLU:HB3	2.32	0.60
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.17	0.60
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.37	0.60
2:H:800:MET:HA	2:H:800:MET:CE	2.32	0.60
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.17	0.60
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.35	0.60
3:D:128:LEU:CD1	3:D:192:MET:HE3	2.28	0.60
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.60
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.84	0.60
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.65	0.60
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.82	0.60
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.83	0.60
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.83	0.60
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.66	0.60
3:D:252:LEU:HD23	3:D:252:LEU:H	1.67	0.60
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.67	0.60
2:H:894:GLN:HE21	3:I:77:ARG:HD3	1.66	0.60
3:D:151:MET:N	3:D:151:MET:SD	2.74	0.60
3:I:1338:ALA:O	3:I:1340:LYS:N	2.35	0.60
2:C:660:VAL:O	2:C:661:VAL:HG22	2.01	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.36	0.59
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.59
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.17	0.59
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.67	0.59
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.84	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
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.83	0.59
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.31	0.59
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.30	0.59
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.83	0.59
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.32	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.85	0.59
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.68	0.59
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.17	0.59
3:I:720:ASN:O	3:I:722:ILE:N	2.35	0.59
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.84	0.59
2:C:619:ALA:HA	2:C:653:MET:HE2	1.84	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.84	0.59
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.85	0.59
2:C:163:LYS:HD3	2:C:163:LYS:N	2.14	0.59
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.33	0.59
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.59
2:H:130:MET:SD	2:H:134:GLY:HA2	2.42	0.59
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.18	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
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.68	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.85	0.59
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.59
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.83	0.59
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.85	0.59
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
4:E:45:LYS:O	4:E:49:ILE:HG12	2.03	0.59
3:D:125:GLY:O	3:D:129:ASP:N	2.36	0.59
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.83	0.59
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.15	0.59
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.36	0.59
2:H:94:ALA:N	2:H:126:GLU:OE2	2.27	0.59
1:G:176:CYS:O	1:G:178:SER:N	2.33	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.34	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
2:C:91:THR:HG22	2:C:138:ILE:HA	1.85	0.59
3:D:313:GLY:H	5:X:38:SER:HB3	1.67	0.59
3:D:389:GLY:O	3:D:391:ALA:N	2.36	0.59
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.50	0.59
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.02	0.59
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.32	0.59
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.85	0.59
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.84	0.59
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.85	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:C:1288:GLN:HE21	2:C:1288:GLN:HA	1.68	0.59
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.84	0.59
5:X:515:GLU:N	5:X:516:ASP:HA	2.18	0.59
3:I:704:GLU:HB2	3:I:718:SER:HG	1.67	0.59
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.18	0.58
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.85	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:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.86	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.86	0.58
3:I:85:CYS:HB3	3:I:88:CYS:O	2.02	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.68	0.58
2:H:99:LYS:H	2:H:99:LYS:HD3	1.68	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
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.83	0.58
2:C:42:ASP:O	2:C:44:GLU:HG2	2.04	0.58
3:D:809:VAL:HG13	3:D:912:GLY:H	1.66	0.58
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.85	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.34	0.58
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.18	0.58
3:I:768:ASN:O	3:I:771:GLN:NE2	2.37	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.84	0.58
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.18	0.58
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.84	0.58
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.86	0.58
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.04	0.58
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.03	0.58
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.84	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.02	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	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
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.58
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.34	0.58
3:D:504:GLN:HA	3:D:730:ALA:HA	1.84	0.58
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.85	0.58
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.68	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.86	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.85	0.58
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.19	0.58
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.84	0.58
3:I:701:LEU:HD23	3:I:723:TYR:HB2	1.86	0.58
2:C:1200:LYS:O	2:C:1202:GLY:N	2.34	0.58
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.86	0.58
2:C:166:SER:O	2:C:168:GLY:N	2.34	0.58
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.37	0.58
1:A:104:LYS:HD3	1:A:105:SER:N	2.19	0.58
2:H:1101:LEU:CD1	3:I:504:GLN:HB2	2.28	0.58
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.39	0.58
1:G:49:SER:HA	1:G:151:GLY:HA2	1.86	0.58
3:D:709:ARG:O	3:D:711:GLY:N	2.37	0.58
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.86	0.58
3:I:591:ILE:HA	3:I:594:GLN:HB2	1.86	0.58
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.68	0.58
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.39	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
2:C:54:ARG:HG2	2:C:55:SER:CB	2.34	0.57
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.27	0.57
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	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
2:C:898:GLU:N	2:C:898:GLU:OE1	2.34	0.57
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.57
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.29	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
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.33	0.57
1:B:176:CYS:C	1:B:178:SER:H	2.08	0.57
2:H:189:ASP:OD1	2:H:193:ASN:N	2.31	0.57
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.57
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.19	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.19	0.57
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.34	0.57
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.86	0.57
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.34	0.57
1:F:181:GLU:OE1	1:F:181:GLU:N	2.38	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
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.81	0.57
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.86	0.57
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.57
3:D:619:ILE:HD13	7:D:1503:O2:O3D	2.05	0.57
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.86	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.86	0.57
1:G:19:VAL:O	1:G:20:SER:OG	2.17	0.57
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.87	0.57
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.37	0.57
2:C:24:VAL:HG11	2:C:704:MET:HE1	1.87	0.57
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.05	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.39	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.33	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	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
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.86	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
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
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.57
2:H:533:LEU:HD23	2:H:533:LEU:H	1.69	0.57
5:X:503:GLU:N	5:X:504:PRO:HA	2.20	0.57
3:I:905:ARG:HG2	3:I:907:HIS:H	1.70	0.57
2:C:106:GLU:H	2:C:107:ARG:HA	1.70	0.57
2:H:753:LEU:O	2:H:753:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.35	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
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.70	0.56
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.05	0.56
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.34	0.56
3:D:417:ARG:HH12	4:E:3:ARG:HH22	1.53	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.85	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
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.20	0.56
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.87	0.56
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.40	0.56
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.05	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
2:C:542:ARG:O	2:C:544:GLY:N	2.34	0.56
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.88	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.56
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.31	0.56
3:I:546:ALA:HB3	3:I:547:ARG:O	2.06	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.35	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.05	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:D:396:ALA:HB2	5:X:606:VAL:HG11	1.87	0.56
2:H:1111:GLN:HG3	2:H:1230:MET:HE2	1.87	0.56
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.70	0.56
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.38	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.05	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.56
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.35	0.56
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.56
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.56
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.86	0.56
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.87	0.56
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.41	0.56
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.26	0.56
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.86	0.56
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.87	0.56
2:H:488:MET:H	2:H:489:PRO:HA	1.70	0.56
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.17	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.56
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.87	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.05	0.56
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.85	0.56
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.36	0.56
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.40	0.56
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.87	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.37	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
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
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.19	0.56
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.88	0.56
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.71	0.56
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.36	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.21	0.56
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.88	0.56
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.87	0.56
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.06	0.56
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.19	0.56
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.41	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.37	0.56
3:D:166:LEU:HD12	3:D:167:ASP:N	2.21	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.87	0.56
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:487:LEU:HD13	2:C:488:MET:H	1.71	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.21	0.55
2:H:505:PHE:O	2:H:512:SER:OG	2.23	0.55
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.88	0.55
2:H:531:SER:OG	2:H:533:LEU:HD23	2.06	0.55
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.88	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.41	0.55
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.35	0.55
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.88	0.55
1:F:10:LYS:HD2	1:G:226:GLU:O	2.06	0.55
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.71	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
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.87	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.20	0.55
3:I:166:LEU:HD12	3:I:167:ASP:N	2.20	0.55
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.36	0.55
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.05	0.55
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.36	0.55
3:I:573:THR:HG22	3:I:576:ARG:CG	2.37	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:D:813:ASP:OD1	3:D:896:ALA:HB3	2.06	0.55
2:C:681:MET:O	2:C:685:MET:HG2	2.06	0.55
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.69	0.55
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.37	0.55
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.88	0.55
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.37	0.55
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.55
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.55
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.71	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.87	0.55
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.72	0.55
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.89	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
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.89	0.55
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.88	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.42	0.55
3:D:473:THR:HB	3:D:476:ALA:CB	2.37	0.55
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.70	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.40	0.55
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.42	0.55
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	1.87	0.55
5:X:379:MET:CE	5:X:379:MET:HA	2.36	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
1:G:42:ALA:O	1:G:46:ILE:HG12	2.07	0.55
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.72	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
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.88	0.55
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.55
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.89	0.55
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.24	0.55
2:C:142:GLU:HG2	2:C:515:MET:SD	2.47	0.55
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.88	0.55
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.35	0.55
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.35	0.55
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.88	0.55
2:H:106:GLU:HG2	2:H:109:ALA:H	1.71	0.55
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
1:G:86:LYS:NZ	3:I:526:VAL:O	2.39	0.55
3:D:609:TYR:CE2	3:D:614:LEU:HD22	2.41	0.54
2:C:163:LYS:H	2:C:163:LYS:CD	2.10	0.54
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.42	0.54
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.72	0.54
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.07	0.54
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.71	0.54
2:H:453:ILE:HG22	2:H:585:GLY:O	2.07	0.54
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.53	0.54
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.88	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:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:514:THR:HG21	3:D:595:ALA:O	2.07	0.54
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.88	0.54
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.89	0.54
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.08	0.54
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.32	0.54
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.89	0.54
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.07	0.54
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.88	0.54
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.37	0.54
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.89	0.54
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.07	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.88	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
2:H:1255:THR:O	2:H:1257:GLN:N	2.38	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
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.23	0.54
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.90	0.54
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.88	0.54
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.90	0.54
4:J:15:ASN:ND2	4:J:18:ASP:H	2.06	0.54
3:I:297:ARG:HH22	5:Y:101:TYR:HB2	1.71	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.90	0.54
2:H:660:VAL:HG22	2:H:661:VAL:N	2.22	0.54
1:F:150:ARG:NH1	1:G:8:PHE:HA	2.20	0.54
2:C:91:THR:HG22	2:C:139:ASN:N	2.23	0.54
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.07	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
2:H:54:ARG:HG2	2:H:55:SER:CB	2.36	0.54
4:E:5:THR:CA	4:E:6:VAL:CB	2.85	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
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.34	0.54
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.08	0.54
3:I:549:LYS:HE2	3:I:571:ASP:OD2	2.07	0.54
2:H:704:MET:HA	2:H:704:MET:HE2	1.90	0.54
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.73	0.54
3:I:405:GLU:O	3:I:407:VAL:N	2.41	0.54
3:D:450:HIS:NE2	3:D:625:MET:SD	2.81	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:151:MET:N	3:I:151:MET:SD	2.81	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.90	0.54
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.54
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.90	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.89	0.54
5:X:556:ALA:O	5:X:560:ARG:HB2	2.08	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
5:X:600:HIS:H	5:X:601:PRO:HD2	1.72	0.54
1:B:176:CYS:O	1:B:178:SER:N	2.41	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.08	0.54
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.90	0.54
3:I:810:THR:HG22	3:I:893:GLY:HA3	1.90	0.54
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.30	0.53
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.08	0.53
3:D:128:LEU:HA	3:D:192:MET:HE3	1.90	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	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
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.20	0.53
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.40	0.53
1:B:118:ASP:OD1	1:B:119:GLY:N	2.41	0.53
2:H:442:VAL:HG12	2:H:443:ASP:H	1.74	0.53
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.34	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:752:ASN:O	2:H:753:LEU:HG	2.08	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:H:728:ASP:OD2	2:H:729:ALA:N	2.41	0.53
2:C:134:GLY:O	2:C:527:LYS:NZ	2.40	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
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.89	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
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
3:D:393:THR:HG23	3:D:396:ALA:H	1.73	0.53
5:X:437:GLN:HA	5:X:440:THR:HG22	1.89	0.53
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.90	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.74	0.53
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.28	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
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.07	0.53
3:I:363:LEU:O	3:I:486:SER:OG	2.20	0.53
2:C:756:TYR:H	2:C:766:ASN:CB	2.22	0.53
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.90	0.53
3:I:1357:ILE:HD12	3:I:1357:ILE:H	1.73	0.53
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.89	0.53
2:H:1332:SER:O	3:I:243:PRO:HG2	2.09	0.53
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.53
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.53
2:C:1119:MET:O	2:C:1123:GLY:N	2.40	0.53
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.53
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.44	0.53
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.91	0.53
2:H:494:ASN:OD1	2:H:495:ALA:N	2.40	0.53
3:D:294:ASN:ND2	3:D:298:MET:SD	2.81	0.53
2:H:1274:GLU:N	2:H:1274:GLU:OE1	2.41	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.41	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
2:C:360:LEU:HD13	2:C:378:ARG:NH1	2.23	0.53
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.39	0.53
2:C:106:GLU:HG2	2:C:109:ALA:H	1.73	0.53
3:D:41:PRO:HB3	3:D:270:ARG:HG3	1.90	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:O	5:X:355:ILE:HD13	2.08	0.53
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.91	0.53
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.30	0.53
2:C:122:VAL:HG22	5:X:472:GLN:HE21	1.72	0.53
1:B:19:VAL:O	1:B:20:SER:HB3	2.08	0.53
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.09	0.53
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.91	0.53
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.90	0.53
2:C:818:VAL:HG22	2:C:819:SER:H	1.74	0.53
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.43	0.53
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.43	0.53
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.39	0.53
3:I:591:ILE:HD12	3:I:592:VAL:N	2.23	0.53
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.91	0.53
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.08	0.53
1:A:42:ALA:O	1:A:46:ILE:HG12	2.08	0.53
1:F:79:LEU:O	1:F:83:LEU:HD13	2.09	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
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.74	0.53
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
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.90	0.53
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.74	0.53
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.90	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
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.90	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.90	0.53
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.09	0.53
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.44	0.53
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.44	0.53
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.23	0.52
2:H:106:GLU:H	2:H:107:ARG:HA	1.74	0.52
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.91	0.52
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.08	0.52
2:H:37:LYS:HE3	2:H:37:LYS:HA	1.91	0.52
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.45	0.52
4:J:45:LYS:O	4:J:49:ILE:HG12	2.09	0.52
2:C:205:PRO:O	2:C:208:ILE:HG22	2.10	0.52
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	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:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.52
3:I:197:GLU:O	3:I:201:LEU:HD23	2.09	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
5:X:264:LYS:HD2	5:X:264:LYS:H	1.73	0.52
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.74	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:D:413:ASP:O	3:D:417:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.73	0.52
4:E:5:THR:HB	4:E:7:GLN:N	2.24	0.52
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.52
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.92	0.52
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.23	0.52
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.74	0.52
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.90	0.52
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.09	0.52
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.44	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	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
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.52
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.42	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.45	0.52
3:I:648:GLU:N	3:I:648:GLU:OE2	2.43	0.52
3:I:393:THR:HG23	3:I:396:ALA:H	1.73	0.52
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.09	0.52
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.91	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
4:E:77:ALA:O	4:E:80:LEU:HD22	2.10	0.52
5:X:493:LYS:O	5:X:497:VAL:HG23	2.09	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:245:LEU:CD1	3:D:246:PRO:HD2	2.39	0.52
5:X:541:ARG:O	5:X:545:HIS:HB2	2.10	0.52
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.09	0.52
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.91	0.52
2:H:131:THR:HG22	2:H:135:THR:HG22	1.91	0.52
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	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
2:H:888:THR:O	2:H:914:LYS:N	2.36	0.52
4:E:82:ALA:O	4:E:86:ILE:HG13	2.10	0.52
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.45	0.52
2:H:699:LEU:H	2:H:799:ASN:HD21	1.56	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:18:ARG:HD3	2:H:619:ALA:O	2.09	0.52
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.91	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
5:X:598:LEU:O	5:X:599:ARG:HD2	2.08	0.52
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.91	0.52
2:H:741:MET:N	2:H:741:MET:SD	2.82	0.52
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.45	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.92	0.52
2:H:694:ARG:O	2:H:798:GLN:NE2	2.37	0.52
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.91	0.52
3:I:504:GLN:HG3	3:I:505:ASP:H	1.75	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.33	0.52
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.90	0.52
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.92	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.52
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.39	0.52
3:D:646:ILE:HG22	3:D:741:ALA:O	2.09	0.52
5:X:119:ILE:O	5:X:123:ILE:HG13	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
2:C:843:THR:HG22	2:C:844:LYS:N	2.24	0.52
2:C:755:LYS:HZ1	2:C:756:TYR:HE2	1.58	0.52
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.09	0.52
2:C:891:GLY:O	2:C:893:THR:HG23	2.10	0.52
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.58	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.40	0.52
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.91	0.52
3:D:504:GLN:HG3	3:D:505:ASP:H	1.75	0.52
3:I:451:PRO:HG2	3:I:625:MET:SD	2.50	0.52
2:H:403:MET:HG3	2:H:414:ILE:HB	1.91	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.24	0.52
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.91	0.52
2:C:80:PHE:O	2:C:84:GLU:HB3	2.10	0.52
2:H:446:ASP:OD1	2:H:547:VAL:N	2.29	0.52
3:I:858:VAL:HB	3:I:859:PRO:CD	2.26	0.51
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.10	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
2:C:487:LEU:CD1	2:C:488:MET:H	2.23	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:703:THR:HA	3:D:717:VAL:HA	1.90	0.51
5:X:400:GLN:O	5:X:404:LEU:HD13	2.11	0.51
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.40	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.51
2:H:496:LYS:HE2	5:Y:471:LEU:CD2	2.39	0.51
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.93	0.51
5:Y:379:MET:CE	5:Y:379:MET:HA	2.41	0.51
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.51
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.92	0.51
2:H:800:MET:HG2	2:H:1096:ILE:HD13	1.91	0.51
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.44	0.51
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.40	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
5:X:484:ALA:HB2	5:X:494:ILE:HD12	1.92	0.51
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.25	0.51
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.51	0.51
2:H:1281:TYR:CZ	3:I:431:ARG:HG2	2.45	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:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.45	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:I:426:ALA:HB3	3:I:427:PRO:CD	2.40	0.51
2:H:634:VAL:H	2:H:645:PHE:HE2	1.59	0.51
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.11	0.51
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.75	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: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:H:153:PRO:HD2	2:H:452:ARG:HD3	1.92	0.51
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.51
2:C:9:LYS:N	2:C:9:LYS:HD3	2.25	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
3:I:482:ALA:C	3:I:483:LEU:HD12	2.31	0.51
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.92	0.51
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.30	0.51
4:E:5:THR:HB	4:E:7:GLN:CB	2.38	0.51
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.92	0.51
3:I:245:LEU:O	3:I:250:ARG:NH1	2.43	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.41	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.39	0.51
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.76	0.51
1:A:248:GLU:N	1:A:248:GLU:OE1	2.42	0.51
1:A:207:THR:OG1	1:A:208:ASN:N	2.44	0.51
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.76	0.51
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.24	0.51
4:E:4:VAL:O	4:E:5:THR:OG1	2.24	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:899:TYR:CE1	3:D:915:ILE:HD12	2.46	0.51
5:X:600:HIS:H	5:X:601:PRO:CD	2.23	0.51
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.44	0.51
3:D:648:GLU:N	3:D:648:GLU:OE2	2.42	0.51
5:X:311:THR:HG21	5:X:348:GLU:CD	2.31	0.51
2:H:1247:SER:O	2:H:1248:THR:HG23	2.11	0.51
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.92	0.51
4:J:5:THR:HB	4:J:7:GLN:H	1.75	0.51
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.20	0.51
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.93	0.51
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.91	0.51
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.93	0.51
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.30	0.51
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.93	0.51
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.44	0.51
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.26	0.51
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.75	0.51
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.10	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.93	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.51
2:H:901:LEU:O	2:H:905:ILE:HG13	2.11	0.51
2:C:49:LEU:HD21	2:C:464:PHE:HB3	1.93	0.51
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.92	0.51
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.92	0.51
2:H:681:MET:O	2:H:685:MET:HG2	2.11	0.51
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.76	0.51
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.92	0.51
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.93	0.51
1:A:303:ILE:O	1:A:307:LEU:HD13	2.10	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.10	0.51
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.93	0.50
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.41	0.50
7:D:1503:OO2:O2'	7:D:1503:OO2: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
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.46	0.50
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.93	0.50
1:A:256:PRO:HA	1:A:277:TYR:HA	1.92	0.50
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.46	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	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
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.12	0.50
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.92	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	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
3:D:262:THR:HG1	3:D:266:ASN:HD22	1.58	0.50
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.10	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
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	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:149:LEU:HD12	2:C:452:ARG:O	2.11	0.50
3:D:910:ASN:HB3	4:E:15:ASN:HA	1.92	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.92	0.50
1:A:263:THR:HG23	1:A:266:SER:H	1.76	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.93	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
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:D:482:ALA:C	3:D:483:LEU:HD12	2.32	0.50
2:H:707:ALA:O	2:H:710:VAL:HG12	2.11	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.50
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.50
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.93	0.50
2:H:38:PHE:O	2:H:39:ILE:HB	2.10	0.50
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.50
3:I:513:MET:CE	3:I:579:LEU:HB2	2.41	0.50
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
5:X:561:MET:HA	5:X:567:MET:SD	2.50	0.50
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.46	0.50
2:H:487:LEU:CB	2:H:488:MET:HG3	2.39	0.50
3:D:545:HIS:O	3:D:573:THR:OG1	2.18	0.50
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.77	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
3:D:57:PHE:HB3	3:D:98:ARG:HH11	1.76	0.50
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.46	0.50
2:H:946:LEU:O	2:H:949:GLU:HG3	2.11	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
3:I:355:ILE:HG21	3:I:466:MET:SD	2.52	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.69	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.40	0.50
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.77	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.11	0.50
3:D:245:LEU:O	3:D:250:ARG:NH1	2.44	0.50
3:I:1171:GLY:N	3:I:1172:LYS:O	2.44	0.50
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.41	0.50
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.94	0.50
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.93	0.50
1:F:151:GLY:O	1:F:177:TYR:HB2	2.12	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.46	0.50
2:C:131:THR:HG22	2:C:135:THR:N	2.27	0.50
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.50
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.92	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.50
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.93	0.50
3:I:316:ILE:N	3:I:316:ILE:HD13	2.27	0.50
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.44	0.50
3:D:173:GLY:O	3:D:175:GLU:HG3	2.11	0.50
3:I:608:CYS:O	3:I:612:LEU:HB2	2.12	0.50
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.93	0.50
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.45	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
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.94	0.50
2:H:1335:ILE:HD12	3:I:1336:ALA:HB2	1.94	0.50
3:I:513:MET:O	3:I:575:GLY:HA3	2.12	0.50
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.50
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.32	0.50
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.50
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.11	0.50
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.50
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.26	0.50
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.12	0.50
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.12	0.49
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.93	0.49
3:I:546:ALA:N	3:I:547:ARG:CA	2.70	0.49
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.35	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
5:X:290:LEU:O	5:X:294:GLN:HB3	2.12	0.49
3:I:678:ARG:O	3:I:681:LYS:HG3	2.11	0.49
2:C:1087:TYR:O	2:C:1213:TYR:N	2.28	0.49
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.94	0.49
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.26	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.12	0.49
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.11	0.49
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.93	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.94	0.49
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.95	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:D:57:PHE:CD1	3:D:247:PRO:HB3	2.46	0.49
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:127:ILE:N	2:H:127:ILE:HD13	2.26	0.49
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.94	0.49
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.26	0.49
7:D:1503:OO2:O3D	7:D:1503:OO2:O2C	2.29	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
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
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.49
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.49
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.13	0.49
2:C:475:VAL:O	2:C:479:LEU:HB2	2.12	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.42	0.49
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.93	0.49
2:C:1288:GLN:CA	2:C:1288:GLN:HE21	2.26	0.49
3:I:840:LEU:HD12	3:I:840:LEU:O	2.11	0.49
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.92	0.49
5:X:278:ASP:OD1	5:X:281:ARG:NH2	2.45	0.49
2:H:1119:MET:O	2:H:1123:GLY:N	2.45	0.49
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.78	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
5:X:108:VAL:HB	5:X:110:LEU:HG	1.94	0.49
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.95	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
5:X:115:GLY:O	5:X:119:ILE:HG12	2.13	0.49
2:H:998:LEU:O	2:H:998:LEU:HD13	2.12	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
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.47	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.77	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.33	0.49
2:C:818:VAL:HG22	2:C:819:SER:N	2.28	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
2:H:590:PRO:O	2:H:659:GLN:NE2	2.46	0.49
3:D:614:LEU:CG	4:E:5:THR:HG21	2.42	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.49
2:H:72:SER:O	2:H:98:VAL:HG23	2.12	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	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
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.48	0.49
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.49
3:I:227:PHE:O	3:I:230:SER:OG	2.24	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
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.95	0.49
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.78	0.49
5:X:379:MET:HE2	5:X:379:MET:HA	1.95	0.49
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.94	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
1:G:9:LEU:HD23	1:G:9:LEU:H	1.78	0.49
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.49
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.49
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.94	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	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
2:H:119:GLU:HG2	2:H:120:GLN:N	2.26	0.49
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.43	0.49
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.28	0.49
2:H:843:THR:HG22	2:H:844:LYS:H	1.78	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
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.77	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.53	0.49
2:C:1335:ILE:HD12	3:D:1336:ALA:HB2	1.95	0.49
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.76	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
1:A:79:LEU:O	1:A:83:LEU:HD13	2.13	0.49
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.94	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.93	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.40	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.13	0.49
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.94	0.49
3:I:317:THR:H	3:I:324:LEU:HD21	1.77	0.49
3:D:644:MET:O	3:D:764:ARG:NH1	2.46	0.49
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.38	0.48
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.13	0.48
3:D:120:LEU:HA	5:X:46:GLN:OE1	2.13	0.48
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.38	0.48
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.48
2:C:740:GLU:HB2	2:C:741:MET:SD	2.53	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.78	0.48
3:I:519:ASN:HD21	3:I:707:ILE:HG21	1.78	0.48
3:D:914:ALA:O	3:D:918:ILE:HG22	2.13	0.48
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.28	0.48
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.94	0.48
1:A:310:ARG:HE	1:A:310:ARG:HA	1.77	0.48
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.48
2:C:866:ASP:HA	2:C:872:TYR:OH	2.12	0.48
5:X:126:GLY:O	5:X:130:VAL:HG23	2.13	0.48
2:C:660:VAL:HG22	2:C:661:VAL:N	2.23	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: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
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.43	0.48
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.26	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
2:C:99:LYS:HG2	2:C:121:GLU:HB3	1.94	0.48
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.48
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.95	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.13	0.48
3:I:531:LYS:NZ	3:I:531:LYS:HB3	2.28	0.48
3:I:221:ILE:HG13	3:I:222:LYS:N	2.28	0.48
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.40	0.48
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.43	0.48
3:D:124:ILE:HA	3:D:237:MET:HE2	1.95	0.48
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.96	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.77	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.12	0.48
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.39	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
2:C:529:ARG:HH22	2:C:687:ARG:NH2	2.12	0.48
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.48
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.48
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.28	0.48
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.95	0.48
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.13	0.48
1:B:192:VAL:HG12	1:B:194:GLN:H	1.78	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.29	0.48
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.37	0.48
3:I:746:LEU:HB3	3:I:754:ILE:HG21	1.96	0.48
5:Y:457:ILE:HG23	5:Y:461:ASN:ND2	2.28	0.48
3:D:450:HIS:HE2	3:D:625:MET:CE	2.27	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.12	0.48
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.94	0.48
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.95	0.48
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.13	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.12	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.12	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.95	0.48
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.28	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
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.24	0.48
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.95	0.48
3:D:915:ILE:HG22	3:D:1255:VAL:HG11	1.96	0.48
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.48
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.94	0.48
3:I:703:THR:O	3:I:718:SER:N	2.47	0.48
1:A:243:LYS:HD3	1:A:243:LYS:N	2.29	0.48
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.94	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.48
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.48
5:X:227:GLN:HA	5:X:230:VAL:HG12	1.96	0.48
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.28	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
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	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
3:D:579:LEU:HD13	3:D:579:LEU:O	2.14	0.48
2:H:747:GLY:C	2:H:748:ILE:HG13	2.34	0.48
3:I:888:CYS:SG	3:I:890:THR:HB	2.54	0.48
1:A:192:VAL:O	1:A:194:GLN:N	2.45	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.79	0.48
3:I:294:ASN:ND2	3:I:298:MET:SD	2.87	0.48
3:D:918:ILE:HD13	3:D:919:ALA:N	2.29	0.48
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.43	0.48
2:H:72:SER:OG	2:H:99:LYS:HE3	2.13	0.48
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.42	0.48
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.78	0.48
3:D:843:VAL:HG11	3:D:897:HIS:HB3	1.96	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.53	0.48
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.14	0.48
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.46	0.48
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.96	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.13	0.48
2:C:59:ILE:HD11	2:C:63:SER:OG	2.14	0.48
2:H:127:ILE:O	2:H:127:ILE:HG12	2.14	0.48
3:D:363:LEU:HD12	3:D:450:HIS:ND1	2.29	0.48
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.96	0.48
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.49	0.48
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.95	0.48
1:G:82:LEU:O	1:G:86:LYS:HG3	2.14	0.48
2:H:818:VAL:HG22	2:H:819:SER:N	2.28	0.48
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.49	0.48
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.96	0.48
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.49	0.48
3:D:120:LEU:HG	5:X:46:GLN:CB	2.42	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
3:I:377:PHE:O	3:I:381:ILE:HG13	2.14	0.48
3:I:265:LEU:HD11	3:I:330:MET:SD	2.54	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.79	0.48
2:C:718:ALA:HB2	2:C:783:LEU:HG	1.96	0.48
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.48	0.48
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.48
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.29	0.48
2:H:356:THR:HG21	2:H:362:ALA:HA	1.95	0.48
3:I:714:GLU:HG2	3:I:715:LYS:H	1.79	0.48
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
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
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.96	0.47
2:H:759:SER:HB3	2:H:763:THR:H	1.80	0.47
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.96	0.47
1:B:195:ARG:HH21	1:B:198:LEU:HD21	1.79	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.14	0.47
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.29	0.47
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.96	0.47
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.29	0.47
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.97	0.47
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.49	0.47
3:D:269:TYR:CD2	3:D:306:LEU:HD11	2.49	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.47
2:H:750:ILE:HD13	2:H:963:GLU:OE2	2.14	0.47
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.40	0.47
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.95	0.47
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.96	0.47
2:C:812:PHE:N	2:C:815:SER:HB2	2.28	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.46	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
4:E:18:ASP:O	4:E:22:VAL:HG12	2.14	0.47
3:I:679:TYR:O	3:I:683:ILE:HG13	2.14	0.47
2:H:963:GLU:O	2:H:967:LEU:HD13	2.14	0.47
3:I:288:PRO:O	3:I:292:VAL:HG12	2.14	0.47
1:F:28:LEU:HD22	1:G:231:PHE:CZ	2.49	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.95	0.47
3:I:161:THR:HG22	3:I:162:GLU:H	1.79	0.47
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.78	0.47
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.47
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
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.47
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.50	0.47
1:A:222:THR:O	1:A:226:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:358:GLY:HA3	3:D:361:LEU:HD23	1.96	0.47
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.96	0.47
2:C:131:THR:HG22	2:C:135:THR:H	1.80	0.47
3:I:201:LEU:HD12	3:I:205:LEU:HD11	1.97	0.47
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.47
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.96	0.47
3:D:714:GLU:HG2	3:D:715:LYS:H	1.79	0.47
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.47
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.95	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
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.14	0.47
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.50	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.43	0.47
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.95	0.47
3:I:514:THR:HG21	3:I:595:ALA:O	2.15	0.47
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.79	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.30	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.28	0.47
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.15	0.47
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.96	0.47
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.55	0.47
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.76	0.47
3:D:310:GLY:O	3:D:314:ARG:HG2	2.14	0.47
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.47
2:H:908:GLU:CD	2:H:908:GLU:H	2.18	0.47
5:X:431:ALA:O	5:X:435:ILE:HG13	2.15	0.47
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.14	0.47
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.49	0.47
2:C:127:ILE:HG12	2:C:127:ILE:O	2.14	0.47
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.49	0.47
3:I:473:THR:CG2	3:I:475:GLU:HG2	2.44	0.47
2:H:1314:GLN:O	3:I:473:THR:HG23	2.15	0.47
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.50	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47
2:H:1106:ARG:O	2:H:1108:ASN:N	2.38	0.47
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:546:GLU:O	2:H:548:ARG:N	2.43	0.47
2:C:237:LEU:HB2	2:C:287:VAL:O	2.14	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.97	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
1:A:234:LEU:HD12	1:A:234:LEU:N	2.29	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.49	0.47
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.47
2:C:941:LYS:O	2:C:941:LYS:HD2	2.14	0.47
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.50	0.47
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.49	0.47
3:I:12:THR:O	3:I:13:LYS:HD2	2.14	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
2:H:59:ILE:HB	2:H:480:SER:OG	2.15	0.47
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.80	0.47
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.47
5:Y:291:CYS:O	5:Y:295:CYS:HB2	2.14	0.47
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.15	0.47
3:D:856:ILE:HG13	3:D:857:LEU:O	2.14	0.47
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.97	0.47
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.32	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.15	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
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.96	0.47
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.77	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.29	0.47
3:D:154:LEU:HD22	3:D:176:PHE:CE1	2.49	0.47
2:C:538:LEU:HD12	2:C:538:LEU:N	2.29	0.47
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.15	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
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.30	0.47
3:D:356:THR:O	3:D:448:GLN:HA	2.15	0.47
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.48	0.47
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.96	0.47
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47
2:C:41:GLN:CD	2:C:42:ASP:H	2.17	0.46
1:G:190:ALA:N	1:G:198:LEU:O	2.37	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.96	0.46
2:H:1017:GLN:HA	2:H:1020:GLU:HB3	1.97	0.46
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.46
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.15	0.46
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.46
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.50	0.46
2:C:28:LEU:HD22	2:C:527:LYS:HD2	1.96	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
3:D:607:THR:O	3:D:611:ILE:HG12	2.15	0.46
3:I:72:CYS:SG	3:I:73:GLY:N	2.88	0.46
3:I:210:SER:O	3:I:214:ARG:HG3	2.15	0.46
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
3:D:524:GLY:HA2	3:D:548:VAL:HG23	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
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
1:F:221:ALA:CB	1:G:228:LEU:HD12	2.37	0.46
3:D:260:PHE:O	5:X:504:PRO:HG2	2.15	0.46
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.46
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.45	0.46
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.46
5:Y:101:TYR:HE2	5:Y:388:ILE:HD11	1.79	0.46
1:G:36:GLY:O	1:G:201:LEU:HD13	2.14	0.46
5:Y:124:GLU:HG2	5:Y:128:ASN:ND2	2.31	0.46
3:I:605:LEU:HD13	3:I:605:LEU:O	2.15	0.46
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.96	0.46
1:B:179:PRO:O	1:B:207:THR:OG1	2.29	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.49	0.46
2:H:697:LYS:HE2	2:H:793:GLU:HB3	1.97	0.46
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.29	0.46
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.48	0.46
5:X:291:CYS:O	5:X:295:CYS:HB2	2.15	0.46
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.80	0.46
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.45	0.46
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
3:D:394:ILE:HG21	5:X:536:THR:HA	1.97	0.46
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.46
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.97	0.46
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.46
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.48	0.46
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.51	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.15	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	1.98	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.27	0.46
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.37	0.46
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.96	0.46
3:D:233:LYS:HB3	3:D:236:TRP:CE2	2.50	0.46
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.97	0.46
1:G:185:TYR:HA	1:G:202:VAL:O	2.15	0.46
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.50	0.46
2:H:1006:GLU:CD	2:H:1006:GLU:H	2.19	0.46
3:I:911:LYS:O	3:I:911:LYS:HD2	2.15	0.46
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.49	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.15	0.46
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.16	0.46
2:C:908:GLU:CG	2:C:909:LYS:H	2.27	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.50	0.46
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.98	0.46
3:I:356:THR:O	3:I:448:GLN:HA	2.16	0.46
2:C:843:THR:HB	2:C:845:LEU:CD2	2.46	0.46
2:C:372:PRO:HB3	5:X:34:ASP:HB3	1.98	0.46
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.97	0.46
3:D:33:TRP:O	3:D:102:MET:HB2	2.15	0.46
3:I:773:PHE:O	3:I:776:THR:HG22	2.15	0.46
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.96	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:382:TYR:HE1	3:I:401:VAL:HG21	1.80	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.50	0.46
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.45	0.46
5:X:139:GLU:HG3	5:X:351:THR:HA	1.97	0.46
3:D:362:ARG:HH22	7:D:1503:O2:H8	1.81	0.46
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.47	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.46
3:I:138:VAL:O	3:I:143:SER:HB3	2.15	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
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.34	0.46
3:D:12:THR:C	3:D:13:LYS:HD2	2.36	0.46
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:369:PRO:HB2	3:D:372:MET:CB	2.46	0.46
2:C:1255:THR:O	2:C:1257:GLN:N	2.42	0.46
2:H:714:VAL:CG2	2:H:787:PRO:HD2	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:1290:MET:SD	3:I:347:VAL:HG11	2.55	0.46
5:X:276:MET:O	5:X:280:VAL:HG23	2.16	0.46
2:C:505:PHE:HA	2:C:509:SER:CB	2.46	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:586:GLY:O	3:D:587:LEU:HB2	2.16	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
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.51	0.46
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.30	0.46
5:Y:585:GLU:O	5:Y:589:GLN:N	2.43	0.46
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.46
3:D:72:CYS:SG	3:D:73:GLY:N	2.87	0.46
3:D:1195:GLN:N	3:D:1195:GLN:OE1	2.48	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.16	0.46
2:C:408:SER:O	2:C:431:LYS:NZ	2.31	0.46
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.46
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.31	0.46
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.97	0.46
2:C:515:MET:HE2	2:C:523:GLU:HB3	1.97	0.46
3:I:539:SER:O	3:I:541:LEU:N	2.49	0.46
3:D:720:ASN:ND2	3:D:720:ASN:O	2.48	0.46
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.45	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
2:H:453:ILE:HG23	2:H:453:ILE:O	2.16	0.46
2:H:205:PRO:O	2:H:208:ILE:HG22	2.16	0.46
2:C:944:ARG:HD3	2:C:944:ARG:O	2.15	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.16	0.46
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.81	0.46
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.56	0.46
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.16	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.16	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.16	0.46
3:D:573:THR:HG23	3:D:576:ARG:H	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:C:475:VAL:HG23	2:C:492:MET:SD	2.56	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.49	0.46
2:H:500:ALA:O	2:H:504:GLU:HB2	2.16	0.46
5:Y:562:ARG:HG3	5:Y:591:GLU:CD	2.36	0.46
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.51	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.98	0.46
2:H:40:GLU:O	2:H:73:TYR:OH	2.33	0.46
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
3:I:613:GLY:O	3:I:617:THR:OG1	2.22	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.97	0.45
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.98	0.45
1:G:218:ARG:HH12	1:G:222:THR:HB	1.81	0.45
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	1.97	0.45
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.80	0.45
2:C:800:MET:HG2	2:C:1096:ILE:HD13	1.98	0.45
2:H:600:THR:HG22	2:H:601:ASP:N	2.28	0.45
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.45
3:I:596:LEU:HD23	3:I:596:LEU:N	2.31	0.45
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	1.98	0.45
2:H:337:PHE:O	2:H:338:THR:OG1	2.26	0.45
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.98	0.45
3:I:800:LEU:O	3:I:803:VAL:HG12	2.16	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.16	0.45
3:I:390:LEU:HD12	3:I:390:LEU:N	2.31	0.45
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.31	0.45
3:D:111:THR:HG23	3:D:300:GLN:NE2	2.30	0.45
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.30	0.45
3:I:620:PHE:O	3:I:624:ILE:HG23	2.16	0.45
3:D:1347:LEU:HD23	3:D:1358:PRO:CG	2.30	0.45
3:I:238:ILE:HG13	3:I:238:ILE:O	2.16	0.45
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.47	0.45
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.16	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:X:112:THR:HG22	5:X:113:ARG:N	2.27	0.45
3:I:589:TYR:O	3:I:591:ILE:HG13	2.16	0.45
2:H:521:LEU:HD22	2:H:667:LEU:HD12	1.99	0.45
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.45
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.45	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:318:LEU:HD13	1:A:318:LEU:N	2.32	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
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.81	0.45
2:C:314:ASN:HD21	2:C:348:SER:HA	1.80	0.45
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.45
2:C:1006:GLU:CD	2:C:1006:GLU:H	2.19	0.45
2:H:1117:LEU:HD11	2:H:1182:ILE:CD1	2.47	0.45
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.15	0.45
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.99	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.98	0.45
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.98	0.45
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.30	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.97	0.45
3:D:290:ILE:O	3:D:293:ARG:HG3	2.15	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
1:A:317:ARG:C	1:A:318:LEU:HD13	2.36	0.45
3:I:214:ARG:O	3:I:218:THR:HG22	2.16	0.45
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.31	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:H	1.81	0.45
3:D:605:LEU:O	3:D:605:LEU:HD13	2.17	0.45
3:I:29:MET:HE3	3:I:29:MET:HA	1.98	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.45
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.48	0.45
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.98	0.45
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.98	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
3:D:514:THR:HG23	3:D:576:ARG:HE	1.80	0.45
2:C:131:THR:HG23	2:C:133:ASN:N	2.30	0.45
3:I:586:GLY:O	3:I:587:LEU:HB2	2.17	0.45
1:F:45:ARG:HD3	1:G:34:GLY:HA3	1.97	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.99	0.45
4:E:15:ASN:ND2	4:E:18:ASP:HB2	2.31	0.45
2:C:1141:LEU:HD22	2:C:1141:LEU:O	2.16	0.45
1:B:129:VAL:HG11	1:B:132:HIS:CE1	2.51	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.99	0.45
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.46	0.45
2:C:620:ASN:HD21	3:D:769:VAL:HG12	1.80	0.45
3:I:846:GLU:HA	3:I:858:VAL:HA	1.98	0.45
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.45
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.47	0.45
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.45
2:C:845:LEU:N	2:C:845:LEU:HD13	2.27	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:N	2.31	0.45
2:C:22:LEU:HD13	2:C:23:ASP:O	2.17	0.45
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.16	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.81	0.45
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	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
5:X:445:ASP:N	5:X:445:ASP:OD1	2.38	0.45
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.30	0.45
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.39	0.45
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.99	0.45
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.38	0.45
2:C:699:LEU:HD11	2:C:1179:GLY:CA	2.43	0.45
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.98	0.45
1:B:48:LEU:HB3	3:D:538:ARG:HD3	1.99	0.45
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.98	0.45
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.98	0.45
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.81	0.45
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.80	0.45
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.76	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45
3:D:513:MET:O	3:D:575:GLY:HA3	2.17	0.45
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.46	0.45
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.98	0.45
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.45
2:C:446:ASP:OD1	2:C:546:GLU:HB3	2.17	0.45
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.32	0.45
3:D:238:ILE:HG13	3:D:238:ILE:O	2.15	0.45
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.98	0.45
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.45
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.45
2:C:49:LEU:CD1	2:C:461:GLU:HA	2.47	0.45
3:I:1297:LYS:HE2	3:I:1297:LYS:HA	1.97	0.45
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:551:HIS:CG	2:C:552:PRO:HD2	2.52	0.45
4:J:60:ASN:H	4:J:63:ILE:HB	1.82	0.45
2:C:958:LYS:O	2:C:962:GLU:HG2	2.17	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.31	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
5:X:451:ARG:O	5:X:452:ILE:HG13	2.17	0.45
5:X:240:ARG:HD3	5:X:244:THR:CB	2.40	0.45
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.16	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.16	0.45
3:D:619:ILE:HD11	3:D:623:GLN:HE21	1.82	0.45
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.52	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.98	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.16	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.98	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.51	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
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.80	0.45
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.17	0.45
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.45
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.99	0.45
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.82	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:H:149:LEU:HD12	2:H:452:ARG:O	2.17	0.45
3:I:704:GLU:O	3:I:705:THR:OG1	2.28	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.99	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.32	0.45
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.45
5:Y:354:THR:HG23	5:Y:357:GLN:HB3	1.97	0.45
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.47	0.45
3:D:210:SER:O	3:D:214:ARG:HG3	2.17	0.45
3:I:527:LEU:HD12	3:I:535:ARG:NE	2.32	0.45
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.47	0.45
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.22	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.82	0.45
3:I:120:LEU:HD22	3:I:1330:ARG:HD2	1.99	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.17	0.45
2:H:475:VAL:O	2:H:479:LEU:HB2	2.16	0.45
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.51	0.45
2:H:756:TYR:H	2:H:766:ASN:HB3	1.82	0.45
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.99	0.45
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.45
3:I:856:ILE:HG13	3:I:857:LEU:O	2.16	0.45
1:A:181:GLU:N	1:A:181:GLU:OE2	2.50	0.45
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.17	0.45
2:H:1081:PRO:O	2:H:1085:MET:HG3	2.17	0.45
2:H:489:PRO:HB2	2:H:492:MET:CB	2.37	0.44
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.45	0.44
5:X:113:ARG:O	5:X:117:ILE:HD13	2.18	0.44
3:D:915:ILE:O	3:D:918:ILE:HG23	2.16	0.44
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.99	0.44
5:Y:119:ILE:CG2	5:Y:379:MET:HG2	2.45	0.44
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.99	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
3:D:596:LEU:HD23	3:D:596:LEU:N	2.32	0.44
2:H:961:SER:O	2:H:965:GLN:HG3	2.17	0.44
3:D:663:GLU:O	3:D:667:GLN:HG3	2.17	0.44
5:Y:555:GLU:OE2	5:Y:597:LYS:NZ	2.33	0.44
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.31	0.44
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.44
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.98	0.44
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.82	0.44
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.32	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.88	0.44
3:D:239:LEU:HD12	3:D:239:LEU:O	2.17	0.44
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.47	0.44
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.18	0.44
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.44
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.32	0.44
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.44
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.98	0.44
3:D:526:VAL:HG12	3:D:549:LYS:O	2.17	0.44
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.44
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.65	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:316:ILE:CG2	3:D:317:THR:H	2.25	0.44
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.44	0.44
2:H:484:LEU:N	2:H:484:LEU:HD22	2.31	0.44
1:G:178:SER:HA	1:G:179:PRO:HD3	1.87	0.44
2:H:1111:GLN:CG	2:H:1230:MET:HE2	2.48	0.44
2:C:88:ARG:NH1	2:C:88:ARG:HB3	2.33	0.44
3:I:161:THR:HG22	3:I:162:GLU:N	2.33	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.98	0.44
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.33	0.44
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.99	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.17	0.44
4:E:30:MET:O	4:E:35:LYS:HG2	2.17	0.44
3:I:490:ILE:O	3:I:499:ILE:HG22	2.18	0.44
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.99	0.44
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	1.99	0.44
2:H:820:GLU:O	2:H:824:GLN:HG3	2.18	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.53	0.44
3:I:909:ILE:O	3:I:909:ILE:HD12	2.18	0.44
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.16	0.44
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.32	0.44
7:D:1503:OO2:O2G	4:E:3:ARG:NH2	2.50	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
3:D:825:VAL:HG23	3:D:835:LEU:HB2	1.99	0.44
2:H:943:LYS:O	2:H:947:GLU:HG2	2.17	0.44
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.44
1:F:185:TYR:HB2	1:F:201:LEU:HD11	1.98	0.44
2:H:429:MET:O	2:H:433:ILE:HG13	2.17	0.44
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.98	0.44
2:H:702:THR:HA	2:H:1184:THR:O	2.16	0.44
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.48	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:A:80:GLU:HG3	2:C:694:ARG:HH12	1.83	0.44
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	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:C:1298:VAL:HG23	2:C:1299:ASN:N	2.29	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	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
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.33	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.80	0.44
2:H:839:VAL:HG11	2:H:841:ARG:HE	1.83	0.44
5:X:61:ASP:HA	5:X:64:ASP:OD2	2.17	0.44
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.33	0.44
4:E:5:THR:CA	4:E:7:GLN:H	2.30	0.44
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.51	0.44
3:I:899:TYR:CE1	3:I:915:ILE:HG23	2.53	0.44
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.46	0.44
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.00	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.18	0.44
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.00	0.44
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.51	0.44
1:F:234:LEU:HD21	1:G:217:ILE:HD11	1.98	0.44
2:C:892:GLU:O	2:C:893:THR:OG1	2.22	0.44
2:H:736:VAL:HG11	2:H:740:GLU:HA	1.98	0.44
3:D:704:GLU:HB2	3:D:718:SER:OG	2.18	0.44
1:G:33:ARG:HD3	2:H:1081:PRO:HG3	1.98	0.44
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.48	0.44
1:G:67:GLU:O	1:G:78:ILE:HB	2.18	0.44
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.51	0.44
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.64	0.44
2:C:177:ILE:HD12	2:C:177:ILE:N	2.33	0.44
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.58	0.44
2:H:845:LEU:N	2:H:845:LEU:HD13	2.30	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.47	0.44
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.44
2:H:202:ARG:NE	2:H:369:MET:HG2	2.33	0.44
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.44
3:I:664:ILE:HG21	3:I:681:LYS:HD2	2.00	0.44
3:D:382:TYR:HE1	3:D:401:VAL:CG2	2.31	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
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
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.53	0.44
2:C:515:MET:HE2	2:C:523:GLU:CG	2.47	0.44
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.18	0.44
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.99	0.44
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.18	0.44
1:A:45:ARG:NE	1:B:38:THR:OG1	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.26	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.21	0.44
2:C:11:ILE:HG21	2:C:697:LYS:HZ1	1.80	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.99	0.44
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.53	0.44
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.82	0.44
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.82	0.44
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.32	0.44
3:I:12:THR:C	3:I:13:LYS:HD2	2.39	0.44
2:C:1233:LEU:HD12	2:C:1233:LEU:O	2.18	0.44
1:B:100:LEU:HD21	1:B:121:VAL:HG21	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
3:D:888:CYS:SG	3:D:890:THR:HB	2.58	0.44
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.46	0.44
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.43	0.44
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.44
1:F:11:PRO:HD2	1:G:227:GLN:HA	1.99	0.44
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.44
2:C:1081:PRO:O	2:C:1085:MET:HG3	2.17	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.33	0.44
2:C:697:LYS:NZ	2:C:791:LEU:HD11	2.32	0.44
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.30	0.44
2:H:106:GLU:CG	2:H:109:ALA:H	2.31	0.44
3:D:490:ILE:HG23	3:D:500:ILE:CD1	2.48	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
3:I:801:VAL:O	3:I:805:GLN:HG2	2.17	0.44
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.32	0.44
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.53	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.75	0.44
2:H:850:ILE:HG23	2:H:885:GLY:O	2.17	0.44
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.99	0.44
3:D:801:VAL:O	3:D:805:GLN:HG2	2.17	0.44
1:B:22:THR:HG22	1:B:208:ASN:O	2.18	0.44
2:H:890:LYS:NZ	2:H:890:LYS:HB3	2.32	0.44
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.51	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.99	0.44
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.00	0.44
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	2.00	0.44
2:H:632:ASP:O	2:H:633:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.44
1:B:190:ALA:N	1:B:198:LEU:O	2.37	0.43
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.43
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.53	0.43
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.83	0.43
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.98	0.43
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.86	0.43
5:Y:477:GLU:N	5:Y:477:GLU:OE1	2.46	0.43
2:C:384:LEU:O	2:C:388:LEU:HG	2.17	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
1:B:180:VAL:HG11	1:B:183:ILE:HG12	2.00	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.51	0.43
2:C:1247:SER:O	2:C:1248:THR:HG23	2.18	0.43
2:C:19:PRO:HA	2:C:1157:GLN:HE21	1.83	0.43
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.69	0.43
1:F:31:LEU:HB2	1:F:199:ASP:O	2.17	0.43
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.82	0.43
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.49	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.00	0.43
3:I:1257:VAL:HA	3:I:1260:MET:CB	2.49	0.43
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.00	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.47	0.43
1:B:46:ILE:HG23	1:B:50:SER:HB2	2.00	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
3:D:62:PHE:O	3:D:101:ARG:HG3	2.18	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.17	0.43
5:X:299:LYS:O	5:X:303:ILE:HG12	2.18	0.43
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.48	0.43
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.18	0.43
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.26	0.43
3:I:508:LEU:HD23	3:I:508:LEU:O	2.19	0.43
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.44	0.43
3:I:52:GLU:OE1	5:Y:451:ARG:HD2	2.17	0.43
2:C:1166:ASP:C	2:C:1168:GLU:H	2.22	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.50	0.43
3:I:905:ARG:NH2	4:J:10:VAL:HG11	2.30	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:X:456:MET:O	5:X:460:ILE:HG13	2.18	0.43
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.50	0.43
2:H:73:TYR:CD2	2:H:73:TYR:N	2.86	0.43
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.01	0.43
2:H:216:THR:O	2:H:220:ILE:HG13	2.18	0.43
2:H:1067:ALA:HB3	2:H:1235:LEU:HD11	2.00	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
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
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.33	0.43
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.84	0.43
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	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
2:C:1002:LEU:HG	2:C:1007:LYS: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: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:D:390:LEU:HD12	3:D:390:LEU:N	2.32	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	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
1:F:77:ASP:O	1:F:81:ILE:HG13	2.18	0.43
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	2.00	0.43
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.18	0.43
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.51	0.43
2:C:533:LEU:N	2:C:533:LEU:HD23	2.31	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
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.00	0.43
3:D:1159:ILE:HD12	3:D:1186:TYR:CE2	2.53	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.00	0.43
3:I:179:LYS:N	3:I:179:LYS:HD3	2.33	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.17	0.43
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	2.00	0.43
3:D:79:LYS:HE3	5:X:568:ASN:C	2.38	0.43
3:D:215:LYS:O	3:D:219:LYS:HG3	2.19	0.43
1:G:227:GLN:O	1:G:228:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.89	0.43
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.54	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
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.83	0.43
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.43
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.43
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
2:H:748:ILE:HD12	2:H:748:ILE:C	2.39	0.43
3:I:796:LEU:HG	3:I:800:LEU:HD23	2.01	0.43
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.54	0.43
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.84	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
2:H:816:ILE:HD13	2:H:1074:GLY:CA	2.43	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
3:D:620:PHE:O	3:D:624:ILE:HG23	2.19	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.52	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
2:C:617:ALA:HB2	2:C:650:VAL:HG21	2.01	0.43
2:C:611:GLU:HG2	2:C:616:ILE:HD11	2.00	0.43
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.18	0.43
3:I:37:GLU:HB2	3:I:104:HIS:HE1	1.83	0.43
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.43
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.43
5:X:469:GLN:O	5:X:473:GLU:N	2.47	0.43
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	2.01	0.43
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.53	0.43
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.33	0.43
2:H:582:ASN:HB3	2:H:586:PHE:C	2.39	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
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.43
2:C:622:ASN:OD1	2:C:623:LEU:N	2.51	0.43
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.00	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.66	0.43
3:D:573:THR:HG22	3:D:576:ARG:CD	2.48	0.43
3:D:259:ARG:HH21	5:X:504:PRO:CB	2.26	0.43
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.19	0.43
1:F:66:HIS:HB3	2:H:874:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.34	0.43
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.19	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.43
3:I:733:SER:O	3:I:737:ILE:HG12	2.19	0.43
3:I:159:ILE:N	3:I:159:ILE:HD12	2.33	0.43
2:H:622:ASN:OD1	2:H:623:LEU:N	2.52	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CD1	2.48	0.43
1:F:219:ARG:O	1:F:223:ILE:HG13	2.18	0.43
3:D:591:ILE:HA	3:D:594:GLN:HB2	2.01	0.43
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.01	0.43
2:H:894:GLN:O	2:H:895:LEU:HB2	2.18	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.53	0.43
3:D:393:THR:H	3:D:396:ALA:HB3	1.83	0.43
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.47	0.43
3:D:491:LEU:HB2	3:D:904:ALA:HA	2.00	0.43
5:X:283:GLN:O	5:X:287:ILE:HG13	2.18	0.43
2:C:17:LYS:N	2:C:17:LYS:HD2	2.34	0.43
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.99	0.43
2:H:768:MET:O	2:H:785:ASP:N	2.50	0.43
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.43
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.43
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.01	0.43
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.34	0.43
2:H:971:LEU:HG	2:H:1018:TYR:HD1	1.84	0.43
3:I:1287:ILE:O	3:I:1290:ARG:HG2	2.18	0.43
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.97	0.43
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
3:D:416:ILE:O	3:D:416:ILE:HD12	2.19	0.43
3:I:809:VAL:CG1	3:I:913:GLU:H	2.32	0.43
2:C:453:ILE:HG22	2:C:585:GLY:O	2.19	0.43
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.43
3:I:655:SER:O	3:I:658:GLU:HG2	2.19	0.43
2:H:1276:TRP:CE2	3:I:801:VAL:HG11	2.54	0.43
3:I:431:ARG:HH21	3:I:493:PRO:HG3	1.83	0.43
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.18	0.43
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.82	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.34	0.43
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.19	0.43
2:H:935:THR:HA	2:H:1048:LYS:HB3	2.00	0.43
1:A:257:VAL:HG13	1:A:276:HIS:O	2.19	0.43
2:C:515:MET:HA	2:C:526:HIS:CE1	2.54	0.42
5:Y:460:ILE:HG12	5:Y:497:VAL:HG13	2.01	0.42
3:D:1284:ARG:HA	3:D:1287:ILE:CD1	2.49	0.42
2:C:794:LEU:HD21	2:C:796:LEU:CG	2.46	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.19	0.42
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.42
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.83	0.42
3:D:377:PHE:O	3:D:381:ILE:HG13	2.18	0.42
3:I:252:LEU:N	3:I:252:LEU:HD23	2.33	0.42
2:H:130:MET:CG	2:H:134:GLY:HA2	2.48	0.42
3:D:704:GLU:O	3:D:705:THR:OG1	2.27	0.42
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.01	0.42
5:X:250:LEU:O	5:X:254:GLU:HG2	2.18	0.42
3:D:508:LEU:HD22	3:D:508:LEU:O	2.18	0.42
2:C:1329:GLU:O	2:C:1332:SER:HB3	2.19	0.42
1:G:222:THR:O	1:G:226:GLU:HG2	2.19	0.42
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.00	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.00	0.42
2:C:556:GLY:O	2:C:579:ALA:HB2	2.18	0.42
2:H:557:ARG:NH2	2:H:607:SER:O	2.51	0.42
3:I:595:ALA:HB1	3:I:596:LEU:HD23	2.01	0.42
3:I:124:ILE:HA	3:I:237:MET:HE2	2.00	0.42
2:C:1252:SER:HB3	2:C:1259:LEU:HD23	2.01	0.42
1:F:134:THR:HG21	2:H:727:VAL:O	2.18	0.42
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.01	0.42
2:C:542:ARG:HG2	2:C:543:ALA:N	2.33	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.18	0.42
2:H:972:PHE:HA	2:H:975:ILE:HG22	2.01	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
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.49	0.42
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.52	0.42
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.01	0.42
2:C:994:ARG:N	2:C:994:ARG:HD3	2.34	0.42
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.50	0.42
3:D:746:LEU:HB3	3:D:754:ILE:CG2	2.49	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
3:D:614:LEU:HD12	4:E:5:THR:HG21	2.01	0.42
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.50	0.42
5:X:448:ARG:HH11	5:X:452:ILE:HD12	1.85	0.42
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.54	0.42
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.49	0.42
2:C:645:PHE:CD1	2:C:650:VAL:HB	2.54	0.42
3:D:789:LYS:HD2	3:D:932:MET:SD	2.59	0.42
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.01	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
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.49	0.42
1:A:152:TYR:CE1	1:A:154:PRO:HD3	2.53	0.42
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
1:B:19:VAL:HG12	1:B:19:VAL:O	2.20	0.42
3:I:805:GLN:HE21	3:I:805:GLN:HB2	1.65	0.42
3:D:843:VAL:HA	3:D:861:ASN:HA	2.01	0.42
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.83	0.42
2:H:941:LYS:O	2:H:941:LYS:HD2	2.19	0.42
3:D:288:PRO:O	3:D:292:VAL:HG12	2.19	0.42
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.00	0.42
2:C:333:ILE:HD12	2:C:333:ILE:N	2.33	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.01	0.42
3:D:201:LEU:HD12	3:D:205:LEU:HD11	2.02	0.42
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.90	0.42
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.49	0.42
3:D:355:ILE:HG12	3:D:464:ASP:O	2.19	0.42
2:H:302:ILE:HA	2:H:309:LEU:HA	2.01	0.42
3:D:909:ILE:HG13	3:D:909:ILE:H	1.56	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
5:Y:469:GLN:O	5:Y:473:GLU:HB2	2.19	0.42
1:A:152:TYR:CD1	1:A:154:PRO:HD3	2.54	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
3:D:114:ILE:CG2	3:D:308:ASP:HB3	2.50	0.42
3:I:403:ARG:O	3:I:405:GLU:N	2.53	0.42
3:I:1282:TYR:HA	3:I:1285:VAL:CG2	2.49	0.42
2:C:51:ALA:C	2:C:53:PHE:H	2.22	0.42
2:C:890:LYS:NZ	2:C:890:LYS:HB3	2.33	0.42
3:I:58:CYS:SG	3:I:61:ILE:HG13	2.60	0.42
2:H:81:ASP:OD1	2:H:83:GLN:HG2	2.19	0.42
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.42
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.30	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	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
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	2.00	0.42
2:H:27:LEU:O	2:H:528:ARG:NH1	2.49	0.42
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.42
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.42
2:H:94:ALA:O	2:H:126:GLU:HG2	2.19	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.02	0.42
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.54	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
5:Y:532:LEU:O	5:Y:536:THR:HG23	2.19	0.42
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.42
1:B:153:VAL:O	1:B:175:ALA:N	2.52	0.42
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.54	0.42
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.42
2:H:22:LEU:HD13	2:H:23:ASP:O	2.19	0.42
2:C:487:LEU:H	2:C:487:LEU:HD12	1.84	0.42
5:X:139:GLU:HA	5:X:142:THR:CG2	2.48	0.42
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.83	0.42
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.42
3:D:77:ARG:CG	3:D:78:LEU:H	2.31	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.39	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.42
3:I:607:THR:O	3:I:611:ILE:HG12	2.19	0.42
5:Y:278:ASP:O	5:Y:282:THR:OG1	2.24	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
3:D:558:ASP:OD1	3:D:559:ALA:N	2.52	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
2:H:1268:GLN:O	3:I:346:ARG:HA	2.20	0.42
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.42
3:I:397:ALA:O	3:I:401:VAL:HG13	2.20	0.42
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.84	0.42
2:H:553:THR:O	2:H:557:ARG:HD3	2.19	0.42
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.42
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:1297:LYS:CA	3:I:1297:LYS:NZ	2.82	0.42
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.01	0.42
3:I:66:LYS:HB3	3:I:66:LYS:NZ	2.34	0.42
3:I:147:ILE:HG13	3:I:149:GLY:H	1.84	0.42
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.55	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.42
2:C:104:ILE:HD11	2:C:115:LYS:HB2	2.02	0.42
2:H:17:LYS:HD2	2:H:17:LYS:N	2.35	0.42
2:C:836:LEU:HB3	2:C:918:LEU:HD21	2.02	0.42
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.42
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.50	0.42
2:H:1073:LYS:HD3	3:I:462:ASP:CB	2.21	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:1146:GLN:CD	2:H:1160:ASP:HB2	2.40	0.42
2:H:766:ASN:H	2:H:787:PRO:HG3	1.85	0.42
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.55	0.42
5:Y:119:ILE:CD1	5:Y:122:ARG:HH21	2.33	0.42
2:C:99:LYS:HZ3	2:C:99:LYS:HB3	1.83	0.42
2:C:348:SER:O	2:C:352:ARG:HG3	2.20	0.42
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.67	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	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
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.42
2:C:632:ASP:O	2:C:633:LEU:HD23	2.20	0.42
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.34	0.42
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.35	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.01	0.42
3:I:1148:ARG:HB2	3:I:1148:ARG:NH2	2.35	0.42
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.84	0.42
3:D:466:MET:HB3	3:D:466:MET:HE2	1.88	0.42
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.19	0.42
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.20	0.42
3:D:154:LEU:HD22	3:D:176:PHE:HE1	1.83	0.42
3:D:843:VAL:HG21	3:D:897:HIS:HA	2.02	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
5:X:608:ARG:HB3	5:X:608:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:80:PHE:O	2:H:84:GLU:HB3	2.19	0.42
2:C:768:MET:O	2:C:785:ASP:N	2.48	0.42
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.00	0.42
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.84	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.50	0.42
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.42
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.54	0.42
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.20	0.42
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.50	0.42
1:F:234:LEU:HD12	1:F:234:LEU:N	2.35	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.59	0.42
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.55	0.42
5:X:477:GLU:H	5:X:477:GLU:CD	2.23	0.42
3:D:574:VAL:O	3:D:578:ILE:HG22	2.20	0.42
5:X:52:GLY:O	5:X:53:ILE:HB	2.20	0.42
2:H:1161:LEU:HD21	2:H:1172:LEU:HD11	2.02	0.42
2:H:549:ASP:OD1	2:H:550:VAL:N	2.53	0.42
2:H:122:VAL:HG22	2:H:123:TYR:N	2.34	0.41
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	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:I:746:LEU:H	3:I:746:LEU:HD22	1.85	0.41
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.46	0.41
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.46	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.41
3:I:326:SER:O	3:I:330:MET:HG3	2.19	0.41
3:I:532:GLU:OE1	3:I:578:ILE:HB	2.20	0.41
3:D:141:PHE:HD2	3:D:141:PHE:HA	1.71	0.41
2:H:469:VAL:O	2:H:472:GLU:HB3	2.20	0.41
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.84	0.41
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.19	0.41
5:Y:363:ARG:HE	5:Y:363:ARG:HA	1.84	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
2:C:72:SER:O	2:C:98:VAL:HG23	2.20	0.41
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.41
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	2.02	0.41
2:H:481:LEU:C	2:H:481:LEU:HD13	2.40	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.20	0.41
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.79	0.41
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	2.02	0.41
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.41
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.35	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.41
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.50	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.41
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.36	0.41
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.33	0.41
1:B:228:LEU:C	1:B:228:LEU:HD12	2.41	0.41
2:H:170:VAL:HG23	2:H:171:LEU:N	2.31	0.41
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.49	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.85	0.41
3:I:290:ILE:O	3:I:293:ARG:HG3	2.20	0.41
2:H:1323:PHE:O	2:H:1327:LEU:HG	2.20	0.41
3:I:500:ILE:CD1	3:I:500:ILE:H	2.33	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
2:H:985:GLU:HG2	2:H:989:LEU:HD13	2.01	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
2:H:103:VAL:HG22	2:H:104:ILE:N	2.34	0.41
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.20	0.41
2:C:135:THR:OG1	2:C:142:GLU:HG3	2.20	0.41
2:H:513:GLN:HA	2:H:513:GLN:NE2	2.24	0.41
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.20	0.41
3:I:120:LEU:HD12	3:I:120:LEU:N	2.35	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.47	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
3:I:141:PHE:O	3:I:297:ARG:HD3	2.21	0.41
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.02	0.41
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.55	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.54	0.41
2:C:230:PHE:HB2	2:C:333:ILE:HB	2.01	0.41
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.55	0.41
2:C:943:LYS:O	2:C:947:GLU:HG2	2.20	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:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.41
1:B:86:LYS:NZ	3:D:526:VAL:O	2.48	0.41
2:H:843:THR:HB	2:H:845:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.41
2:H:619:ALA:HA	2:H:653:MET:CE	2.51	0.41
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.55	0.41
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.36	0.41
2:H:142:GLU:O	2:H:143:ARG:HB2	2.21	0.41
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.34	0.41
2:C:27:LEU:O	2:C:528:ARG:NH1	2.52	0.41
3:D:369:PRO:HB2	3:D:372:MET:HB2	2.01	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB2	1.89	0.41
1:A:22:THR:O	1:A:207:THR:N	2.50	0.41
3:D:805:GLN:HB2	3:D:805:GLN:HE21	1.72	0.41
2:H:518:ASN:ND2	2:H:761:GLN:HG2	2.35	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.20	0.41
3:I:219:LYS:O	3:I:223:LEU:HG	2.20	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.21	0.41
2:H:1199:LEU:HD13	2:H:1206:THR:HA	2.02	0.41
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.90	0.41
3:I:217:LEU:O	3:I:221:ILE:HG23	2.21	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.41
1:F:46:ILE:O	1:F:50:SER:HB2	2.20	0.41
3:I:135:ILE:O	3:I:139:LEU:HD12	2.20	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
3:I:279:LEU:HD23	3:I:295:GLU:HB3	2.02	0.41
1:A:166:ARG:HG3	1:A:166:ARG:O	2.21	0.41
3:I:1193:TRP:CD1	3:I:1194:ARG:HD2	2.55	0.41
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.55	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
1:B:47:LEU:HD13	1:B:205:MET:HE2	2.03	0.41
2:C:546:GLU:O	2:C:548:ARG:N	2.48	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.41
5:Y:528:LEU:O	5:Y:528:LEU:HD12	2.20	0.41
3:I:303:VAL:O	3:I:307:LEU:HG	2.20	0.41
5:X:133:SER:OG	5:X:365:MET:HB2	2.21	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:I:392:THR:HG22	5:Y:606:VAL:HG11	2.01	0.41
4:E:16:ARG:O	4:E:19:LEU:HB3	2.20	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.96	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1165:SER:O	2:H:1168:GLU:HB3	2.21	0.41
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.50	0.41
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.56	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.19	0.41
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.54	0.41
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.50	0.41
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.41
3:D:649:LYS:O	3:D:653:ILE:HG12	2.21	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.20	0.41
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.41
5:Y:453:PRO:CD	5:Y:456:MET:HB2	2.42	0.41
2:H:843:THR:HB	2:H:845:LEU:CD2	2.51	0.41
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.69	0.41
3:I:382:TYR:CE1	3:I:398:LYS:HA	2.56	0.41
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.84	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
2:C:901:LEU:HD13	5:X:559:LEU:HD22	2.02	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:I:1322:ALA:O	3:I:1326:GLN:HG3	2.21	0.41
5:X:363:ARG:HE	5:X:363:ARG:HA	1.85	0.41
5:Y:476:ARG:HB2	5:Y:477:GLU:OE1	2.20	0.41
3:I:494:ALA:HA	3:I:1252:HIS:CE1	2.53	0.41
2:C:99:LYS:HA	2:C:121:GLU:HA	2.02	0.41
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.03	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.21	0.41
2:H:680:LEU:HD23	2:H:680:LEU:O	2.21	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.54	0.41
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.41
1:F:89:ALA:HB3	1:F:124:VAL:HB	2.03	0.41
3:D:746:LEU:H	3:D:746:LEU:HD22	1.85	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.41
5:X:35:ILE:HG13	5:X:36:VAL:N	2.21	0.41
3:D:1149:ARG:CD	3:D:1149:ARG:H	2.23	0.41
3:I:422:LEU:O	3:I:422:LEU:HD12	2.20	0.41
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.02	0.41
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.30	0.41
2:H:1285:TYR:HA	2:H:1288:GLN:HB3	2.02	0.41
3:D:27:PRO:HD3	3:D:236:TRP:CE3	2.56	0.41
2:C:975:ILE:O	2:C:978:VAL:HG12	2.21	0.41
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.01	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.61	0.41
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.41
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.56	0.41
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.20	0.41
3:I:873:GLU:HG3	3:I:873:GLU:H	1.64	0.41
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.41
5:X:261:LEU:HD12	5:X:261:LEU:N	2.36	0.41
3:D:53:ARG:HA	3:D:53:ARG:HD2	1.96	0.41
5:Y:261:LEU:HD12	5:Y:261:LEU:N	2.36	0.41
5:X:270:VAL:HA	5:X:273:MET:HE3	2.01	0.41
2:H:977:ALA:O	2:H:980:VAL:HG12	2.20	0.41
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.03	0.41
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.41
3:I:1173:ARG:CA	3:I:1174:ARG:CB	2.86	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
3:D:128:LEU:HD12	3:D:192:MET:CE	2.35	0.41
3:I:746:LEU:HD22	3:I:746:LEU:N	2.36	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.20	0.41
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.35	0.41
2:C:773:LEU:HD22	2:C:773:LEU:C	2.41	0.41
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.89	0.41
2:H:618:GLN:HG2	2:H:637:ARG:NH2	2.36	0.41
5:X:262:VAL:HG13	5:X:263:PRO:CD	2.48	0.41
3:D:362:ARG:NH1	7:D:1503:O2:H8	2.33	0.41
3:I:116:PHE:HB3	3:I:237:MET:HE3	2.03	0.41
2:C:752:ASN:C	2:C:753:LEU:HG	2.40	0.41
3:I:552:ILE:HD13	3:I:570:LYS:HB2	2.03	0.41
3:I:526:VAL:HG12	3:I:549:LYS:O	2.20	0.41
2:C:122:VAL:CG2	5:X:472:GLN:HE21	2.34	0.41
3:D:647:PRO:HG3	3:D:697:MET:HA	2.03	0.41
2:C:442:VAL:HG12	2:C:443:ASP:N	2.36	0.41
2:C:688:GLN:O	2:C:1236:ASN:N	2.54	0.41
3:I:155:GLU:H	3:I:155:GLU:CD	2.24	0.41
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.21	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB2	2.01	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.41
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.41
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.41	0.41
2:C:82:VAL:O	2:C:86:GLN:HG3	2.20	0.41
2:H:690:VAL:HA	2:H:691:PRO:HD3	1.91	0.41
2:H:374:GLU:HA	2:H:375:PRO:HD3	1.93	0.41
2:H:1138:VAL:O	2:H:1139:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.20	0.41
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.55	0.41
5:Y:374:ARG:O	5:Y:378:GLU:HG3	2.21	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.21	0.41
2:H:812:PHE:H	2:H:815:SER:HB2	1.86	0.41
2:C:661:VAL:HG23	2:C:662:SER:O	2.22	0.41
3:I:527:LEU:HB3	3:I:528:THR:H	1.72	0.41
3:I:903:LEU:HD11	3:I:909:ILE:CG2	2.45	0.41
3:D:681:LYS:HD3	3:D:682:VAL:N	2.36	0.41
3:I:128:LEU:HD12	3:I:192:MET:HE1	2.02	0.41
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.20	0.41
3:D:409:TRP:O	3:D:412:LEU:HB3	2.21	0.41
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
2:H:31:GLN:HG3	2:H:130:MET:HE1	2.03	0.41
4:E:15:ASN:HD21	4:E:18:ASP:CB	2.32	0.41
2:H:698:PRO:HB3	2:H:1231:TYR:CE1	2.56	0.41
1:B:176:CYS:C	1:B:178:SER:N	2.74	0.41
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.50	0.41
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
2:C:84:GLU:HG3	2:C:88:ARG:HD3	2.03	0.41
3:I:856:ILE:HD12	3:I:857:LEU:H	1.86	0.41
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.41
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.21	0.41
3:D:361:LEU:HD22	3:D:361:LEU:N	2.36	0.41
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.54	0.41
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.02	0.41
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
2:H:691:PRO:HA	2:H:788:SER:OG	2.21	0.41
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.61	0.41
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.20	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
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.21	0.40
5:Y:591:GLU:O	5:Y:595:LEU:HG	2.21	0.40
2:H:892:GLU:C	2:H:894:GLN:H	2.24	0.40
2:H:130:MET:HG3	2:H:134:GLY:HA2	2.03	0.40
3:D:1274:PHE:CD2	3:D:1275:LEU:HG	2.50	0.40
2:H:740:GLU:CD	2:H:740:GLU:H	2.24	0.40
2:C:73:TYR:HA	2:C:98:VAL:HA	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.86	0.40
2:C:854:ILE:HB	2:C:857:VAL:HG11	2.03	0.40
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.02	0.40
1:F:59:VAL:HG21	1:F:85:LEU:HD13	2.03	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:1269:ARG:HD2	3:D:344:GLY:N	2.35	0.40
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.86	0.40
3:D:836:ARG:HA	3:D:836:ARG:HD2	1.88	0.40
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.40
3:I:519:ASN:HD21	3:I:707:ILE:CG2	2.33	0.40
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.86	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.86	0.40
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.21	0.40
1:A:323:PRO:HA	1:A:324:ALA:HA	1.77	0.40
3:D:697:MET:SD	3:D:741:ALA:HB3	2.62	0.40
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.52	0.40
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.03	0.40
2:C:538:LEU:HD12	2:C:538:LEU:H	1.86	0.40
3:I:385:LEU:HD23	3:I:411:ILE:HG13	2.03	0.40
2:H:821:ARG:HB2	2:H:1082:ILE:HD13	2.04	0.40
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	2.03	0.40
2:H:870:ILE:HD12	2:H:870:ILE:N	2.36	0.40
5:X:253:SER:O	5:X:257:LYS:HG3	2.21	0.40
2:C:848:GLU:HG2	2:C:888:THR:HA	2.02	0.40
2:H:219:GLN:O	2:H:223:LEU:HG	2.21	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
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.02	0.40
1:A:102:LEU:HD12	1:A:115:ILE:HG12	2.03	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
3:I:545:HIS:HA	3:I:546:ALA:HA	1.80	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:517:GLN:HG3	2:C:759:SER:OG	2.21	0.40
3:D:395:LYS:NZ	5:X:607:LEU:O	2.50	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.22	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
5:X:283:GLN:CD	5:X:343:LYS:HD2	2.41	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:18:ARG:HG3	2:C:19:PRO:HD2	2.03	0.40
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.55	0.40
3:I:1243:LEU:O	3:I:1243:LEU:HD23	2.22	0.40
1:A:313:SER:OG	1:A:314:LEU:N	2.53	0.40
3:I:510:LEU:HD12	3:I:601:ILE:HD11	2.03	0.40
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.21	0.40
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.50	0.40
3:D:746:LEU:N	3:D:746:LEU:HD22	2.36	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:I:325:LYS:NZ	3:I:325:LYS:HB3	2.36	0.40
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.52	0.40
5:X:559:LEU:HD23	5:X:559:LEU:HA	1.90	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
3:D:483:LEU:HD11	4:E:20:VAL:HG21	2.03	0.40
3:D:679:TYR:O	3:D:683:ILE:HG13	2.21	0.40
2:C:505:PHE:HA	2:C:509:SER:HB3	2.04	0.40
3:I:310:GLY:HA2	3:I:314:ARG:HG2	2.04	0.40
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.87	0.40
2:C:115:LYS:O	2:C:116:ASP:HB2	2.21	0.40
2:H:623:LEU:HD12	2:H:623:LEU:N	2.36	0.40
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.03	0.40
5:X:410:ILE:O	5:X:414:LYS:HG3	2.22	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.85	0.40
2:C:409:LEU:HD11	2:C:428:VAL:HA	2.04	0.40
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.91	0.40
3:I:609:TYR:HE2	3:I:614:LEU:HD13	1.86	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.37	0.40
3:I:915:ILE:O	3:I:918:ILE:HG23	2.22	0.40
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.86	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:355:ILE:HG21	3:D:466:MET:SD	2.61	0.40
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.46	0.40
3:D:678:ARG:O	3:D:682:VAL:HG13	2.21	0.40
5:X:558:VAL:O	5:X:562:ARG:HB2	2.22	0.40
3:D:709:ARG:O	3:D:712:GLN:N	2.53	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.04	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.52	0.40
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:894:GLN:NE2	3:I:77:ARG:HD3	2.32	0.40
1:A:50:SER:HA	1:A:150:ARG:HD2	2.02	0.40
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.40
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.40
5:X:400:GLN:HE21	5:X:403:ASP:CG	2.25	0.40
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.40
2:C:1195:ILE:O	2:C:1199:LEU:HG	2.22	0.40
2:C:465:ARG:O	2:C:469:VAL:HG23	2.21	0.40
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.87	0.40
5:X:530:LEU:H	5:X:530:LEU:HD12	1.86	0.40
3:D:84:ILE:H	3:D:84:ILE:HG13	1.76	0.40
3:I:417:ARG:NH1	4:J:43:ASN:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	4	45
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	5	53
1	F	227/329 (69%)	193 (85%)	28 (12%)	6 (3%)	8	61
1	G	213/329 (65%)	186 (87%)	22 (10%)	5 (2%)	10	64
2	C	1333/1342 (99%)	1073 (80%)	208 (16%)	52 (4%)	5	50
2	H	1333/1342 (99%)	1078 (81%)	206 (16%)	49 (4%)	5	53
3	D	1154/1407 (82%)	926 (80%)	182 (16%)	46 (4%)	5	49
3	I	1154/1407 (82%)	925 (80%)	184 (16%)	45 (4%)	5	50
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	3	39
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	3	41
5	X	511/613 (83%)	450 (88%)	46 (9%)	15 (3%)	7	59
5	Y	454/613 (74%)	409 (90%)	34 (8%)	11 (2%)	9	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7079/8222 (86%)	5834 (82%)	984 (14%)	261 (4%)	5	53

All (261) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	56	89
1	B	189/286 (66%)	186 (98%)	3 (2%)	75	94
1	F	197/286 (69%)	194 (98%)	3 (2%)	76	94
1	G	185/286 (65%)	182 (98%)	3 (2%)	75	94
2	C	1150/1157 (99%)	1094 (95%)	56 (5%)	35	80
2	H	1150/1157 (99%)	1097 (95%)	53 (5%)	37	81
3	D	971/1168 (83%)	921 (95%)	50 (5%)	33	79
3	I	971/1168 (83%)	918 (94%)	53 (6%)	30	77
4	E	74/75 (99%)	72 (97%)	2 (3%)	57	89
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	447 (97%)	13 (3%)	56	89
5	Y	407/540 (75%)	392 (96%)	15 (4%)	45	86
All	All	6100/7024 (87%)	5841 (96%)	259 (4%)	40	83

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
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

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Mol	Chain	Res	Type
2	C	964	LEU
2	C	975	ILE
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

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Mol	Chain	Res	Type
3	D	309	ASN
3	D	430	HIS
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

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Mol	Chain	Res	Type
5	X	476	ARG
5	X	495	ARG
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

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Mol	Chain	Res	Type
2	H	944	ARG
2	H	955	GLN
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

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Mol	Chain	Res	Type
3	I	416	ILE
3	I	430	HIS
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

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Mol	Chain	Res	Type
5	Y	495	ARG
5	Y	545	HIS
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

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Mol	Chain	Res	Type
3	D	519	ASN
3	D	623	GLN
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

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Mol	Chain	Res	Type
3	I	274	ASN
3	I	300	GLN
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	42,42,42	2.57	17 (40%)	64,68,68	12.68	14 (21%)

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	-	-	0/33/49/49	0/1/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	002	C2-N2	6.86	1.43	1.32
7	D	1503	002	O6-C6	6.14	1.36	1.24
7	D	1503	002	PD-O3C	-4.99	1.51	1.60
7	D	1503	002	C2'-C1'	-4.43	1.47	1.53
7	D	1503	002	PC-O3C	-4.41	1.51	1.59
7	D	1503	002	O2'-C2'	-4.31	1.32	1.43
7	D	1503	002	C6-C5	-3.74	1.35	1.41
7	D	1503	002	C4-N3	-3.66	1.32	1.37
7	D	1503	002	C8-N7	3.29	1.41	1.34
7	D	1503	002	C4-N9	2.69	1.44	1.38
7	D	1503	002	PA-O3A	-2.68	1.55	1.59
7	D	1503	002	PB-O3A	-2.67	1.55	1.59
7	D	1503	002	C2'-C3'	-2.52	1.47	1.53
7	D	1503	002	O4'-C4'	-2.50	1.39	1.45
7	D	1503	002	O4'-C1'	-2.34	1.37	1.41
7	D	1503	002	PC-O3'	-2.21	1.54	1.60
7	D	1503	002	C8-N9	2.15	1.39	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	002	C6-C5-N7	-98.25	129.01	134.24
7	D	1503	002	N3-C4-N9	17.53	132.62	126.41
7	D	1503	002	C4'-O4'-C1'	-9.59	99.33	109.75
7	D	1503	002	O3A-PB-O3B	7.90	117.72	101.66
7	D	1503	002	PA-O3A-PB	-6.32	113.14	131.68
7	D	1503	002	PC-O3C-PD	-5.94	114.28	131.68
7	D	1503	002	C8-N9-C4	-3.01	104.60	106.90
7	D	1503	002	O3'-C3'-C2'	2.56	121.55	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	0O2	C1'-N9-C4	2.53	130.43	126.29
7	D	1503	0O2	PB-O3B-PG	-2.44	124.52	131.68
7	D	1503	0O2	O3G-PG-O3B	2.35	116.28	105.14
7	D	1503	0O2	O4'-C4'-C3'	2.28	110.06	104.88
7	D	1503	0O2	O1G-PG-O2G	-2.24	103.14	110.44
7	D	1503	0O2	PC-O3'-C3'	2.09	127.36	119.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	323/329 (98%)	0.29	12 (3%)	39	33	0, 55, 172, 230	0
1	B	221/329 (67%)	0.53	14 (6%)	19	20	0, 86, 193, 260	0
1	F	229/329 (69%)	0.54	19 (8%)	11	14	2, 123, 212, 293	0
1	G	217/329 (65%)	0.53	10 (4%)	31	27	5, 113, 204, 271	0
2	C	1335/1342 (99%)	0.20	41 (3%)	47	38	0, 38, 168, 304	0
2	H	1335/1342 (99%)	0.36	73 (5%)	24	22	0, 78, 206, 346	0
3	D	1160/1407 (82%)	0.23	28 (2%)	56	44	0, 28, 152, 297	0
3	I	1160/1407 (82%)	0.37	58 (5%)	28	25	0, 54, 183, 316	0
4	E	90/91 (98%)	0.14	1 (1%)	77	63	0, 33, 116, 167	0
4	J	76/91 (83%)	0.54	2 (2%)	53	42	12, 83, 181, 230	0
5	X	517/613 (84%)	0.45	42 (8%)	12	14	0, 98, 238, 341	0
5	Y	458/613 (74%)	0.36	28 (6%)	21	21	1, 100, 216, 296	0
All	All	7121/8222 (86%)	0.33	328 (4%)	31	27	0, 63, 198, 346	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	521	LYS	10.9
3	I	10	ALA	9.7
2	H	981	ALA	8.4
2	H	982	GLY	7.5
3	I	208	THR	6.9
1	F	162	GLU	6.1
5	X	35	ILE	5.8
3	I	207	GLU	5.8
2	C	251	ALA	5.7
3	I	9	LYS	5.7
2	H	1000	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
3	D	1133	ASP	5.4
3	I	1294	ALA	5.4
2	H	1002	LEU	5.3
5	Y	311	THR	5.2
1	F	148	ARG	5.2
3	I	11	GLN	5.2
2	H	1003	THR	5.0
5	X	24	TYR	4.9
3	D	1199	PHE	4.8
2	H	983	GLY	4.8
2	H	1001	GLY	4.6
5	Y	310	GLU	4.6
2	H	163	LYS	4.6
3	I	1167	LYS	4.6
5	Y	478	PRO	4.5
3	I	1203	ARG	4.4
3	I	13	LYS	4.4
2	H	999	GLU	4.4
3	D	1171	GLY	4.4
3	I	1172	LYS	4.3
5	Y	315	TRP	4.3
2	H	1020	GLU	4.3
3	I	1376	GLY	4.2
1	G	157	THR	4.1
5	X	36	VAL	4.1
2	H	742	TYR	4.1
3	I	12	THR	4.1
2	H	113	THR	4.0
1	F	193	GLU	4.0
3	D	81	ARG	4.0
2	H	332	ARG	4.0
3	I	1204	VAL	4.0
5	X	54	GLN	4.0
2	C	232	ILE	3.9
2	C	252	SER	3.9
5	X	318	ALA	3.9
1	A	193	GLU	3.9
2	H	979	LEU	3.8
2	C	238	GLN	3.8
5	X	56	MET	3.8
5	X	339	ARG	3.8
1	B	74	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	282	VAL	3.7
3	I	1168	GLU	3.7
1	F	195	ARG	3.7
3	I	1295	ASN	3.7
2	C	311	CYS	3.7
5	X	34	ASP	3.7
2	C	265	LYS	3.7
2	C	231	GLU	3.6
1	G	54	CYS	3.6
2	C	272	ARG	3.6
5	X	16	GLY	3.6
4	E	91	ARG	3.6
2	C	1002	LEU	3.6
5	Y	305	LEU	3.6
2	H	172	TYR	3.6
5	X	6	GLN	3.6
1	F	194	GLN	3.5
2	H	1008	GLN	3.5
5	Y	320	ILE	3.5
2	C	233	ARG	3.5
5	X	305	LEU	3.5
2	C	165	HIS	3.5
3	D	80	HIS	3.4
2	C	310	ILE	3.4
3	I	151	MET	3.4
5	Y	212	ILE	3.4
1	B	75	GLN	3.4
2	C	266	GLY	3.4
1	A	196	THR	3.4
3	I	1375	ALA	3.4
1	F	95	LYS	3.3
3	D	1170	LYS	3.3
1	B	169	GLY	3.3
2	H	986	ALA	3.3
3	D	1168	GLU	3.3
3	I	205	LEU	3.3
2	C	267	ARG	3.2
1	A	262	LEU	3.2
5	X	53	ILE	3.2
3	I	1201	GLY	3.2
5	X	64	ASP	3.2
3	I	1170	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	1134	GLN	3.2
1	F	163	GLU	3.2
2	H	996	ARG	3.2
2	H	375	PRO	3.2
1	B	73	GLY	3.2
2	H	115	LYS	3.1
5	Y	489	MET	3.1
2	H	988	LYS	3.1
5	Y	319	ALA	3.1
2	C	67	GLU	3.1
1	A	191	ARG	3.1
3	D	1172	LYS	3.1
5	Y	316	PHE	3.1
5	X	317	ASN	3.1
5	X	57	GLU	3.0
5	X	336	GLU	3.0
1	B	97	GLU	3.0
2	H	998	LEU	3.0
5	Y	309	ASN	3.0
2	H	376	PRO	3.0
5	Y	321	ALA	3.0
1	F	19	VAL	3.0
2	H	978	VAL	3.0
5	X	522	PHE	3.0
3	I	542	ALA	3.0
2	H	987	GLU	3.0
5	X	423	ARG	3.0
3	I	213	LYS	3.0
3	D	314	ARG	2.9
2	H	744	GLY	2.9
3	D	1134	ILE	2.9
5	Y	425	TYR	2.9
2	H	1012	GLU	2.9
5	X	303	ILE	2.9
5	X	288	MET	2.9
2	H	1004	ASP	2.8
2	H	1019	ASP	2.8
2	C	271	ALA	2.8
3	D	1198	VAL	2.8
2	C	981	ALA	2.8
5	Y	515	GLU	2.8
1	B	91	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
5	X	425	TYR	2.8
3	I	732	GLY	2.8
3	I	212	THR	2.8
1	G	172	LEU	2.8
5	Y	328	GLU	2.8
1	A	25	LYS	2.8
1	F	164	ASP	2.8
2	H	1006	GLU	2.8
3	D	208	THR	2.7
4	J	12	LYS	2.7
2	C	1000	LEU	2.7
2	H	975	ILE	2.7
3	I	672	LEU	2.7
3	D	1203	ARG	2.7
1	B	95	LYS	2.7
1	B	172	LEU	2.7
2	C	116	ASP	2.7
3	I	1161	GLY	2.7
5	X	328	GLU	2.7
2	H	265	LYS	2.7
2	H	331	LYS	2.7
1	G	86	LYS	2.7
2	C	909	LYS	2.7
3	I	830	ASP	2.7
5	X	240	ARG	2.7
2	H	1151	LEU	2.7
1	G	23	HIS	2.7
5	X	239	GLY	2.7
5	X	304	THR	2.7
2	C	304	GLU	2.6
5	X	236	LYS	2.6
2	H	1152	GLY	2.6
2	C	991	LYS	2.6
5	X	315	TRP	2.6
5	Y	477	GLU	2.6
1	G	18	GLN	2.6
2	H	974	ARG	2.6
3	I	831	VAL	2.6
1	A	241	GLU	2.6
3	I	80	HIS	2.6
2	C	250	THR	2.6
2	C	1001	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	414	ILE	2.6
3	D	834	PRO	2.6
2	C	908	GLU	2.6
1	G	194	GLN	2.6
3	I	1171	GLY	2.6
1	F	192	VAL	2.6
3	I	1169	THR	2.6
2	C	403	MET	2.6
1	G	148	ARG	2.6
2	C	854	ILE	2.6
5	X	422	ARG	2.6
2	H	105	TYR	2.6
3	I	217	LEU	2.6
2	H	254	ASP	2.5
3	D	1268	ASN	2.5
3	I	520	ALA	2.5
1	F	127	GLN	2.5
1	F	234	LEU	2.5
2	H	264	GLU	2.5
2	H	252	SER	2.5
3	I	1166	GLY	2.5
5	Y	306	PHE	2.5
3	I	1133	ASP	2.4
2	H	311	CYS	2.4
5	Y	600	HIS	2.4
2	H	1070	HIS	2.4
2	C	1263	ALA	2.4
1	B	147	GLN	2.4
1	G	195	ARG	2.4
3	D	390	LEU	2.4
5	X	319	ALA	2.4
1	B	92	VAL	2.4
3	I	1162	ILE	2.4
1	F	126	PRO	2.4
1	F	113	ALA	2.4
3	D	829	GLY	2.4
2	H	773	LEU	2.4
2	C	333	ILE	2.4
3	D	1376	GLY	2.4
2	H	1023	HIS	2.4
3	I	8	LEU	2.4
2	H	1009	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	176	CYS	2.3
3	I	832	LYS	2.3
5	X	424	GLY	2.3
2	C	910	ALA	2.3
2	H	169	LYS	2.3
2	H	103	VAL	2.3
3	I	1297	LYS	2.3
3	D	826	ILE	2.3
2	H	1005	GLU	2.3
3	I	874	GLU	2.3
1	B	168	ILE	2.3
2	H	1010	GLN	2.3
2	C	257	ALA	2.3
1	A	95	LYS	2.3
2	C	306	THR	2.3
3	I	314	ARG	2.3
2	H	1153	ALA	2.3
3	I	855	ASP	2.3
5	X	519	LEU	2.3
2	H	746	ALA	2.3
3	I	834	PRO	2.3
3	D	832	LYS	2.3
5	Y	488	LEU	2.3
2	C	982	GLY	2.3
2	H	253	PHE	2.3
3	I	563	LEU	2.3
1	A	4	SER	2.3
3	I	564	VAL	2.3
5	X	21	TYR	2.3
3	I	675	ALA	2.3
3	D	344	GLY	2.3
5	Y	154	GLU	2.3
2	H	269	ILE	2.2
3	D	207	GLU	2.2
5	X	33	GLU	2.2
2	H	1202	GLY	2.2
5	X	10	LYS	2.2
3	I	211	GLU	2.2
1	A	5	VAL	2.2
5	Y	293	GLU	2.2
2	H	745	GLU	2.2
2	H	980	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	1137	GLU	2.2
1	F	149	GLY	2.2
2	H	374	GLU	2.2
2	H	725	GLN	2.2
2	C	258	ASN	2.2
5	X	584	ARG	2.2
3	I	175	GLU	2.2
1	A	324	ALA	2.2
3	D	565	ALA	2.2
3	D	831	VAL	2.2
2	H	990	ASP	2.2
5	Y	214	PRO	2.2
1	G	24	ALA	2.2
2	C	66	SER	2.2
5	X	420	GLU	2.2
1	B	171	LEU	2.2
1	A	269	CYS	2.2
5	Y	317	ASN	2.2
5	X	310	GLU	2.2
2	C	332	ARG	2.2
1	F	191	ARG	2.2
5	X	213	ASP	2.2
2	C	270	THR	2.1
3	I	445	LYS	2.1
5	X	322	MET	2.1
3	I	709	ARG	2.1
5	Y	307	THR	2.1
3	I	1327	GLU	2.1
2	H	301	TYR	2.1
2	H	1155	VAL	2.1
1	F	112	ALA	2.1
3	I	876	SER	2.1
2	H	114	VAL	2.1
4	J	59	ILE	2.1
5	X	20	GLY	2.1
5	Y	511	ILE	2.1
1	F	97	GLU	2.1
2	H	782	VAL	2.1
2	C	597	GLY	2.1
3	D	1200	GLU	2.1
2	H	989	LEU	2.1
2	H	233	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	1138	VAL	2.1
2	C	645	PHE	2.1
1	B	54	CYS	2.0
2	H	1316	GLU	2.0
3	D	333	GLY	2.0
3	D	563	LEU	2.0
3	I	849	LEU	2.0
2	C	375	PRO	2.0
3	I	209	ASN	2.0
3	I	747	MET	2.0
5	X	333	VAL	2.0
5	Y	318	ALA	2.0
2	H	867	GLU	2.0
2	H	969	ALA	2.0
1	A	133	LEU	2.0
5	X	15	ARG	2.0
3	I	1215	GLU	2.0
1	B	94	GLY	2.0
3	I	746	LEU	2.0
5	Y	584	ARG	2.0
2	H	614	TYR	2.0
5	Y	322	MET	2.0
3	D	1202	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	I	1502	1/1	0.17	-0.38	49,49,49,49	0
6	ZN	D	1502	1/1	0.22	-0.66	8,8,8,8	0
6	ZN	I	1501	1/1	0.04	-1.58	60,60,60,60	0
6	ZN	D	1501	1/1	0.05	-1.71	54,54,54,54	0
7	0O2	D	1503	40/40	0.14	-1.77	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.