



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 17, 2017 – 05:26 AM EDT

PDB ID : 5JUY
EMDB ID: : EMD-8178
Title : Active human apoptosome with procaspase-9
Authors : Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.
Deposited on : unknown
Resolution : 4.10 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

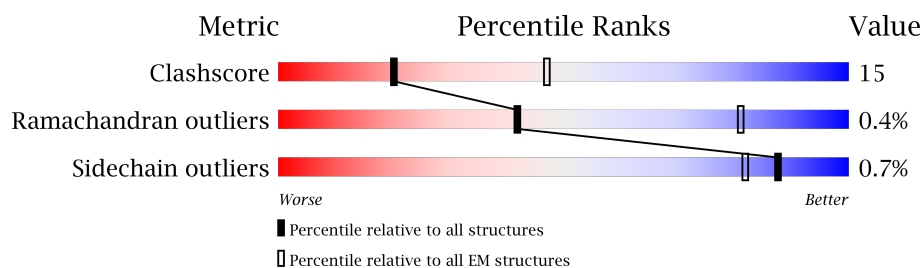
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1248	65% 26% 9%
1	B	1248	72% 26% ..
1	C	1248	65% 26% 9%
1	D	1248	72% 27% ..
1	E	1248	72% 27% ..
1	F	1248	65% 26% 9%
1	G	1248	72% 26% ..
2	H	104	57% 43%
2	I	104	56% 44%

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Mol	Chain	Length	Quality of chain
2	J	104	 58% 42%
2	K	104	 58% 42%
2	L	104	 58% 42%
2	M	104	 59% 41%
2	N	104	 60% 40%
3	O	95	 76% 20% .
3	P	95	 76% 19% 5%
3	Q	95	 77% 19% .
3	R	95	 77% 19% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 76058 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	B	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	C	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	D	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	E	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		
1	F	1139	Total	C	N	O	S	0	0
			9099	5764	1563	1711	61		
1	G	1234	Total	C	N	O	S	0	0
			9861	6243	1694	1857	67		

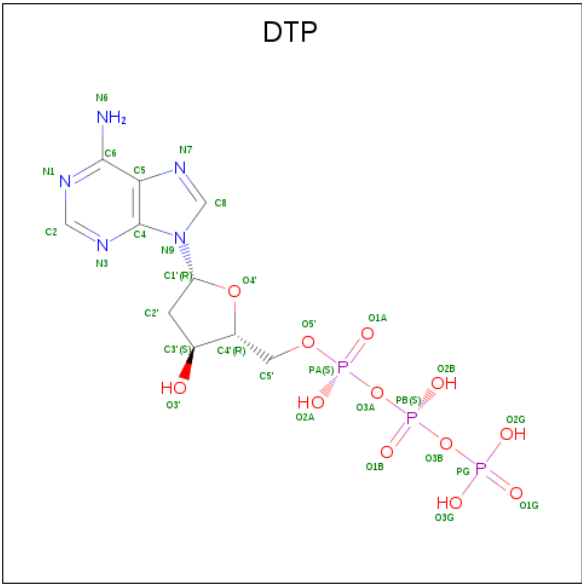
- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is a protein called Caspase-9.

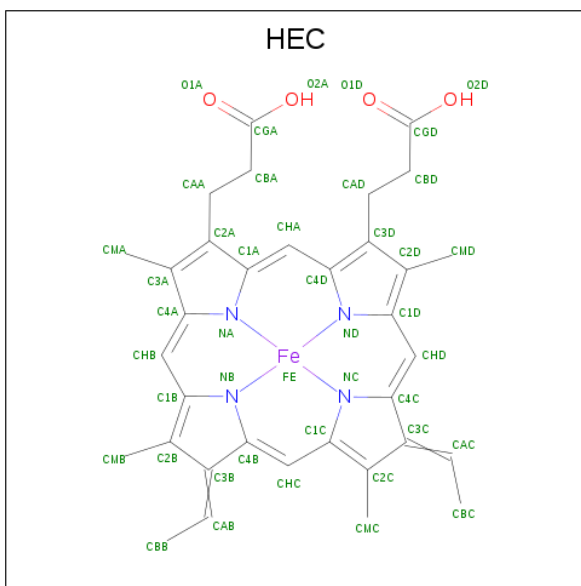
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	P	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	Q	95	Total	C	N	O	S	0	0
			777	475	152	145	5		
3	R	95	Total	C	N	O	S	0	0
			777	475	152	145	5		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	G	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



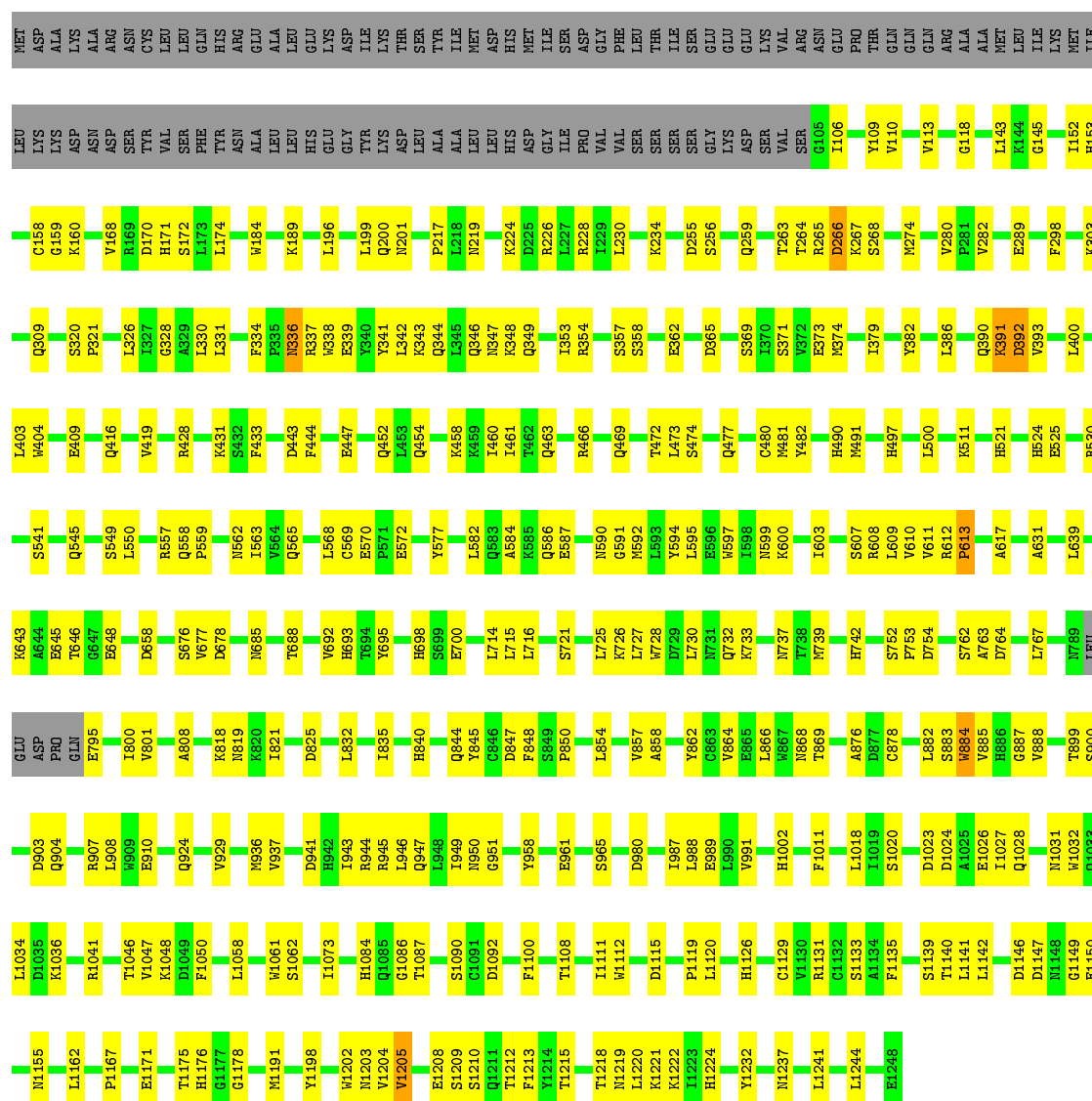
Mol	Chain	Residues	Atoms					AltConf
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	I	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	K	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

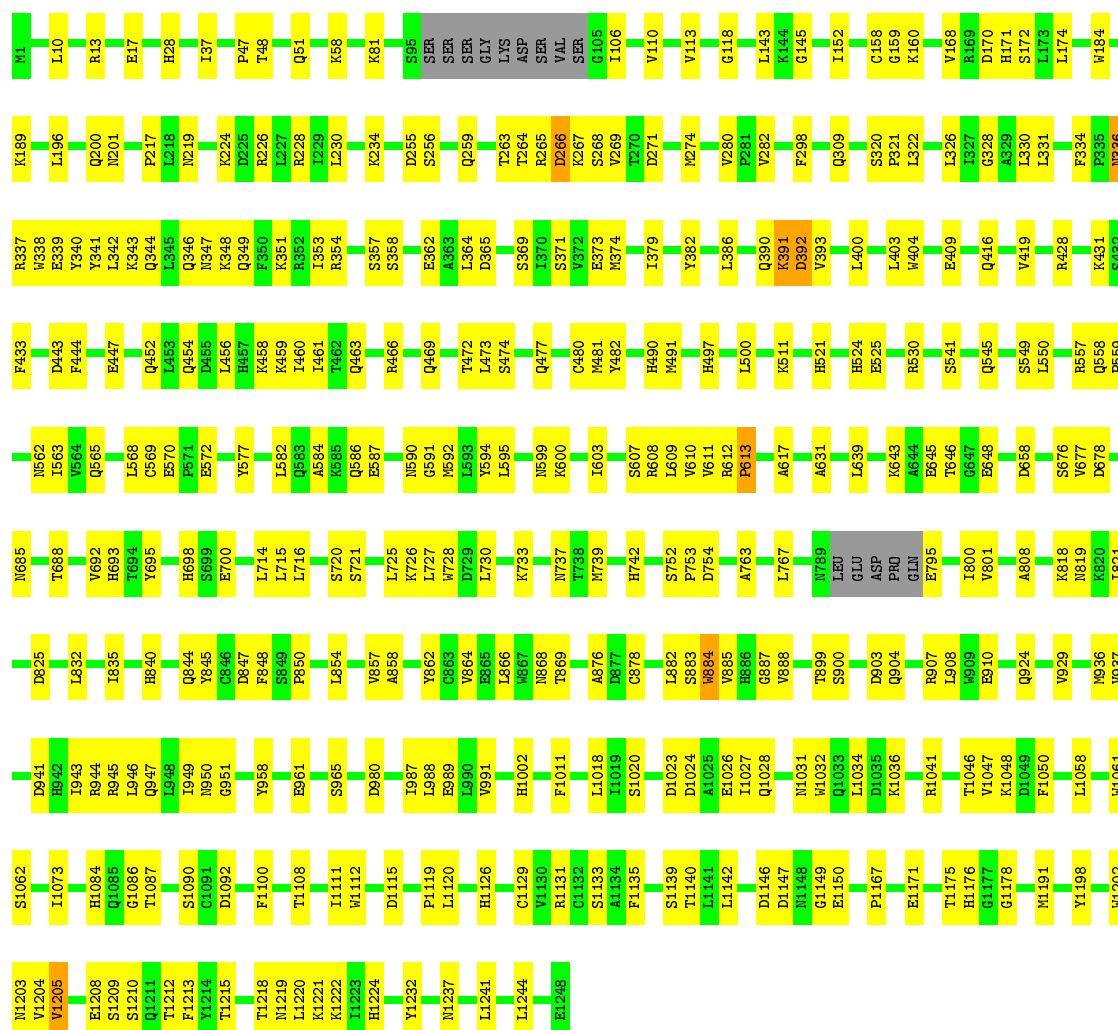
- Molecule 1: Apoptotic protease-activating factor 1

Chain A: 



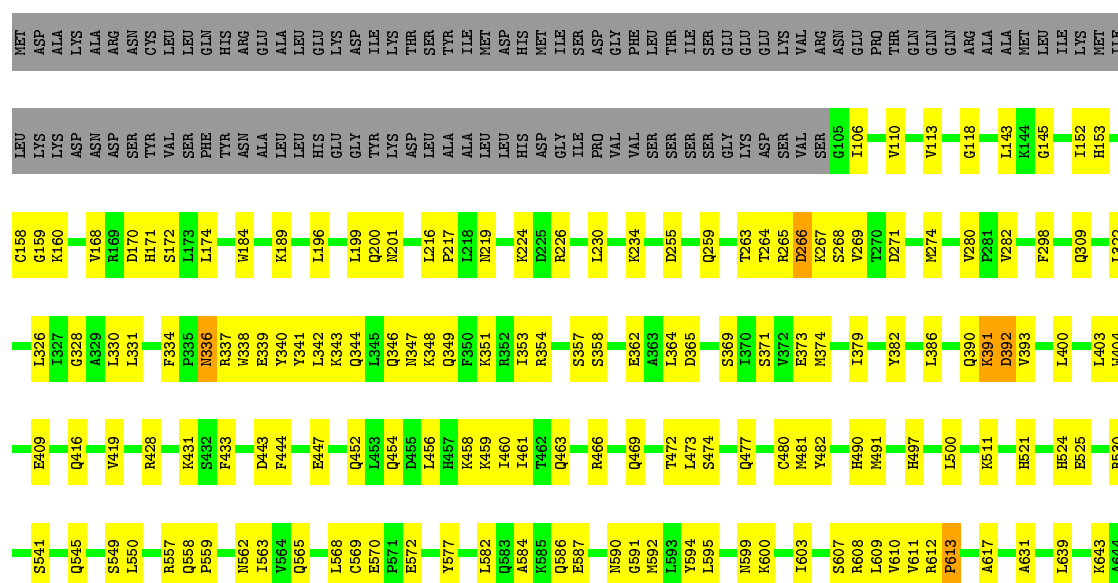
- Molecule 1: Apoptotic protease-activating factor 1

Chain B: 



• Molecule 1: Apoptotic protease-activating factor 1

Chain C: 65% 26% 9%



E645	T646	G647	E648	D658	S676	V677	D678	N685	T688	V692	H693	T694	Y695	H698	S699	E700	L714	L715	L716	S720	S721	L725	K726	L727	W728	D729	L730	K733	N737	L738	W739	H742	S752	P753	D754	S762	A763	D764	L767	L789	LEU	GLU	ASP	
PRU	GLN	E795	I800	R801	A808	K818	N819	K820	I821	D825	L832	H835	H840	Q844	N845	C846	D847	F848	S849	P850	L854	V857	A858	Y862	C863	V864	E865	L866	N867	N868	T869	A876	D877	C878	L882	S883	W884	W885	H886	G887	V888	T889	S900	D903
Q904	R907	L908	H909	E910	Q924	V929	M936	V937	D941	H942	I943	R944	R945	L946	L948	L949	N950	G951	Y958	E961	S965	D980	I987	L988	E989	L990	V991	H1002	F1011	L1018	I1019	S1020	D1023	D1024	A1025	E1026	I1027	Q1028	N1031	W1032	Q1033	L1034	D1035	
K1036	R1041	T1046	V1047	K1048	D1049	F1050	L1058	W1061	S1062	I1073	H1084	Q1085	G1086	T1087	S1090	C1091	D1092	F1100	T1108	I1111	W1112	D1115	P1119	L1120	H1126	C1129	V1130	R1131	C1132	S1133	A1134	F1135	S1139	T1140	L1141	L1142	D1146	W1148	G1149	E1150	N1155			
P1167	E1171	T1175	H1176	G1177	G1178	M1191	Y1198	W1202	N1203	V1204	E1208	S1209	Q1210	Q1211	T1212	F1213	Y1214	T1215	T1218	N1219	K1221	K1222	H1224	Y1232	N1237	L1241	L1244	E1246																

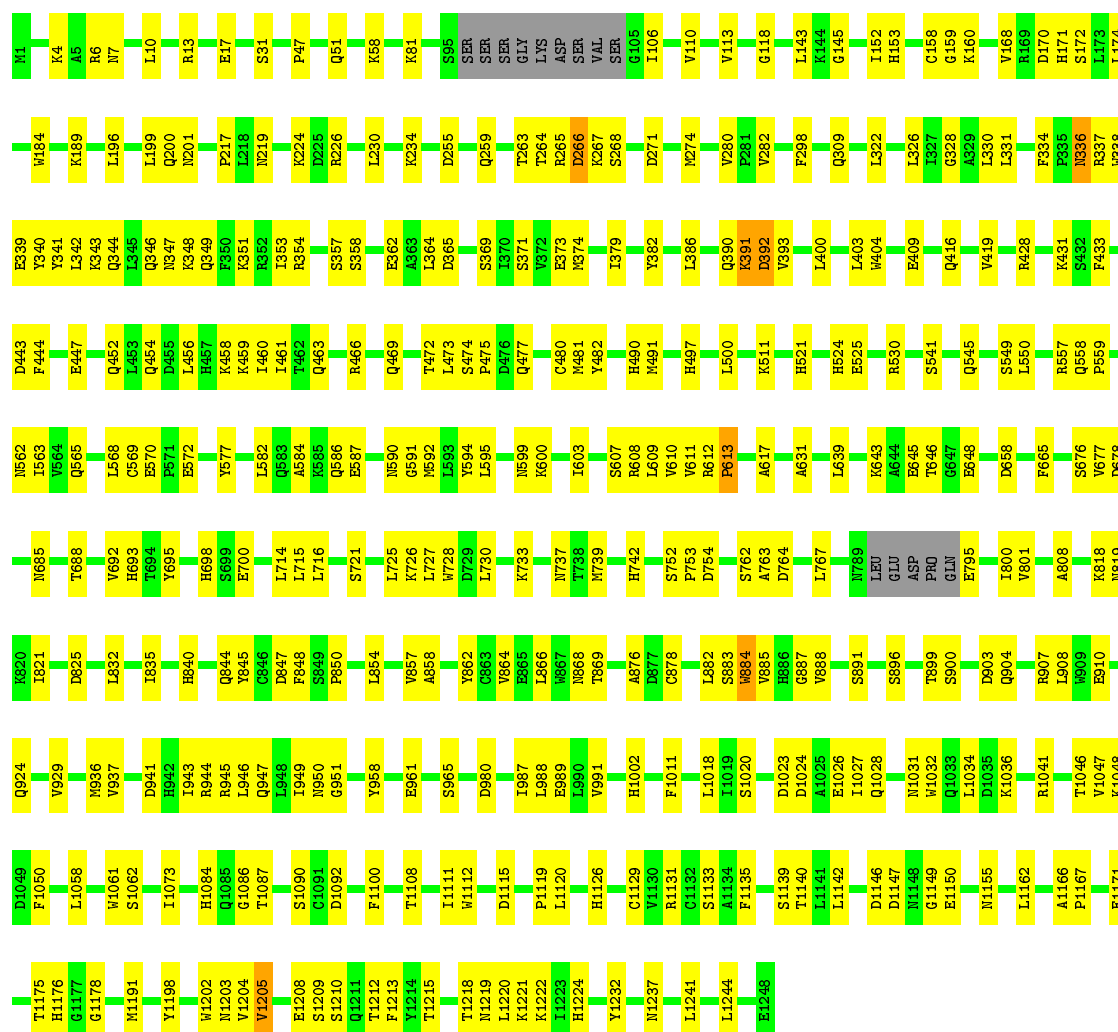
• Molecule 1: Apoptotic protease-activating factor 1

Chain D:  72% 27% **

Y1198	S1062	D941	D825	T688	Q565	E447	E339	L174	M1
W1202	I1073	H942	V692	V692	L568	Q452	Y340	W184	L10
N1203	N1073	I943	L832	H693	C569	L453	Y341	W184	L10
V1204	H1084	R944	L832	T694	E570	Q454	K343	K189	R13
V1205	Q1085	R945	I835	V695	P571	D455	Q344	K189	E14
E1208	T1087	L946	H840	H698	E572	L456	L345	L196	E17
S1209	L948	Q947	H840	S699	Y577	H457	Q346	L199	E17
S1210	L948	Q947	H840	S699	Y577	H457	Q346	L199	E17
S1210	L948	Q947	H840	S699	Y577	H457	Q346	L199	E17
S1210	L948	Q947	H840	S699	Y577	H457	Q346	L199	E17
Q1211	C1091	N950	Y845	E700	L582	K458	N347	Q200	I30
D1092	D1092	G951	C846	L714	Q583	T462	Q349	N201	S31
F1100	F1100	Y958	D847	L715	A584	Q463	Q354	L216	I37
T1108	T1108	E961	F848	L716	K585	Q463	R354	P217	M45
T1218	T1218	E961	S849	L716	Q586	Q466	N219	L218	E46
N1219	I1111	S965	P850	S720	E587	R466	S357	N219	P47
K1221	W1112	S965	L854	S721	N590	Q469	S358	K224	P47
K1222	D1115	D980	V857	L725	G591	Q469	E362	K224	Q51
I1223	D1115	D980	A858	L726	M592	T472	R226	R226	Q51
H1224	P1119	L987	W728	L727	L593	L473	D365	R226	K58
	L1120	L988	Y862	W728	Y594	S474	L230	L230	K31
		E989	C863	D729	L595	P475	S369	K234	K31
Y1232	H1126	L990	V864	L730	E596	P476	I370	K234	S95
		V991	E865	K733	H597	Q477	S371	D255	SER
N1237	C1129	H1002	L866	N737	I598	C480	V372	D255	SER
L1241	W1130	F1011	N867	W738	K600	N481	N374	Q259	SER
L1244	C1132	R1131	N868	T739	I603	Y482	I379	T263	GLY
E1246	A1134	L1018	A876	H742	S607	H490	Y382	T264	LVS
	F1135	I1019	D877	H742	R608	N491	R265	R264	ASP
		S1020	C878	S752	L609	H497	D266	K267	SER
				P763	V610	L500	L386	S268	VAL
				D754	R612	L500	Q390	S268	G105
				S762	P613	R511	K391	D271	I106
				A763	P613	R511	D392	M274	V110
				D764	A617	H521	V393		V113
							L400	V280	V113
							L400	F281	G118
							L403	V282	G118
							W404		L143
							F298		K144
							E409		G145
							Q416		G145
							V419		I152
							R428		H153
							L327		C158
							A329		G159
							L330		K160
							L331		
							K431		
							F432		V168
							S432		R169
							D443		D170
							N336		H171
							R337		S172
							F444		L173
							I563		
							V564		
					</				

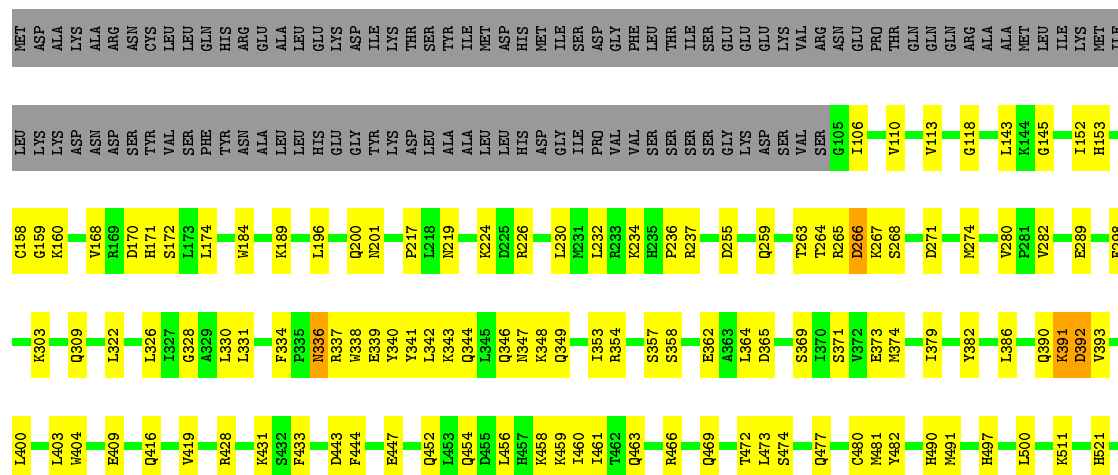
• Molecule 1: Apoptotic protease-activating factor 1

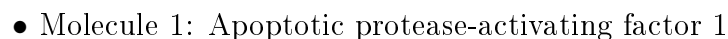
Chain E:  72% 27% ..



• Molecule 1: Apoptotic protease-activating factor 1

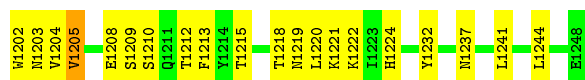
Chain F:  65% 26% 9%





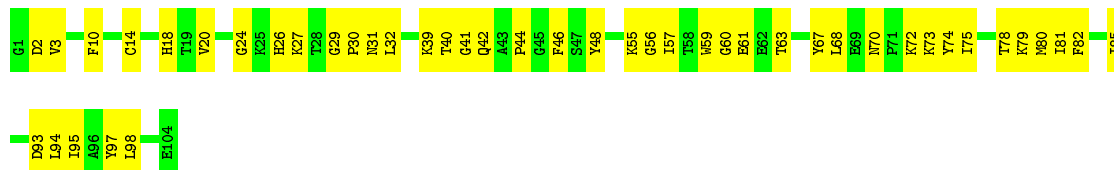
Opinion	Percentage
Doing a good job	72%
Doing a bad job	26%





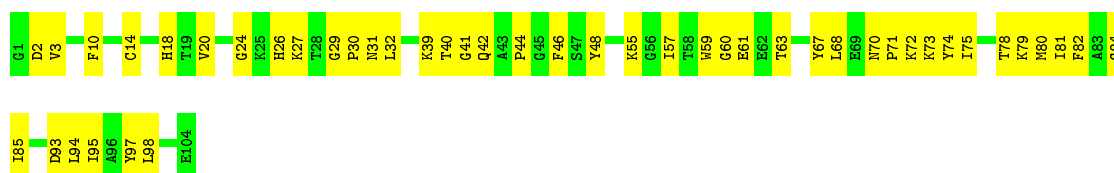
• Molecule 2: Cytochrome c

Chain H: 57% 43%



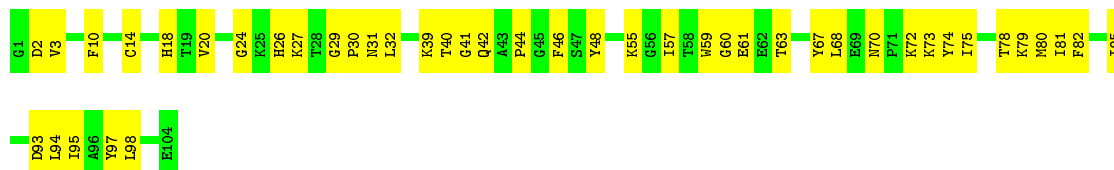
• Molecule 2: Cytochrome c

Chain I: 56% 44%



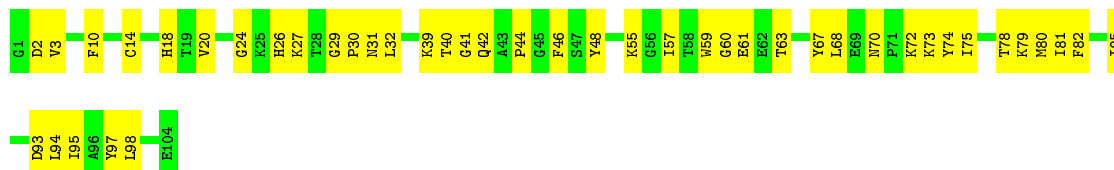
• Molecule 2: Cytochrome c

Chain J: 58% 42%



• Molecule 2: Cytochrome c

Chain K: 58% 42%



• Molecule 2: Cytochrome c

Chain L: 58% 42%





• Molecule 2: Cytochrome c

Chain M: 59% 41%



• Molecule 2: Cytochrome c

Chain N: 60% 40%



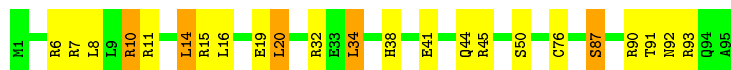
• Molecule 3: Caspase-9

Chain O: 76% 20% .



• Molecule 3: Caspase-9

Chain P: 76% 19% 5%



• Molecule 3: Caspase-9

Chain Q: 77% 19% .



• Molecule 3: Caspase-9

Chain R: 77% 19% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	92867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2	RMSZ	# Z >2
1	A	0.33	1/9295 (0.0%)	0.46	0/12575
1	B	0.37	1/10068 (0.0%)	0.47	0/13613
1	C	0.33	1/9295 (0.0%)	0.46	0/12575
1	D	0.36	1/10068 (0.0%)	0.47	0/13613
1	E	0.36	1/10068 (0.0%)	0.47	0/13613
1	F	0.33	1/9295 (0.0%)	0.47	0/12575
1	G	0.37	1/10068 (0.0%)	0.47	0/13613
2	H	0.25	0/830	0.42	0/1105
2	I	0.25	0/830	0.42	0/1105
2	J	0.25	0/830	0.42	0/1105
2	K	0.25	0/830	0.42	0/1105
2	L	0.25	0/830	0.42	0/1105
2	M	0.25	0/830	0.42	0/1105
2	N	0.25	0/830	0.42	0/1105
3	O	0.60	0/784	0.61	0/1051
3	P	0.60	0/784	0.61	0/1051
3	Q	0.60	0/784	0.61	0/1051
3	R	0.60	0/784	0.61	0/1051
All	All	0.36	7/77103 (0.0%)	0.47	0/104116

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	168	VAL	C-N	6.96	1.50	1.34
1	B	168	VAL	C-N	6.94	1.50	1.34
1	A	168	VAL	C-N	6.94	1.50	1.34
1	E	168	VAL	C-N	6.94	1.50	1.34
1	D	168	VAL	C-N	6.93	1.50	1.34
1	G	168	VAL	C-N	6.91	1.50	1.34
1	C	168	VAL	C-N	6.91	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASN	Peptide
1	B	336	ASN	Peptide
1	C	336	ASN	Peptide
1	D	336	ASN	Peptide
1	E	336	ASN	Peptide
1	F	336	ASN	Peptide
1	G	336	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9099	0	8967	296	0
1	B	9861	0	9736	300	0
1	C	9099	0	8968	293	0
1	D	9861	0	9736	310	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	9861	0	9736	313	0
1	F	9099	0	8968	300	0
1	G	9861	0	9736	300	0
2	H	814	0	833	59	0
2	I	814	0	833	58	0
2	J	814	0	833	59	0
2	K	814	0	833	57	0
2	L	814	0	833	58	0
2	M	814	0	833	59	0
2	N	814	0	833	56	0
3	O	777	0	787	21	0
3	P	777	0	787	28	0
3	Q	777	0	786	39	0
3	R	777	0	787	29	0
4	A	30	0	9	3	0
4	B	30	0	9	3	0
4	C	30	0	9	3	0
4	D	30	0	9	3	0
4	E	30	0	9	3	0
4	F	30	0	9	3	0
4	G	30	0	9	3	0
5	H	43	0	32	4	0
5	I	43	0	32	4	0
5	J	43	0	32	4	0
5	K	43	0	32	4	0
5	L	43	0	32	4	0
5	M	43	0	32	4	0
5	N	43	0	32	4	0
All	All	76058	0	75112	2327	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:HD3	3:R:38:HIS:CE1	1.20	1.66
3:Q:52:ARG:CD	3:R:38:HIS:CE1	2.01	1.40
1:E:884:TRP:CH2	2:L:79:LYS:HA	1.68	1.28
1:D:884:TRP:CH2	2:K:79:LYS:HA	1.68	1.28
1:G:884:TRP:CH2	2:N:79:LYS:HA	1.68	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:TRP:CH2	2:H:79:LYS:HA	1.68	1.27
1:E:7:ASN:HB2	1:F:236:PRO:CG	1.63	1.26
1:C:884:TRP:CH2	2:J:79:LYS:HA	1.68	1.26
1:F:884:TRP:CH2	2:M:79:LYS:HA	1.68	1.26
1:B:884:TRP:CH2	2:I:79:LYS:HA	1.68	1.26
1:C:884:TRP:CZ3	2:J:79:LYS:HD2	1.74	1.22
1:B:884:TRP:CZ3	2:I:79:LYS:HD2	1.74	1.22
1:D:884:TRP:CZ3	2:K:79:LYS:HD2	1.74	1.21
1:E:884:TRP:CZ3	2:L:79:LYS:HD2	1.74	1.21
1:A:884:TRP:CZ3	2:H:79:LYS:HD2	1.74	1.21
1:F:884:TRP:CZ3	2:M:79:LYS:HD2	1.74	1.21
1:G:884:TRP:CZ3	2:N:79:LYS:HD2	1.74	1.21
1:B:884:TRP:CZ3	2:I:79:LYS:HA	1.82	1.15
1:A:884:TRP:CZ3	2:H:79:LYS:HA	1.82	1.15
1:C:884:TRP:CZ3	2:J:79:LYS:HA	1.82	1.15
1:G:884:TRP:CZ3	2:N:79:LYS:HA	1.81	1.14
1:D:884:TRP:CZ3	2:K:79:LYS:HA	1.82	1.14
1:E:884:TRP:CZ3	2:L:79:LYS:HA	1.82	1.14
1:F:884:TRP:CZ3	2:M:79:LYS:HA	1.82	1.13
1:E:7:ASN:HB2	1:F:236:PRO:HG3	1.28	1.10
1:G:1086:GLY:HA2	2:N:39:LYS:HZ1	1.22	1.04
1:E:7:ASN:HB2	1:F:236:PRO:HG2	1.36	1.01
1:G:569:CYS:SG	1:G:1213:PHE:HE1	1.85	0.99
1:A:565:GLN:NE2	1:A:1213:PHE:H	1.60	0.99
1:F:569:CYS:SG	1:F:1213:PHE:CE1	2.56	0.99
1:B:569:CYS:SG	1:B:600:LYS:NZ	2.36	0.99
1:C:565:GLN:NE2	1:C:1213:PHE:H	1.60	0.99
1:G:569:CYS:SG	1:G:1213:PHE:CE1	2.56	0.99
1:D:569:CYS:SG	1:D:1213:PHE:HE1	1.85	0.99
1:E:569:CYS:SG	1:E:600:LYS:NZ	2.36	0.99
1:F:569:CYS:SG	1:F:600:LYS:NZ	2.36	0.99
1:B:569:CYS:SG	1:B:1213:PHE:CE1	2.56	0.99
1:B:569:CYS:SG	1:B:1213:PHE:HE1	1.85	0.99
1:C:569:CYS:SG	1:C:1213:PHE:CE1	2.56	0.99
1:C:569:CYS:SG	1:C:1213:PHE:HE1	1.85	0.99
1:C:569:CYS:SG	1:C:600:LYS:NZ	2.36	0.99
1:E:569:CYS:SG	1:E:1213:PHE:CE1	2.56	0.99
1:G:569:CYS:SG	1:G:600:LYS:NZ	2.36	0.99
1:A:569:CYS:SG	1:A:1213:PHE:CE1	2.56	0.99
1:B:565:GLN:NE2	1:B:1213:PHE:H	1.60	0.99
1:F:569:CYS:SG	1:F:1213:PHE:HE1	1.85	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:569:CYS:SG	1:E:1213:PHE:HE1	1.85	0.98
1:G:565:GLN:NE2	1:G:1213:PHE:H	1.60	0.98
1:G:884:TRP:HH2	2:N:79:LYS:HA	1.28	0.98
1:D:569:CYS:SG	1:D:1213:PHE:CE1	2.56	0.98
1:A:569:CYS:SG	1:A:1213:PHE:HE1	1.85	0.98
1:A:569:CYS:SG	1:A:600:LYS:NZ	2.36	0.98
1:E:565:GLN:NE2	1:E:1213:PHE:H	1.60	0.97
1:D:569:CYS:SG	1:D:600:LYS:NZ	2.36	0.97
1:F:565:GLN:NE2	1:F:1213:PHE:H	1.60	0.97
1:A:109:TYR:HE1	1:G:4:LYS:NZ	1.34	0.97
1:A:884:TRP:HH2	2:H:79:LYS:HA	1.28	0.97
1:D:565:GLN:NE2	1:D:1213:PHE:H	1.60	0.97
3:O:52:ARG:CB	3:P:38:HIS:CE1	2.48	0.96
3:Q:52:ARG:HD3	3:R:38:HIS:ND1	1.79	0.96
1:E:884:TRP:HH2	2:L:79:LYS:HA	1.28	0.95
1:E:565:GLN:CD	1:E:1213:PHE:H	1.71	0.94
1:F:565:GLN:CD	1:F:1213:PHE:H	1.71	0.94
1:D:565:GLN:CD	1:D:1213:PHE:H	1.71	0.94
1:G:565:GLN:CD	1:G:1213:PHE:H	1.71	0.94
1:E:7:ASN:CB	1:F:236:PRO:HG2	1.97	0.94
1:C:565:GLN:CD	1:C:1213:PHE:H	1.71	0.93
1:D:884:TRP:HH2	2:K:79:LYS:HA	1.28	0.93
1:A:565:GLN:CD	1:A:1213:PHE:H	1.71	0.93
1:C:884:TRP:HH2	2:J:79:LYS:HA	1.28	0.93
1:B:565:GLN:CD	1:B:1213:PHE:H	1.71	0.93
1:B:1086:GLY:HA2	2:I:39:LYS:HZ1	1.30	0.93
1:D:30:ILE:CG2	3:Q:10:ARG:HB3	1.97	0.93
1:F:884:TRP:HH2	2:M:79:LYS:HA	1.28	0.93
1:C:1086:GLY:HA2	2:J:39:LYS:HZ1	1.34	0.93
1:F:1086:GLY:HA2	2:M:39:LYS:HZ1	1.30	0.93
1:E:550:LEU:CD2	1:E:607:SER:HB2	2.00	0.92
1:E:7:ASN:CB	1:F:236:PRO:CG	2.46	0.92
1:G:550:LEU:CD2	1:G:607:SER:HB2	2.00	0.92
1:B:884:TRP:HH2	2:I:79:LYS:HA	1.28	0.92
1:B:550:LEU:CD2	1:B:607:SER:HB2	2.00	0.92
1:F:550:LEU:CD2	1:F:607:SER:HB2	2.00	0.92
1:D:1086:GLY:HA2	2:K:39:LYS:HZ1	1.32	0.92
1:A:550:LEU:CD2	1:A:607:SER:HB2	2.00	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:HZ1	1.32	0.91
1:D:524:HIS:HB2	1:D:646:THR:HG21	1.52	0.91
1:C:1086:GLY:HA2	2:J:39:LYS:NZ	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:LEU:CD2	1:C:607:SER:HB2	2.00	0.91
1:B:1086:GLY:HA2	2:I:39:LYS:NZ	1.86	0.91
1:C:524:HIS:HB2	1:C:646:THR:HG21	1.52	0.91
1:D:1086:GLY:HA2	2:K:39:LYS:NZ	1.85	0.91
1:A:1086:GLY:HA2	2:H:39:LYS:NZ	1.86	0.90
3:O:52:ARG:HB2	3:P:38:HIS:CE1	2.06	0.90
1:E:524:HIS:HB2	1:E:646:THR:HG21	1.52	0.90
1:D:550:LEU:CD2	1:D:607:SER:HB2	2.00	0.90
3:O:52:ARG:HB3	3:P:38:HIS:CE1	2.07	0.90
1:B:524:HIS:HB2	1:B:646:THR:HG21	1.52	0.90
1:E:1086:GLY:HA2	2:L:39:LYS:NZ	1.85	0.90
1:G:1086:GLY:HA2	2:N:39:LYS:NZ	1.85	0.90
1:G:524:HIS:HB2	1:G:646:THR:HG21	1.52	0.89
1:F:1086:GLY:HA2	2:M:39:LYS:NZ	1.85	0.89
1:A:524:HIS:HB2	1:A:646:THR:HG21	1.52	0.89
1:F:524:HIS:HB2	1:F:646:THR:HG21	1.52	0.88
1:F:884:TRP:CZ3	2:M:79:LYS:CD	2.57	0.88
1:B:884:TRP:CZ3	2:I:79:LYS:CD	2.57	0.88
1:A:884:TRP:CZ3	2:H:79:LYS:CD	2.57	0.88
1:E:884:TRP:CZ3	2:L:79:LYS:CD	2.57	0.88
1:C:884:TRP:CZ3	2:J:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:NZ	2.04	0.87
1:D:884:TRP:CZ3	2:K:79:LYS:CD	2.57	0.87
1:A:109:TYR:CE1	1:G:4:LYS:HD2	2.11	0.86
3:Q:52:ARG:CD	3:R:38:HIS:HE1	1.89	0.86
3:Q:52:ARG:CB	3:R:38:HIS:HE1	1.88	0.86
3:P:50:SER:CB	3:Q:45:ARG:HH12	1.89	0.85
1:A:884:TRP:CH2	2:H:79:LYS:CA	2.59	0.85
3:Q:52:ARG:HD3	3:R:38:HIS:NE2	1.88	0.85
1:B:884:TRP:CH2	2:I:79:LYS:CA	2.59	0.85
1:E:885:VAL:HG11	1:E:888:VAL:HG13	1.59	0.85
1:G:885:VAL:HG11	1:G:888:VAL:HG13	1.59	0.85
1:G:884:TRP:CH2	2:N:79:LYS:CA	2.59	0.85
1:G:884:TRP:CZ3	2:N:79:LYS:CD	2.57	0.85
1:E:1086:GLY:HA2	2:L:39:LYS:HZ1	1.41	0.85
1:A:885:VAL:HG11	1:A:888:VAL:HG13	1.59	0.85
1:D:885:VAL:HG11	1:D:888:VAL:HG13	1.59	0.85
1:F:885:VAL:HG11	1:F:888:VAL:HG13	1.59	0.85
1:B:882:LEU:HB2	1:B:903:ASP:HB3	1.59	0.84
1:A:882:LEU:HB2	1:A:903:ASP:HB3	1.59	0.84
1:B:885:VAL:HG11	1:B:888:VAL:HG13	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TRP:CH2	2:J:79:LYS:CA	2.58	0.84
1:G:550:LEU:HD21	1:G:607:SER:HB2	1.60	0.84
1:C:885:VAL:HG11	1:C:888:VAL:HG13	1.59	0.84
1:A:550:LEU:HD21	1:A:607:SER:HB2	1.60	0.83
1:F:884:TRP:CH2	2:M:79:LYS:CA	2.59	0.83
1:F:550:LEU:HD21	1:F:607:SER:HB2	1.60	0.83
1:G:882:LEU:HB2	1:G:903:ASP:HB3	1.59	0.83
1:C:882:LEU:HB2	1:C:903:ASP:HB3	1.59	0.83
1:F:565:GLN:NE2	1:F:1213:PHE:N	2.27	0.82
1:C:550:LEU:HD21	1:C:607:SER:HB2	1.60	0.82
1:E:550:LEU:HD21	1:E:607:SER:HB2	1.60	0.82
1:B:565:GLN:NE2	1:B:1213:PHE:N	2.27	0.82
1:E:565:GLN:NE2	1:E:1213:PHE:N	2.27	0.82
1:E:882:LEU:HB2	1:E:903:ASP:HB3	1.59	0.82
1:B:550:LEU:HD21	1:B:607:SER:HB2	1.60	0.82
1:D:550:LEU:HD21	1:D:607:SER:HB2	1.60	0.82
1:A:565:GLN:NE2	1:A:1213:PHE:N	2.27	0.82
1:C:565:GLN:NE2	1:C:1213:PHE:N	2.27	0.82
1:F:882:LEU:HB2	1:F:903:ASP:HB3	1.59	0.82
1:D:565:GLN:NE2	1:D:1213:PHE:N	2.27	0.81
1:D:884:TRP:CH2	2:K:79:LYS:CA	2.59	0.81
1:G:584:ALA:HA	1:G:594:TYR:CE2	2.16	0.81
1:G:565:GLN:NE2	1:G:1213:PHE:N	2.27	0.81
1:E:584:ALA:HA	1:E:594:TYR:CE2	2.16	0.81
1:D:882:LEU:HB2	1:D:903:ASP:HB3	1.59	0.81
1:D:584:ALA:HA	1:D:594:TYR:CE2	2.16	0.81
1:A:862:TYR:CA	1:A:884:TRP:HA	2.11	0.80
1:B:584:ALA:HA	1:B:594:TYR:CE2	2.16	0.80
1:F:584:ALA:HA	1:F:594:TYR:CE2	2.16	0.80
1:F:862:TYR:CA	1:F:884:TRP:HA	2.11	0.80
1:C:862:TYR:HA	1:C:884:TRP:HA	1.63	0.80
1:E:884:TRP:CH2	2:L:79:LYS:CA	2.59	0.80
1:E:862:TYR:CA	1:E:884:TRP:HA	2.11	0.80
1:A:584:ALA:HA	1:A:594:TYR:CE2	2.16	0.80
1:B:862:TYR:HA	1:B:884:TRP:HA	1.63	0.80
1:D:862:TYR:HA	1:D:884:TRP:HA	1.63	0.80
1:E:862:TYR:HA	1:E:884:TRP:HA	1.63	0.80
1:E:7:ASN:CB	1:F:236:PRO:HG3	2.11	0.80
1:A:862:TYR:HA	1:A:884:TRP:HA	1.63	0.80
3:Q:52:ARG:CD	3:R:38:HIS:ND1	2.40	0.80
1:D:862:TYR:CA	1:D:884:TRP:HA	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ARG:NH2	1:F:232:LEU:O	2.15	0.79
1:G:862:TYR:CA	1:G:884:TRP:HA	2.11	0.79
1:F:882:LEU:HD13	1:F:1176:HIS:NE2	1.98	0.79
1:F:862:TYR:HA	1:F:884:TRP:HA	1.64	0.79
3:O:15:ARG:CD	3:O:19:GLU:OE2	2.30	0.79
1:B:862:TYR:CA	1:B:884:TRP:HA	2.11	0.79
1:C:584:ALA:HA	1:C:594:TYR:CE2	2.16	0.79
1:E:1084:HIS:HE2	1:E:1108:THR:HG1	1.30	0.79
1:B:882:LEU:HD13	1:B:1176:HIS:NE2	1.98	0.79
1:G:862:TYR:HA	1:G:884:TRP:HA	1.63	0.79
3:Q:15:ARG:CD	3:Q:19:GLU:OE2	2.30	0.79
1:C:862:TYR:CA	1:C:884:TRP:HA	2.11	0.79
1:D:1084:HIS:HE2	1:D:1108:THR:HG1	1.31	0.79
3:P:15:ARG:CD	3:P:19:GLU:OE2	2.30	0.79
3:R:15:ARG:CD	3:R:19:GLU:OE2	2.30	0.79
1:D:882:LEU:HD13	1:D:1176:HIS:NE2	1.98	0.78
1:C:882:LEU:HD13	1:C:1176:HIS:NE2	1.98	0.78
1:A:882:LEU:HD13	1:A:1176:HIS:NE2	1.98	0.78
1:G:882:LEU:HD13	1:G:1176:HIS:NE2	1.98	0.78
1:E:882:LEU:HD13	1:E:1176:HIS:NE2	1.98	0.77
3:P:50:SER:HB2	3:Q:45:ARG:HH12	1.48	0.77
1:A:565:GLN:HE22	1:A:1213:PHE:H	1.33	0.77
1:E:349:GLN:HA	1:E:447:GLU:OE2	1.86	0.76
1:A:349:GLN:HA	1:A:447:GLU:OE2	1.85	0.76
1:B:884:TRP:HH2	2:I:79:LYS:CA	1.97	0.76
1:B:349:GLN:HA	1:B:447:GLU:OE2	1.85	0.76
1:F:884:TRP:HH2	2:M:79:LYS:CA	1.97	0.76
1:G:47:PRO:HG2	1:G:51:GLN:HE22	1.51	0.76
1:C:1084:HIS:HE2	1:C:1108:THR:HG1	1.33	0.76
1:G:1086:GLY:CA	2:N:39:LYS:HZ1	1.98	0.76
1:C:565:GLN:HE22	1:C:1213:PHE:H	1.33	0.76
1:G:884:TRP:HH2	2:N:79:LYS:CA	1.97	0.76
1:A:1084:HIS:HE2	1:A:1108:THR:HG1	1.31	0.76
1:F:349:GLN:HA	1:F:447:GLU:OE2	1.85	0.76
1:E:47:PRO:HG2	1:E:51:GLN:HE22	1.51	0.76
1:B:565:GLN:HE22	1:B:1213:PHE:H	1.33	0.75
1:D:349:GLN:HA	1:D:447:GLU:OE2	1.85	0.75
1:E:7:ASN:CG	1:F:236:PRO:HG2	2.06	0.75
1:C:1112:TRP:HB3	1:C:1119:PRO:HA	1.68	0.75
1:A:882:LEU:CD1	1:A:1176:HIS:NE2	2.50	0.75
1:F:1084:HIS:HE2	1:F:1108:THR:HG1	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:7:ARG:O	3:Q:11:ARG:HG3	1.87	0.75
1:A:557:ARG:NH2	1:A:1175:THR:HG23	2.02	0.75
1:E:882:LEU:CD1	1:E:1176:HIS:NE2	2.50	0.75
1:G:882:LEU:CD1	1:G:1176:HIS:NE2	2.50	0.75
1:B:47:PRO:HG2	1:B:51:GLN:HE22	1.51	0.75
1:B:557:ARG:NH2	1:B:1175:THR:HG23	2.01	0.75
1:E:884:TRP:HH2	2:L:79:LYS:CA	1.97	0.75
1:C:349:GLN:HA	1:C:447:GLU:OE2	1.85	0.75
1:D:1112:TRP:HB3	1:D:1119:PRO:HA	1.68	0.75
3:R:7:ARG:O	3:R:11:ARG:HG3	1.87	0.75
1:B:882:LEU:CD1	1:B:1176:HIS:NE2	2.50	0.75
1:F:882:LEU:CD1	1:F:1176:HIS:NE2	2.50	0.75
2:N:24:GLY:O	2:N:31:ASN:ND2	2.20	0.75
1:E:1112:TRP:HB3	1:E:1119:PRO:HA	1.68	0.75
1:F:1112:TRP:HB3	1:F:1119:PRO:HA	1.68	0.74
1:G:565:GLN:HE22	1:G:1213:PHE:H	1.33	0.74
2:H:24:GLY:O	2:H:31:ASN:ND2	2.20	0.74
1:D:309:GLN:NE2	1:D:339:GLU:OE1	2.21	0.74
1:E:309:GLN:NE2	1:E:339:GLU:OE1	2.21	0.74
1:F:557:ARG:NH2	1:F:1175:THR:HG23	2.01	0.74
1:G:557:ARG:NH2	1:G:1175:THR:HG23	2.01	0.74
1:G:349:GLN:HA	1:G:447:GLU:OE2	1.85	0.74
1:B:884:TRP:HZ3	2:I:79:LYS:HD2	1.51	0.74
3:P:7:ARG:O	3:P:11:ARG:HG3	1.87	0.74
1:B:339:GLU:OE2	1:B:343:LYS:NZ	2.20	0.74
1:F:941:ASP:H	1:F:946:LEU:HA	1.53	0.74
1:A:884:TRP:HH2	2:H:79:LYS:CA	1.97	0.74
1:C:309:GLN:NE2	1:C:339:GLU:OE1	2.21	0.74
1:D:882:LEU:CD1	1:D:1176:HIS:NE2	2.50	0.74
1:F:309:GLN:NE2	1:F:339:GLU:OE1	2.21	0.74
1:A:1112:TRP:HB3	1:A:1119:PRO:HA	1.68	0.74
1:C:339:GLU:OE2	1:C:343:LYS:NZ	2.20	0.74
2:L:24:GLY:O	2:L:31:ASN:ND2	2.20	0.74
1:C:557:ARG:NH2	1:C:1175:THR:HG23	2.01	0.74
1:C:882:LEU:CD1	1:C:1176:HIS:NE2	2.50	0.74
1:D:47:PRO:HG2	1:D:51:GLN:HE22	1.51	0.74
1:D:557:ARG:NH2	1:D:1175:THR:HG23	2.01	0.74
1:D:941:ASP:H	1:D:946:LEU:HA	1.53	0.74
1:F:565:GLN:HE22	1:F:1213:PHE:H	1.33	0.74
1:A:274:MET:HE3	1:G:358:SER:HB3	1.70	0.74
2:I:24:GLY:O	2:I:31:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TRP:HH2	2:J:79:LYS:CA	1.97	0.74
1:C:941:ASP:H	1:C:946:LEU:HA	1.53	0.74
1:E:565:GLN:HE22	1:E:1213:PHE:H	1.33	0.74
1:G:1112:TRP:HB3	1:G:1119:PRO:HA	1.68	0.74
2:K:24:GLY:O	2:K:31:ASN:ND2	2.20	0.74
1:E:884:TRP:HZ3	2:L:79:LYS:HD2	1.51	0.74
2:M:24:GLY:O	2:M:31:ASN:ND2	2.20	0.74
3:Q:52:ARG:HD2	3:R:38:HIS:CE1	2.17	0.74
1:B:1112:TRP:HB3	1:B:1119:PRO:HA	1.68	0.74
1:A:274:MET:CE	1:G:358:SER:HB3	2.17	0.74
1:D:339:GLU:OE2	1:D:343:LYS:NZ	2.20	0.73
1:G:941:ASP:H	1:G:946:LEU:HA	1.53	0.73
3:O:7:ARG:O	3:O:11:ARG:HG3	1.87	0.73
1:D:884:TRP:HH2	2:K:79:LYS:CA	1.97	0.73
1:E:557:ARG:NH2	1:E:1175:THR:HG23	2.01	0.73
2:J:24:GLY:O	2:J:31:ASN:ND2	2.20	0.73
1:A:309:GLN:NE2	1:A:339:GLU:OE1	2.21	0.73
1:C:358:SER:HB3	1:D:274:MET:HE3	1.71	0.73
1:B:309:GLN:NE2	1:B:339:GLU:OE1	2.21	0.73
1:C:884:TRP:HZ3	2:J:79:LYS:HD2	1.51	0.73
1:E:339:GLU:OE2	1:E:343:LYS:NZ	2.20	0.73
1:G:309:GLN:NE2	1:G:339:GLU:OE1	2.21	0.73
3:Q:52:ARG:CB	3:R:38:HIS:CE1	2.72	0.73
1:A:339:GLU:OE2	1:A:343:LYS:NZ	2.20	0.73
1:D:884:TRP:HZ3	2:K:79:LYS:HD2	1.52	0.73
3:R:87:SER:O	3:R:91:THR:HG23	1.89	0.73
1:B:1084:HIS:HE2	1:B:1108:THR:HG1	1.34	0.73
3:Q:87:SER:O	3:Q:91:THR:HG23	1.89	0.72
1:E:941:ASP:H	1:E:946:LEU:HA	1.53	0.72
1:G:339:GLU:OE2	1:G:343:LYS:NZ	2.20	0.72
1:A:941:ASP:H	1:A:946:LEU:HA	1.53	0.72
1:C:358:SER:HB3	1:D:274:MET:CE	2.19	0.72
1:B:941:ASP:H	1:B:946:LEU:HA	1.53	0.72
3:P:87:SER:O	3:P:91:THR:HG23	1.89	0.72
1:B:609:LEU:HB3	1:B:908:LEU:HB2	1.71	0.72
1:C:609:LEU:HB3	1:C:908:LEU:HB2	1.71	0.72
1:D:565:GLN:HE22	1:D:1213:PHE:H	1.33	0.72
2:K:26:HIS:NE2	2:K:44:PRO:O	2.23	0.72
1:B:882:LEU:HB2	1:B:903:ASP:CB	2.20	0.71
1:F:339:GLU:OE2	1:F:343:LYS:NZ	2.20	0.71
1:G:882:LEU:HB2	1:G:903:ASP:CB	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1084:HIS:HE2	1:G:1108:THR:HG1	1.35	0.71
2:I:26:HIS:NE2	2:I:44:PRO:O	2.23	0.71
1:D:609:LEU:HB3	1:D:908:LEU:HB2	1.71	0.71
2:H:26:HIS:NE2	2:H:44:PRO:O	2.23	0.71
2:J:26:HIS:NE2	2:J:44:PRO:O	2.23	0.71
2:L:26:HIS:NE2	2:L:44:PRO:O	2.23	0.71
1:D:1034:LEU:HB3	1:D:1036:LYS:HD3	1.73	0.71
1:E:609:LEU:HB3	1:E:908:LEU:HB2	1.71	0.71
3:O:87:SER:O	3:O:91:THR:HG23	1.89	0.71
1:C:1034:LEU:HB3	1:C:1036:LYS:HD3	1.73	0.71
1:D:358:SER:HB3	1:E:274:MET:CE	2.19	0.71
2:M:26:HIS:NE2	2:M:44:PRO:O	2.23	0.71
1:A:609:LEU:HB3	1:A:908:LEU:HB2	1.71	0.71
1:G:565:GLN:HE22	1:G:1213:PHE:N	1.89	0.71
1:A:1034:LEU:HB3	1:A:1036:LYS:HD3	1.73	0.71
1:G:549:SER:O	1:G:610:VAL:HB	1.91	0.71
1:D:30:ILE:HG23	3:Q:10:ARG:HB3	1.73	0.71
1:A:549:SER:O	1:A:610:VAL:HB	1.91	0.71
1:D:882:LEU:HB2	1:D:903:ASP:CB	2.20	0.71
1:E:549:SER:O	1:E:610:VAL:HB	1.91	0.71
2:N:26:HIS:NE2	2:N:44:PRO:O	2.23	0.71
3:P:41:GLU:HB3	3:P:45:ARG:HH12	1.56	0.71
1:B:1034:LEU:HB3	1:B:1036:LYS:HD3	1.73	0.71
1:B:346:GLN:O	1:B:348:LYS:HG3	1.91	0.71
1:B:549:SER:O	1:B:610:VAL:HB	1.91	0.71
1:F:609:LEU:HB3	1:F:908:LEU:HB2	1.71	0.71
1:G:1034:LEU:HB3	1:G:1036:LYS:HD3	1.73	0.71
1:B:28:HIS:CE1	3:P:14:LEU:HD21	2.26	0.71
1:C:346:GLN:O	1:C:348:LYS:HG3	1.91	0.70
1:D:47:PRO:HG2	1:D:51:GLN:NE2	2.07	0.70
1:E:882:LEU:HB2	1:E:903:ASP:CB	2.20	0.70
1:F:346:GLN:O	1:F:348:LYS:HG3	1.91	0.70
1:G:609:LEU:HB3	1:G:908:LEU:HB2	1.71	0.70
1:A:882:LEU:HB2	1:A:903:ASP:CB	2.20	0.70
1:C:549:SER:O	1:C:610:VAL:HB	1.91	0.70
1:D:569:CYS:SG	1:D:1213:PHE:CZ	2.85	0.70
1:D:346:GLN:O	1:D:348:LYS:HG3	1.91	0.70
1:D:403:LEU:HD13	1:D:460:ILE:HG22	1.73	0.70
1:E:47:PRO:HG2	1:E:51:GLN:NE2	2.07	0.70
1:F:549:SER:O	1:F:610:VAL:HB	1.91	0.70
1:A:569:CYS:SG	1:A:1213:PHE:CZ	2.85	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:GLN:HE22	1:C:1213:PHE:N	1.89	0.70
1:E:884:TRP:CE3	2:L:79:LYS:HD2	2.27	0.70
1:A:358:SER:HB3	1:B:274:MET:CE	2.20	0.70
1:E:1034:LEU:HB3	1:E:1036:LYS:HD3	1.73	0.70
1:E:346:GLN:O	1:E:348:LYS:HG3	1.91	0.70
1:E:358:SER:HB3	1:F:274:MET:CE	2.21	0.70
1:E:189:LYS:NZ	1:E:374:MET:SD	2.65	0.70
1:E:403:LEU:HD13	1:E:460:ILE:HG22	1.73	0.70
1:G:569:CYS:SG	1:G:1213:PHE:CZ	2.85	0.70
1:C:569:CYS:SG	1:C:1213:PHE:CZ	2.85	0.70
1:B:358:SER:HB3	1:C:274:MET:CE	2.21	0.70
1:C:403:LEU:HD13	1:C:460:ILE:HG22	1.73	0.70
1:D:189:LYS:NZ	1:D:374:MET:SD	2.65	0.70
1:D:854:LEU:HB3	1:D:866:LEU:HD11	1.74	0.70
1:A:854:LEU:HB3	1:A:866:LEU:HD11	1.74	0.70
1:G:346:GLN:O	1:G:348:LYS:HG3	1.91	0.70
1:C:854:LEU:HB3	1:C:866:LEU:HD11	1.74	0.70
1:C:882:LEU:HB2	1:C:903:ASP:CB	2.21	0.70
1:E:569:CYS:SG	1:E:1213:PHE:CZ	2.85	0.70
1:D:884:TRP:CE3	2:K:79:LYS:HD2	2.27	0.70
1:B:565:GLN:HE22	1:B:1213:PHE:N	1.89	0.69
1:G:854:LEU:HB3	1:G:866:LEU:HD11	1.74	0.69
1:B:884:TRP:CE3	2:I:79:LYS:HD2	2.27	0.69
1:A:346:GLN:O	1:A:348:LYS:HG3	1.91	0.69
1:D:14:GLU:OE1	1:E:31:SER:OG	2.10	0.69
1:E:854:LEU:HB3	1:E:866:LEU:HD11	1.74	0.69
1:F:1034:LEU:HB3	1:F:1036:LYS:HD3	1.73	0.69
1:F:882:LEU:HB2	1:F:903:ASP:CB	2.20	0.69
1:G:884:TRP:CE3	2:N:79:LYS:HD2	2.27	0.69
3:P:15:ARG:HD3	3:P:19:GLU:OE2	1.92	0.69
1:G:47:PRO:HG2	1:G:51:GLN:NE2	2.07	0.69
1:A:844:GLN:HE22	2:H:79:LYS:NZ	1.91	0.69
1:B:854:LEU:HB3	1:B:866:LEU:HD11	1.74	0.69
1:E:844:GLN:HE22	2:L:79:LYS:NZ	1.91	0.69
1:B:569:CYS:SG	1:B:1213:PHE:CZ	2.85	0.69
1:D:549:SER:O	1:D:610:VAL:HB	1.91	0.69
1:C:844:GLN:HE22	2:J:79:LYS:NZ	1.91	0.69
3:Q:15:ARG:HD3	3:Q:19:GLU:OE2	1.92	0.69
1:B:47:PRO:HG2	1:B:51:GLN:NE2	2.07	0.69
1:F:854:LEU:HB3	1:F:866:LEU:HD11	1.74	0.69
1:F:569:CYS:SG	1:F:1213:PHE:CZ	2.85	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:LYS:NZ	1:F:374:MET:SD	2.65	0.69
1:F:403:LEU:HD13	1:F:460:ILE:HG22	1.74	0.69
1:B:844:GLN:HE22	2:I:79:LYS:NZ	1.90	0.69
1:D:844:GLN:HE22	2:K:79:LYS:NZ	1.91	0.69
1:G:844:GLN:HE22	2:N:79:LYS:NZ	1.91	0.69
1:F:565:GLN:HE22	1:F:1213:PHE:N	1.89	0.68
1:B:403:LEU:HD13	1:B:460:ILE:HG22	1.73	0.68
1:F:844:GLN:HE22	2:M:79:LYS:NZ	1.91	0.68
1:A:403:LEU:HD13	1:A:460:ILE:HG22	1.73	0.68
1:B:37:ILE:HG13	3:P:10:ARG:NH1	2.08	0.68
1:B:590:ASN:C	1:B:592:MET:H	1.97	0.68
1:C:189:LYS:NZ	1:C:374:MET:SD	2.65	0.68
1:G:403:LEU:HD13	1:G:460:ILE:HG22	1.74	0.68
2:I:61:GLU:HA	2:I:95:ILE:HG21	1.76	0.68
3:R:15:ARG:HD3	3:R:19:GLU:OE2	1.93	0.68
1:F:884:TRP:CE3	2:M:79:LYS:HD2	2.27	0.68
2:J:61:GLU:HA	2:J:95:ILE:HG21	1.76	0.68
1:B:611:VAL:HG12	1:B:613:PRO:HD3	1.75	0.68
2:H:61:GLU:HA	2:H:95:ILE:HG21	1.75	0.68
1:C:590:ASN:C	1:C:592:MET:H	1.97	0.68
1:D:565:GLN:HE22	1:D:1213:PHE:N	1.89	0.68
1:F:611:VAL:HG12	1:F:613:PRO:HD3	1.75	0.68
1:G:611:VAL:HG12	1:G:613:PRO:HD3	1.75	0.68
1:D:1204:VAL:HG12	1:D:1205:VAL:HG23	1.76	0.68
1:G:189:LYS:NZ	1:G:374:MET:SD	2.65	0.68
1:E:565:GLN:HE22	1:E:1213:PHE:N	1.89	0.67
2:H:20:VAL:HG12	2:H:32:LEU:HB2	1.77	0.67
1:C:1204:VAL:HG12	1:C:1205:VAL:HG23	1.76	0.67
1:C:611:VAL:HG12	1:C:613:PRO:HD3	1.75	0.67
1:D:590:ASN:C	1:D:592:MET:H	1.97	0.67
1:A:884:TRP:CE3	2:H:79:LYS:HD2	2.27	0.67
1:C:884:TRP:CE3	2:J:79:LYS:HD2	2.27	0.67
1:G:565:GLN:CD	1:G:1213:PHE:N	2.48	0.67
1:C:1086:GLY:HA2	2:J:39:LYS:CE	2.24	0.67
2:K:61:GLU:HA	2:K:95:ILE:HG21	1.75	0.67
2:N:61:GLU:HA	2:N:95:ILE:HG21	1.75	0.67
3:O:15:ARG:HD3	3:O:19:GLU:OE2	1.93	0.67
3:O:52:ARG:CB	3:P:38:HIS:HE1	2.07	0.67
1:A:590:ASN:C	1:A:592:MET:H	1.97	0.67
2:I:20:VAL:HG12	2:I:32:LEU:HB2	1.77	0.67
1:E:1204:VAL:HG12	1:E:1205:VAL:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:VAL:HG12	2:N:32:LEU:HB2	1.77	0.67
1:D:358:SER:HB3	1:E:274:MET:HE2	1.76	0.67
1:E:590:ASN:C	1:E:592:MET:H	1.97	0.67
1:F:565:GLN:CD	1:F:1213:PHE:N	2.48	0.67
1:B:1086:GLY:HA2	2:I:39:LYS:CE	2.24	0.67
1:A:189:LYS:NZ	1:A:374:MET:SD	2.65	0.67
2:J:18:HIS:NE2	5:J:500:HEC:NB	2.43	0.67
2:K:18:HIS:NE2	5:K:500:HEC:NB	2.43	0.67
2:M:61:GLU:HA	2:M:95:ILE:HG21	1.76	0.67
3:O:6:ARG:O	3:O:10:ARG:HG2	1.95	0.67
1:A:611:VAL:HG12	1:A:613:PRO:HD3	1.75	0.67
2:L:61:GLU:HA	2:L:95:ILE:HG21	1.75	0.67
1:A:565:GLN:CD	1:A:1213:PHE:N	2.48	0.67
1:B:189:LYS:NZ	1:B:374:MET:SD	2.65	0.67
2:L:18:HIS:NE2	5:L:500:HEC:NB	2.43	0.67
1:B:1204:VAL:HG12	1:B:1205:VAL:HG23	1.76	0.66
1:D:611:VAL:HG12	1:D:613:PRO:HD3	1.75	0.66
2:N:18:HIS:NE2	5:N:500:HEC:NB	2.43	0.66
1:E:611:VAL:HG12	1:E:613:PRO:HD3	1.75	0.66
1:E:1086:GLY:HA2	2:L:39:LYS:CE	2.24	0.66
3:Q:6:ARG:O	3:Q:10:ARG:HG2	1.95	0.66
1:A:569:CYS:HG	1:A:1213:PHE:HE1	1.43	0.66
1:B:474:SER:HB2	1:B:477:GLN:HG2	1.78	0.66
1:E:565:GLN:CD	1:E:1213:PHE:N	2.48	0.66
1:F:590:ASN:C	1:F:592:MET:H	1.97	0.66
1:B:565:GLN:CD	1:B:1213:PHE:N	2.48	0.66
1:A:1086:GLY:HA2	2:H:39:LYS:CE	2.24	0.66
2:H:18:HIS:NE2	5:H:500:HEC:NB	2.43	0.66
1:F:1086:GLY:HA2	2:M:39:LYS:CE	2.25	0.66
1:C:565:GLN:CD	1:C:1213:PHE:N	2.48	0.66
1:D:1027:ILE:HD11	1:D:1047:VAL:HG11	1.78	0.66
1:D:565:GLN:CD	1:D:1213:PHE:N	2.48	0.66
1:E:1027:ILE:HD11	1:E:1047:VAL:HG11	1.78	0.66
1:F:1027:ILE:HD11	1:F:1047:VAL:HG11	1.78	0.66
1:G:1086:GLY:HA2	2:N:39:LYS:CE	2.24	0.66
1:F:358:SER:HB3	1:G:274:MET:CE	2.25	0.66
1:A:474:SER:HB2	1:A:477:GLN:HG2	1.78	0.66
1:G:590:ASN:C	1:G:592:MET:H	1.97	0.66
2:I:18:HIS:NE2	5:I:500:HEC:NB	2.43	0.66
2:L:20:VAL:HG12	2:L:32:LEU:HB2	1.77	0.66
1:F:1204:VAL:HG12	1:F:1205:VAL:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:844:GLN:NE2	2:L:79:LYS:HE3	2.11	0.66
3:R:6:ARG:O	3:R:10:ARG:HG2	1.95	0.66
2:J:20:VAL:HG12	2:J:32:LEU:HB2	1.77	0.66
1:D:1086:GLY:HA2	2:K:39:LYS:CE	2.24	0.66
1:F:844:GLN:NE2	2:M:79:LYS:HE3	2.11	0.66
3:P:6:ARG:O	3:P:10:ARG:HG2	1.95	0.66
1:D:844:GLN:NE2	2:K:79:LYS:HE3	2.11	0.65
1:F:354:ARG:NH1	1:F:362:GLU:OE1	2.30	0.65
1:G:1027:ILE:HD11	1:G:1047:VAL:HG11	1.78	0.65
1:G:844:GLN:NE2	2:N:79:LYS:HE3	2.11	0.65
2:K:20:VAL:HG12	2:K:32:LEU:HB2	1.77	0.65
2:M:18:HIS:NE2	5:M:500:HEC:NB	2.43	0.65
1:E:391:LYS:O	1:E:392:ASP:HB2	1.96	0.65
1:F:391:LYS:O	1:F:392:ASP:HB2	1.96	0.65
1:A:1204:VAL:HG12	1:A:1205:VAL:HG23	1.76	0.65
1:B:354:ARG:NH1	1:B:362:GLU:OE1	2.30	0.65
1:C:474:SER:HB2	1:C:477:GLN:HG2	1.78	0.65
1:D:943:ILE:HG22	1:D:944:ARG:HG2	1.78	0.65
1:E:569:CYS:HG	1:E:1213:PHE:HE1	1.42	0.65
1:E:943:ILE:HG22	1:E:944:ARG:HG2	1.78	0.65
1:F:201:ASN:HD21	1:G:219:ASN:HD21	1.44	0.65
1:F:943:ILE:HG22	1:F:944:ARG:HG2	1.78	0.65
1:G:1204:VAL:HG12	1:G:1205:VAL:HG23	1.76	0.65
1:A:866:LEU:HB3	1:A:876:ALA:HB3	1.77	0.65
1:B:590:ASN:O	1:B:592:MET:N	2.30	0.65
1:C:1027:ILE:HD11	1:C:1047:VAL:HG11	1.78	0.65
1:C:590:ASN:O	1:C:592:MET:N	2.30	0.65
1:E:354:ARG:NH1	1:E:362:GLU:OE1	2.30	0.65
1:F:590:ASN:O	1:F:592:MET:N	2.30	0.65
1:G:354:ARG:NH1	1:G:362:GLU:OE1	2.30	0.65
1:C:943:ILE:HG22	1:C:944:ARG:HG2	1.78	0.65
1:G:866:LEU:HB3	1:G:876:ALA:HB3	1.77	0.65
1:G:943:ILE:HG22	1:G:944:ARG:HG2	1.78	0.65
1:C:844:GLN:NE2	2:J:79:LYS:HE3	2.11	0.65
2:M:20:VAL:HG12	2:M:32:LEU:HB2	1.77	0.65
1:A:943:ILE:HG22	1:A:944:ARG:HG2	1.78	0.65
1:B:391:LYS:O	1:B:392:ASP:HB2	1.96	0.65
1:C:354:ARG:NH1	1:C:362:GLU:OE1	2.30	0.65
1:B:884:TRP:HZ3	2:I:79:LYS:HA	1.56	0.65
1:C:266:ASP:OD2	1:C:268:SER:OG	2.16	0.64
1:D:866:LEU:HB3	1:D:876:ALA:HB3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:GLN:HE22	1:A:1213:PHE:N	1.89	0.64
1:B:943:ILE:HG22	1:B:944:ARG:HG2	1.78	0.64
1:D:160:LYS:N	4:D:1301:DTP:O1A	2.21	0.64
1:D:266:ASP:OD2	1:D:268:SER:OG	2.16	0.64
1:D:391:LYS:O	1:D:392:ASP:HB2	1.96	0.64
1:F:1133:SER:HB2	1:F:1142:LEU:HD11	1.79	0.64
1:F:469:GLN:HB2	1:F:472:THR:HB	1.79	0.64
1:G:474:SER:HB2	1:G:477:GLN:HG2	1.78	0.64
1:A:1133:SER:HB2	1:A:1142:LEU:HD11	1.79	0.64
1:A:590:ASN:O	1:A:592:MET:N	2.30	0.64
1:C:866:LEU:HB3	1:C:876:ALA:HB3	1.77	0.64
1:D:643:LYS:HE3	1:D:645:GLU:HB3	1.79	0.64
1:D:715:LEU:HD13	1:D:727:LEU:HD21	1.79	0.64
1:G:1133:SER:HB2	1:G:1142:LEU:HD11	1.79	0.64
2:J:2:ASP:N	2:J:93:ASP:OD1	2.28	0.64
1:A:160:LYS:N	4:A:1301:DTP:O1A	2.21	0.64
1:A:643:LYS:HE3	1:A:645:GLU:HB3	1.79	0.64
1:B:266:ASP:OD2	1:B:268:SER:OG	2.16	0.64
1:D:590:ASN:O	1:D:592:MET:N	2.30	0.64
1:E:469:GLN:HB2	1:E:472:THR:HB	1.79	0.64
2:N:2:ASP:N	2:N:93:ASP:OD1	2.28	0.64
1:A:354:ARG:NH1	1:A:362:GLU:OE1	2.30	0.64
1:B:866:LEU:HB3	1:B:876:ALA:HB3	1.77	0.64
1:F:866:LEU:HB3	1:F:876:ALA:HB3	1.77	0.64
1:B:844:GLN:NE2	2:I:79:LYS:HE3	2.11	0.64
1:A:1027:ILE:HD11	1:A:1047:VAL:HG11	1.78	0.64
1:C:643:LYS:HE3	1:C:645:GLU:HB3	1.79	0.64
1:D:354:ARG:NH1	1:D:362:GLU:OE1	2.30	0.64
1:A:844:GLN:NE2	2:H:79:LYS:HE3	2.11	0.64
1:E:715:LEU:HD13	1:E:727:LEU:HD21	1.79	0.64
1:G:391:LYS:O	1:G:392:ASP:HB2	1.96	0.64
1:G:884:TRP:HZ3	2:N:79:LYS:HD2	1.52	0.64
1:A:1232:TYR:HB2	1:A:1244:LEU:HB2	1.80	0.64
1:B:1027:ILE:HD11	1:B:1047:VAL:HG11	1.78	0.64
1:B:1232:TYR:HB2	1:B:1244:LEU:HB2	1.80	0.64
1:C:1232:TYR:HB2	1:C:1244:LEU:HB2	1.80	0.64
1:E:160:LYS:N	4:E:1301:DTP:O1A	2.21	0.64
1:E:643:LYS:HE3	1:E:645:GLU:HB3	1.79	0.64
1:A:884:TRP:HZ3	2:H:79:LYS:HA	1.56	0.64
1:E:474:SER:HB2	1:E:477:GLN:HG2	1.78	0.64
2:I:2:ASP:N	2:I:93:ASP:OD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1086:GLY:CA	2:M:39:LYS:HZ1	2.07	0.64
1:B:643:LYS:HE3	1:B:645:GLU:HB3	1.79	0.64
1:D:474:SER:HB2	1:D:477:GLN:HG2	1.78	0.64
1:E:866:LEU:HB3	1:E:876:ALA:HB3	1.77	0.64
1:A:391:LYS:O	1:A:392:ASP:HB2	1.96	0.63
1:B:1133:SER:HB2	1:B:1142:LEU:HD11	1.79	0.63
1:C:715:LEU:HD13	1:C:727:LEU:HD21	1.79	0.63
1:G:1232:TYR:HB2	1:G:1244:LEU:HB2	1.80	0.63
1:G:469:GLN:HB2	1:G:472:THR:HB	1.79	0.63
1:G:643:LYS:HE3	1:G:645:GLU:HB3	1.79	0.63
1:D:469:GLN:HB2	1:D:472:THR:HB	1.79	0.63
1:E:1133:SER:HB2	1:E:1142:LEU:HD11	1.79	0.63
1:E:945:ARG:HH22	1:E:988:LEU:HD22	1.64	0.63
1:F:474:SER:HB2	1:F:477:GLN:HG2	1.78	0.63
1:C:1133:SER:HB2	1:C:1142:LEU:HD11	1.79	0.63
1:C:391:LYS:O	1:C:392:ASP:HB2	1.96	0.63
1:A:266:ASP:OD2	1:A:268:SER:OG	2.16	0.63
1:C:884:TRP:HZ3	2:J:79:LYS:HA	1.56	0.63
1:G:715:LEU:HD13	1:G:727:LEU:HD21	1.79	0.63
1:D:1133:SER:HB2	1:D:1142:LEU:HD11	1.79	0.63
1:D:1232:TYR:HB2	1:D:1244:LEU:HB2	1.80	0.63
1:A:109:TYR:HE1	1:G:4:LYS:HZ3	0.70	0.63
1:F:565:GLN:OE1	1:F:1213:PHE:N	2.32	0.63
1:F:1232:TYR:HB2	1:F:1244:LEU:HB2	1.80	0.63
1:F:715:LEU:HD13	1:F:727:LEU:HD21	1.79	0.63
1:G:565:GLN:OE1	1:G:1213:PHE:N	2.32	0.63
1:D:565:GLN:OE1	1:D:1213:PHE:N	2.32	0.63
1:A:715:LEU:HD13	1:A:727:LEU:HD21	1.79	0.62
1:D:945:ARG:HH22	1:D:988:LEU:HD22	1.64	0.62
1:E:590:ASN:O	1:E:592:MET:N	2.30	0.62
1:F:643:LYS:HE3	1:F:645:GLU:HB3	1.79	0.62
1:G:945:ARG:HH22	1:G:988:LEU:HD22	1.64	0.62
1:B:715:LEU:HD13	1:B:727:LEU:HD21	1.79	0.62
1:C:903:ASP:OD2	1:C:907:ARG:NH1	2.28	0.62
1:E:1232:TYR:HB2	1:E:1244:LEU:HB2	1.80	0.62
1:G:590:ASN:O	1:G:592:MET:N	2.30	0.62
3:O:52:ARG:HB2	3:P:38:HIS:HE1	1.61	0.62
1:A:945:ARG:HH22	1:A:988:LEU:HD22	1.64	0.62
1:B:469:GLN:HB2	1:B:472:THR:HB	1.79	0.62
1:B:945:ARG:HH22	1:B:988:LEU:HD22	1.64	0.62
1:G:160:LYS:N	4:G:1301:DTP:O1A	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:ASP:N	2:K:93:ASP:OD1	2.28	0.62
1:A:1031:ASN:HB2	1:A:1036:LYS:HB2	1.82	0.62
1:A:565:GLN:OE1	1:A:1213:PHE:N	2.32	0.62
1:C:945:ARG:HH22	1:C:988:LEU:HD22	1.64	0.62
1:F:569:CYS:HG	1:F:1213:PHE:HE1	1.47	0.62
1:F:266:ASP:OD2	1:F:268:SER:OG	2.16	0.62
1:A:557:ARG:HH22	1:A:1175:THR:HG23	1.64	0.62
1:C:565:GLN:OE1	1:C:1213:PHE:N	2.32	0.62
1:F:945:ARG:HH22	1:F:988:LEU:HD22	1.64	0.62
2:M:2:ASP:N	2:M:93:ASP:OD1	2.28	0.62
1:A:469:GLN:HB2	1:A:472:THR:HB	1.79	0.62
1:B:1031:ASN:HB2	1:B:1036:LYS:HB2	1.82	0.62
1:B:924:GLN:NE2	1:B:965:SER:O	2.33	0.62
1:C:469:GLN:HB2	1:C:472:THR:HB	1.79	0.62
1:G:1031:ASN:HB2	1:G:1036:LYS:HB2	1.82	0.62
1:G:569:CYS:HG	1:G:1213:PHE:HE1	1.44	0.62
1:B:557:ARG:HH22	1:B:1175:THR:HG23	1.64	0.62
1:B:565:GLN:OE1	1:B:1213:PHE:N	2.32	0.62
1:C:924:GLN:NE2	1:C:965:SER:O	2.33	0.62
1:D:862:TYR:HB3	1:D:884:TRP:HA	1.82	0.62
1:F:924:GLN:NE2	1:F:965:SER:O	2.33	0.62
1:A:1086:GLY:CA	2:H:39:LYS:HZ1	2.10	0.62
1:A:924:GLN:NE2	1:A:965:SER:O	2.33	0.62
1:E:924:GLN:NE2	1:E:965:SER:O	2.33	0.62
1:E:587:GLU:OE1	1:E:594:TYR:OH	2.18	0.62
1:G:559:PRO:HD3	1:G:1171:GLU:OE1	2.00	0.62
1:G:714:LEU:HB3	1:G:730:LEU:HD12	1.82	0.62
1:A:145:GLY:HA2	1:A:259:GLN:NE2	2.15	0.61
1:D:569:CYS:HG	1:D:1213:PHE:HE1	1.48	0.61
1:E:565:GLN:OE1	1:E:1213:PHE:N	2.32	0.61
1:G:266:ASP:OD2	1:G:268:SER:OG	2.16	0.61
1:G:587:GLU:OE1	1:G:594:TYR:OH	2.17	0.61
1:A:358:SER:HB3	1:B:274:MET:HE3	1.81	0.61
1:C:1031:ASN:HB2	1:C:1036:LYS:HB2	1.82	0.61
1:G:557:ARG:HH22	1:G:1175:THR:HG23	1.64	0.61
1:D:559:PRO:HD3	1:D:1171:GLU:OE1	2.00	0.61
1:F:714:LEU:HB3	1:F:730:LEU:HD12	1.82	0.61
1:G:924:GLN:NE2	1:G:965:SER:O	2.33	0.61
2:L:2:ASP:N	2:L:93:ASP:OD1	2.28	0.61
1:G:884:TRP:HZ3	2:N:79:LYS:HA	1.56	0.61
1:A:274:MET:HG2	1:G:358:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:PRO:HD3	1:C:1171:GLU:OE1	2.00	0.61
1:C:862:TYR:HB3	1:C:884:TRP:HA	1.82	0.61
1:D:924:GLN:NE2	1:D:965:SER:O	2.33	0.61
1:E:145:GLY:HA2	1:E:259:GLN:NE2	2.15	0.61
1:F:559:PRO:HD3	1:F:1171:GLU:OE1	2.00	0.61
1:A:587:GLU:OE1	1:A:594:TYR:OH	2.18	0.61
1:D:145:GLY:HA2	1:D:259:GLN:NE2	2.15	0.61
1:E:862:TYR:HB3	1:E:884:TRP:HA	1.82	0.61
1:F:1031:ASN:HB2	1:F:1036:LYS:HB2	1.82	0.61
1:F:587:GLU:OE1	1:F:594:TYR:OH	2.18	0.61
1:F:882:LEU:HD12	1:F:903:ASP:HB2	1.83	0.61
1:A:884:TRP:HZ3	2:H:79:LYS:HD2	1.52	0.61
2:H:2:ASP:N	2:H:93:ASP:OD1	2.28	0.61
1:A:862:TYR:HB3	1:A:884:TRP:HA	1.82	0.61
1:B:160:LYS:N	4:B:1301:DTP:O1A	2.21	0.61
1:B:882:LEU:HD13	1:B:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD13	1:A:1176:HIS:CE1	2.36	0.61
1:A:882:LEU:HD12	1:A:903:ASP:HB2	1.83	0.61
1:D:882:LEU:HD13	1:D:1176:HIS:CE1	2.36	0.61
1:D:599:ASN:ND2	1:D:1241:LEU:O	2.34	0.61
1:E:714:LEU:HB3	1:E:730:LEU:HD12	1.82	0.61
1:E:882:LEU:HD12	1:E:903:ASP:HB2	1.83	0.61
1:F:1092:ASP:OD2	1:F:1133:SER:OG	2.17	0.61
1:F:145:GLY:HA2	1:F:259:GLN:NE2	2.15	0.61
1:F:862:TYR:CB	1:F:884:TRP:HA	2.31	0.61
1:G:145:GLY:HA2	1:G:259:GLN:NE2	2.16	0.61
1:A:752:SER:OG	1:A:754:ASP:O	2.19	0.61
1:B:145:GLY:HA2	1:B:259:GLN:NE2	2.16	0.61
1:B:599:ASN:ND2	1:B:1241:LEU:O	2.34	0.61
1:E:559:PRO:HD3	1:E:1171:GLU:OE1	2.00	0.61
1:G:599:ASN:ND2	1:G:1241:LEU:O	2.34	0.61
1:A:714:LEU:HB3	1:A:730:LEU:HD12	1.82	0.61
1:B:882:LEU:HD12	1:B:903:ASP:HB2	1.83	0.61
1:C:265:ARG:NH2	4:C:1301:DTP:O2G	2.31	0.61
1:E:266:ASP:OD2	1:E:268:SER:OG	2.16	0.61
1:E:358:SER:HB3	1:F:274:MET:HE3	1.82	0.61
1:G:862:TYR:HB3	1:G:884:TRP:HA	1.82	0.61
1:F:844:GLN:HE22	2:M:79:LYS:CE	2.14	0.61
1:C:557:ARG:HH22	1:C:1175:THR:HG23	1.64	0.61
1:C:714:LEU:HB3	1:C:730:LEU:HD12	1.82	0.61
1:C:882:LEU:HD13	1:C:1176:HIS:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:844:GLN:HE22	2:K:79:LYS:CE	2.14	0.61
1:F:482:TYR:HH	1:F:490:HIS:HE2	1.45	0.61
1:B:844:GLN:HE22	2:I:79:LYS:CE	2.14	0.61
3:Q:52:ARG:HB2	3:R:38:HIS:HE1	1.65	0.61
1:C:160:LYS:N	4:C:1301:DTP:O1A	2.21	0.60
1:B:358:SER:HB3	1:C:274:MET:HE2	1.82	0.60
1:D:1031:ASN:HB2	1:D:1036:LYS:HB2	1.82	0.60
1:G:752:SER:OG	1:G:754:ASP:O	2.19	0.60
1:G:882:LEU:HD12	1:G:903:ASP:HB2	1.83	0.60
1:A:559:PRO:HD3	1:A:1171:GLU:OE1	2.00	0.60
1:B:714:LEU:HB3	1:B:730:LEU:HD12	1.82	0.60
1:C:1092:ASP:OD2	1:C:1133:SER:OG	2.17	0.60
1:D:882:LEU:HD12	1:D:903:ASP:HB2	1.83	0.60
1:E:1031:ASN:HB2	1:E:1036:LYS:HB2	1.82	0.60
1:E:557:ARG:HH22	1:E:1175:THR:HG23	1.64	0.60
1:E:201:ASN:HD21	1:F:219:ASN:HD21	1.49	0.60
1:E:752:SER:OG	1:E:754:ASP:O	2.19	0.60
1:G:265:ARG:NH2	4:G:1301:DTP:O2G	2.31	0.60
1:F:358:SER:HB3	1:G:274:MET:HE3	1.83	0.60
1:D:1086:GLY:CA	2:K:39:LYS:HZ1	2.10	0.60
1:D:844:GLN:NE2	2:K:79:LYS:CE	2.64	0.60
1:E:844:GLN:NE2	2:L:79:LYS:CE	2.64	0.60
1:B:903:ASP:OD2	1:B:907:ARG:NH1	2.28	0.60
1:D:1092:ASP:OD2	1:D:1133:SER:OG	2.17	0.60
1:F:599:ASN:ND2	1:F:1241:LEU:O	2.34	0.60
1:B:1086:GLY:CA	2:I:39:LYS:HZ1	2.07	0.60
1:E:844:GLN:HE22	2:L:79:LYS:CE	2.14	0.60
1:G:844:GLN:HE22	2:N:79:LYS:CE	2.14	0.60
1:C:882:LEU:HD12	1:C:903:ASP:HB2	1.83	0.60
1:C:862:TYR:CB	1:C:884:TRP:HA	2.31	0.60
1:E:1087:THR:N	2:L:39:LYS:HZ3	2.00	0.60
1:G:844:GLN:NE2	2:N:79:LYS:CE	2.65	0.60
1:C:844:GLN:NE2	2:J:79:LYS:CE	2.65	0.60
1:D:884:TRP:HZ3	2:K:79:LYS:HA	1.56	0.60
1:B:559:PRO:HD3	1:B:1171:GLU:OE1	2.00	0.60
1:B:862:TYR:HB3	1:B:884:TRP:HA	1.82	0.60
1:D:714:LEU:HB3	1:D:730:LEU:HD12	1.82	0.60
1:D:752:SER:OG	1:D:754:ASP:O	2.19	0.60
1:E:862:TYR:CB	1:E:884:TRP:HA	2.31	0.60
1:F:557:ARG:HH22	1:F:1175:THR:HG23	1.64	0.60
1:F:1210:SER:HB2	1:F:1212:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ASN:ND2	1:A:1241:LEU:O	2.34	0.60
1:B:569:CYS:HG	1:B:1213:PHE:HE1	1.50	0.60
1:B:862:TYR:CB	1:B:884:TRP:HA	2.31	0.60
1:C:145:GLY:HA2	1:C:259:GLN:NE2	2.15	0.60
1:D:557:ARG:HH22	1:D:1175:THR:HG23	1.64	0.60
1:E:882:LEU:HD13	1:E:1176:HIS:CE1	2.36	0.60
1:F:862:TYR:HB3	1:F:884:TRP:HA	1.82	0.60
1:F:884:TRP:HZ3	2:M:79:LYS:HD2	1.51	0.60
1:B:587:GLU:OE1	1:B:594:TYR:OH	2.18	0.60
1:B:752:SER:OG	1:B:754:ASP:O	2.19	0.60
1:D:862:TYR:CB	1:D:884:TRP:HA	2.31	0.60
1:A:862:TYR:CB	1:A:884:TRP:HA	2.31	0.60
1:B:844:GLN:NE2	2:I:79:LYS:CE	2.65	0.60
1:G:1210:SER:HB2	1:G:1212:THR:HG23	1.84	0.60
1:A:844:GLN:HE22	2:H:79:LYS:CE	2.14	0.60
1:A:844:GLN:NE2	2:H:79:LYS:CE	2.65	0.60
1:E:265:ARG:NH2	4:E:1301:DTP:O2G	2.31	0.60
1:F:882:LEU:HD13	1:F:1176:HIS:CE1	2.36	0.60
1:G:882:LEU:HD13	1:G:1176:HIS:CE1	2.36	0.60
1:G:862:TYR:CB	1:G:884:TRP:HA	2.31	0.60
1:C:358:SER:OG	1:D:274:MET:HG2	2.02	0.60
1:D:1210:SER:HB2	1:D:1212:THR:HG23	1.84	0.60
1:E:599:ASN:ND2	1:E:1241:LEU:O	2.34	0.60
1:F:844:GLN:NE2	2:M:79:LYS:CE	2.64	0.60
1:C:599:ASN:ND2	1:C:1241:LEU:O	2.34	0.59
1:E:1115:ASP:HB2	1:E:1120:LEU:HD11	1.84	0.59
1:F:882:LEU:HD13	1:F:1176:HIS:CD2	2.37	0.59
1:A:1115:ASP:HB2	1:A:1120:LEU:HD11	1.84	0.59
1:A:903:ASP:OD2	1:A:907:ARG:NH1	2.28	0.59
1:B:201:ASN:HD21	1:C:219:ASN:HD21	1.50	0.59
1:E:1210:SER:HB2	1:E:1212:THR:HG23	1.84	0.59
1:F:752:SER:OG	1:F:754:ASP:O	2.19	0.59
1:F:903:ASP:OD2	1:F:907:ARG:NH1	2.28	0.59
1:B:1115:ASP:HB2	1:B:1120:LEU:HD11	1.84	0.59
1:G:903:ASP:OD2	1:G:907:ARG:NH1	2.28	0.59
1:A:882:LEU:HD13	1:A:1176:HIS:CD2	2.38	0.59
1:A:201:ASN:HD21	1:B:219:ASN:HD21	1.50	0.59
1:C:844:GLN:HE22	2:J:79:LYS:CE	2.14	0.59
1:D:1115:ASP:HB2	1:D:1120:LEU:HD11	1.84	0.59
1:E:715:LEU:HB3	1:E:727:LEU:HD11	1.85	0.59
1:B:882:LEU:HD13	1:B:1176:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1210:SER:HB2	1:C:1212:THR:HG23	1.84	0.59
1:C:752:SER:OG	1:C:754:ASP:O	2.19	0.59
1:D:1131:ARG:NH2	1:D:1147:ASP:OD1	2.36	0.59
1:D:482:TYR:HH	1:D:490:HIS:HE2	1.50	0.59
1:D:715:LEU:HB3	1:D:727:LEU:HD11	1.85	0.59
1:E:903:ASP:OD2	1:E:907:ARG:NH1	2.28	0.59
1:F:1115:ASP:HB2	1:F:1120:LEU:HD11	1.84	0.59
3:Q:52:ARG:CG	3:R:38:HIS:CE1	2.82	0.59
1:F:715:LEU:HB3	1:F:727:LEU:HD11	1.85	0.59
1:A:1210:SER:HB2	1:A:1212:THR:HG23	1.84	0.59
1:C:1131:ARG:NH2	1:C:1147:ASP:OD1	2.36	0.59
1:E:1131:ARG:NH2	1:E:1147:ASP:OD1	2.36	0.59
1:G:1115:ASP:HB2	1:G:1120:LEU:HD11	1.84	0.59
3:P:41:GLU:HB3	3:P:45:ARG:NH1	2.17	0.59
1:B:358:SER:HB3	1:C:274:MET:HE3	1.84	0.59
1:D:882:LEU:HD13	1:D:1176:HIS:CD2	2.37	0.59
1:C:1031:ASN:HB3	1:C:1034:LEU:HD12	1.85	0.59
1:C:521:HIS:NE2	1:C:525:GLU:OE2	2.36	0.59
1:E:882:LEU:HD13	1:E:1176:HIS:CD2	2.37	0.59
1:G:463:GLN:OE1	1:G:466:ARG:NH2	2.28	0.59
1:A:358:SER:HB3	1:B:274:MET:HE2	1.84	0.58
1:A:521:HIS:NE2	1:A:525:GLU:OE2	2.36	0.58
1:F:160:LYS:N	4:F:1301:DTP:O1A	2.20	0.58
1:G:882:LEU:HD13	1:G:1176:HIS:CD2	2.38	0.58
1:D:358:SER:OG	1:E:274:MET:HG2	2.03	0.58
1:E:1202:TRP:HA	1:E:1208:GLU:HB2	1.85	0.58
1:F:1202:TRP:HA	1:F:1208:GLU:HB2	1.85	0.58
1:B:1031:ASN:HB3	1:B:1034:LEU:HD12	1.85	0.58
1:B:1210:SER:HB2	1:B:1212:THR:HG23	1.84	0.58
1:B:48:THR:HG22	1:D:45:ASN:OD1	2.04	0.58
1:C:1115:ASP:HB2	1:C:1120:LEU:HD11	1.84	0.58
1:C:715:LEU:HB3	1:C:727:LEU:HD11	1.85	0.58
1:C:201:ASN:HD21	1:D:219:ASN:HD21	1.51	0.58
1:D:903:ASP:OD2	1:D:907:ARG:NH1	2.28	0.58
1:E:4:LYS:HA	1:F:237:ARG:HH21	1.68	0.58
2:J:67:TYR:OH	2:J:80:MET:SD	2.57	0.58
1:F:884:TRP:HZ3	2:M:79:LYS:HA	1.56	0.58
3:Q:52:ARG:HB3	3:R:38:HIS:CE1	2.37	0.58
1:C:1202:TRP:HA	1:C:1208:GLU:HB2	1.85	0.58
1:C:882:LEU:HD13	1:C:1176:HIS:CD2	2.38	0.58
1:D:1202:TRP:HA	1:D:1208:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1086:GLY:CA	2:J:39:LYS:HZ1	2.12	0.58
1:B:1131:ARG:NH2	1:B:1147:ASP:OD1	2.36	0.58
1:F:1131:ARG:NH2	1:F:1147:ASP:OD1	2.36	0.58
1:G:884:TRP:CZ3	2:N:79:LYS:CA	2.74	0.58
1:E:884:TRP:HZ3	2:L:79:LYS:HA	1.56	0.58
1:A:1031:ASN:HB3	1:A:1034:LEU:HD12	1.85	0.58
1:B:265:ARG:NH2	4:B:1301:DTP:O2G	2.31	0.58
1:B:482:TYR:HH	1:B:490:HIS:HE2	1.50	0.58
1:D:265:ARG:NH2	4:D:1301:DTP:O2G	2.31	0.58
1:F:1031:ASN:HB3	1:F:1034:LEU:HD12	1.85	0.58
1:G:1131:ARG:NH2	1:G:1147:ASP:OD1	2.36	0.58
1:A:1131:ARG:NH2	1:A:1147:ASP:OD1	2.36	0.58
1:C:884:TRP:CH2	2:J:78:THR:O	2.57	0.58
1:D:1031:ASN:HB3	1:D:1034:LEU:HD12	1.85	0.58
1:E:358:SER:HB3	1:F:274:MET:HE2	1.85	0.58
1:G:1048:LYS:H	1:G:1062:SER:HA	1.69	0.58
1:B:1202:TRP:HA	1:B:1208:GLU:HB2	1.85	0.58
1:C:587:GLU:OE1	1:C:594:TYR:OH	2.18	0.58
1:E:482:TYR:HH	1:E:490:HIS:HE2	1.48	0.58
1:F:1048:LYS:H	1:F:1062:SER:HA	1.69	0.58
1:G:715:LEU:HB3	1:G:727:LEU:HD11	1.85	0.58
1:B:521:HIS:NE2	1:B:525:GLU:OE2	2.36	0.57
1:D:521:HIS:NE2	1:D:525:GLU:OE2	2.36	0.57
1:E:482:TYR:OH	1:E:490:HIS:NE2	2.35	0.57
1:F:521:HIS:NE2	1:F:525:GLU:OE2	2.36	0.57
1:G:482:TYR:OH	1:G:490:HIS:NE2	2.36	0.57
1:A:715:LEU:HB3	1:A:727:LEU:HD11	1.85	0.57
1:B:884:TRP:CH2	2:I:78:THR:O	2.57	0.57
1:G:1202:TRP:HA	1:G:1208:GLU:HB2	1.86	0.57
1:D:884:TRP:CH2	2:K:78:THR:O	2.57	0.57
1:B:715:LEU:HB3	1:B:727:LEU:HD11	1.85	0.57
1:D:201:ASN:HD21	1:E:219:ASN:HD21	1.52	0.57
1:B:454:GLN:OE1	1:B:458:LYS:NZ	2.38	0.57
1:D:454:GLN:OE1	1:D:458:LYS:NZ	2.38	0.57
1:E:521:HIS:NE2	1:E:525:GLU:OE2	2.36	0.57
1:E:358:SER:OG	1:F:274:MET:HG2	2.04	0.57
1:B:1048:LYS:H	1:B:1062:SER:HA	1.69	0.57
1:C:454:GLN:OE1	1:C:458:LYS:NZ	2.38	0.57
1:E:454:GLN:OE1	1:E:458:LYS:NZ	2.38	0.57
1:G:521:HIS:NE2	1:G:525:GLU:OE2	2.36	0.57
1:F:884:TRP:CH2	2:M:78:THR:O	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:OE1	1:A:458:LYS:NZ	2.38	0.57
1:B:884:TRP:CZ3	2:I:79:LYS:CA	2.74	0.57
1:D:1048:LYS:H	1:D:1062:SER:HA	1.69	0.57
1:E:1048:LYS:H	1:E:1062:SER:HA	1.69	0.57
1:G:1031:ASN:HB3	1:G:1034:LEU:HD12	1.85	0.57
1:G:884:TRP:CH2	2:N:78:THR:O	2.57	0.57
1:A:1202:TRP:HA	1:A:1208:GLU:HB2	1.85	0.57
1:B:358:SER:OG	1:C:274:MET:HG2	2.04	0.57
1:D:482:TYR:OH	1:D:490:HIS:NE2	2.35	0.57
1:G:454:GLN:OE1	1:G:458:LYS:NZ	2.38	0.57
1:A:884:TRP:CH2	2:H:78:THR:O	2.57	0.57
1:D:1139:SER:O	1:D:1140:THR:HG22	2.05	0.57
1:G:264:THR:OG1	1:G:265:ARG:N	2.37	0.57
1:A:358:SER:OG	1:B:274:MET:HG2	2.04	0.57
1:C:1048:LYS:H	1:C:1062:SER:HA	1.69	0.57
1:C:763:ALA:HA	1:C:801:VAL:H	1.70	0.57
1:D:264:THR:OG1	1:D:265:ARG:N	2.37	0.57
1:E:1031:ASN:HB3	1:E:1034:LEU:HD12	1.85	0.57
1:E:763:ALA:HA	1:E:801:VAL:H	1.70	0.57
1:F:265:ARG:NH2	4:F:1301:DTP:O2G	2.31	0.57
1:F:454:GLN:OE1	1:F:458:LYS:NZ	2.38	0.57
1:G:1092:ASP:OD2	1:G:1133:SER:OG	2.17	0.57
1:G:1139:SER:O	1:G:1140:THR:HG22	2.05	0.57
1:B:264:THR:OG1	1:B:265:ARG:N	2.37	0.56
1:B:524:HIS:HB2	1:B:646:THR:CG2	2.32	0.56
1:F:264:THR:OG1	1:F:265:ARG:N	2.38	0.56
1:A:1139:SER:O	1:A:1140:THR:HG22	2.05	0.56
1:C:1139:SER:O	1:C:1140:THR:HG22	2.05	0.56
1:C:482:TYR:HH	1:C:490:HIS:HE2	1.53	0.56
1:D:587:GLU:OE1	1:D:594:TYR:OH	2.18	0.56
1:E:1092:ASP:OD2	1:E:1133:SER:OG	2.17	0.56
1:B:1139:SER:O	1:B:1140:THR:HG22	2.05	0.56
1:E:524:HIS:HB2	1:E:646:THR:CG2	2.32	0.56
1:B:1023:ASP:OD1	1:B:1046:THR:OG1	2.24	0.56
1:C:482:TYR:OH	1:C:490:HIS:NE2	2.35	0.56
1:C:884:TRP:CZ3	2:J:79:LYS:CA	2.74	0.56
1:D:569:CYS:HB3	1:D:600:LYS:HZ3	1.71	0.56
1:E:884:TRP:CH2	2:L:78:THR:O	2.57	0.56
1:A:264:THR:OG1	1:A:265:ARG:N	2.37	0.56
1:C:716:LEU:HB3	1:C:728:TRP:HB2	1.87	0.56
1:D:463:GLN:OE1	1:D:466:ARG:NH2	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:THR:OG1	1:E:265:ARG:N	2.37	0.56
1:A:1048:LYS:H	1:A:1062:SER:HA	1.69	0.56
1:A:565:GLN:NE2	1:A:1213:PHE:CA	2.69	0.56
1:A:524:HIS:HB2	1:A:646:THR:CG2	2.32	0.56
1:F:1139:SER:O	1:F:1140:THR:HG22	2.05	0.56
1:C:1087:THR:N	2:J:39:LYS:HZ3	2.04	0.56
1:G:565:GLN:NE2	1:G:1213:PHE:CA	2.69	0.56
1:G:716:LEU:HB3	1:G:728:TRP:HB2	1.87	0.56
1:C:1086:GLY:CA	2:J:39:LYS:NZ	2.66	0.56
1:A:1023:ASP:OD1	1:A:1046:THR:OG1	2.24	0.56
1:B:763:ALA:HA	1:B:801:VAL:H	1.70	0.56
1:D:716:LEU:HB3	1:D:728:TRP:HB2	1.87	0.56
1:E:1139:SER:O	1:E:1140:THR:HG22	2.05	0.56
1:A:844:GLN:HE22	2:H:79:LYS:HE3	1.71	0.56
2:M:67:TYR:OH	2:M:80:MET:SD	2.57	0.56
1:A:170:ASP:OD1	1:A:171:HIS:N	2.39	0.56
1:B:143:LEU:C	1:B:145:GLY:H	2.09	0.56
1:C:264:THR:OG1	1:C:265:ARG:N	2.37	0.56
1:C:326:LEU:HD13	1:C:353:ILE:CG2	2.37	0.56
1:D:326:LEU:HD13	1:D:353:ILE:CG2	2.36	0.56
1:F:143:LEU:C	1:F:145:GLY:H	2.09	0.56
1:B:844:GLN:HE22	2:I:79:LYS:HE3	1.71	0.56
3:P:50:SER:CB	3:Q:45:ARG:NH1	2.64	0.56
1:C:1023:ASP:OD1	1:C:1046:THR:OG1	2.24	0.55
1:D:884:TRP:CZ3	2:K:79:LYS:CA	2.74	0.55
1:E:326:LEU:HD13	1:E:353:ILE:CG2	2.36	0.55
1:F:336:ASN:HB2	1:G:431:LYS:HE3	1.87	0.55
1:G:844:GLN:HE22	2:N:79:LYS:HE3	1.71	0.55
1:A:463:GLN:OE1	1:A:466:ARG:NH2	2.28	0.55
1:B:1092:ASP:OD2	1:B:1133:SER:OG	2.17	0.55
1:B:170:ASP:OD1	1:B:171:HIS:N	2.39	0.55
1:B:326:LEU:HD13	1:B:353:ILE:CG2	2.37	0.55
1:G:170:ASP:OD1	1:G:171:HIS:N	2.39	0.55
1:A:326:LEU:HD13	1:A:353:ILE:CG2	2.37	0.55
1:A:716:LEU:HB3	1:A:728:TRP:HB2	1.87	0.55
1:A:884:TRP:CZ3	2:H:79:LYS:CA	2.74	0.55
1:B:845:TYR:HB3	1:B:858:ALA:HB3	1.89	0.55
1:C:217:PRO:HG3	1:C:226:ARG:HH12	1.72	0.55
1:C:844:GLN:HE22	2:J:79:LYS:HE3	1.71	0.55
1:D:217:PRO:HG3	1:D:226:ARG:HH12	1.71	0.55
1:A:763:ALA:HA	1:A:801:VAL:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:845:TYR:HB3	1:C:858:ALA:HB3	1.89	0.55
1:C:617:ALA:HA	1:C:904:GLN:HG2	1.89	0.55
1:D:572:GLU:HA	1:D:577:TYR:CD2	2.42	0.55
1:E:884:TRP:CD1	1:E:884:TRP:N	2.73	0.55
1:F:572:GLU:HA	1:F:577:TYR:CD2	2.42	0.55
1:F:716:LEU:HB3	1:F:728:TRP:HB2	1.87	0.55
1:F:763:ALA:HA	1:F:801:VAL:H	1.70	0.55
1:G:763:ALA:HA	1:G:801:VAL:H	1.70	0.55
1:A:845:TYR:HB3	1:A:858:ALA:HB3	1.89	0.55
1:B:572:GLU:HA	1:B:577:TYR:CD2	2.42	0.55
1:C:170:ASP:OD1	1:C:171:HIS:N	2.39	0.55
1:C:463:GLN:OE1	1:C:466:ARG:NH2	2.28	0.55
1:C:572:GLU:HA	1:C:577:TYR:CD2	2.42	0.55
1:D:763:ALA:HA	1:D:801:VAL:H	1.70	0.55
1:E:572:GLU:HA	1:E:577:TYR:CD2	2.42	0.55
1:F:326:LEU:HD13	1:F:353:ILE:CG2	2.36	0.55
1:A:572:GLU:HA	1:A:577:TYR:CD2	2.42	0.55
1:B:28:HIS:CE1	3:P:14:LEU:CD2	2.90	0.55
1:B:565:GLN:NE2	1:B:1213:PHE:CA	2.69	0.55
1:C:565:GLN:NE2	1:C:1213:PHE:CA	2.69	0.55
1:D:143:LEU:C	1:D:145:GLY:H	2.09	0.55
1:D:617:ALA:HA	1:D:904:GLN:HG2	1.89	0.55
1:F:217:PRO:HG3	1:F:226:ARG:HH12	1.71	0.55
1:G:326:LEU:HD13	1:G:353:ILE:CG2	2.36	0.55
1:G:572:GLU:HA	1:G:577:TYR:CD2	2.42	0.55
1:B:1086:GLY:CA	2:I:39:LYS:NZ	2.66	0.55
1:D:844:GLN:HE22	2:K:79:LYS:HE3	1.71	0.55
1:E:716:LEU:HB3	1:E:728:TRP:HB2	1.87	0.55
3:O:27:ASP:OD1	3:R:13:ARG:HG2	2.06	0.55
1:A:1092:ASP:OD2	1:A:1133:SER:OG	2.17	0.55
1:D:565:GLN:NE2	1:D:1213:PHE:CA	2.69	0.55
1:D:170:ASP:OD1	1:D:171:HIS:N	2.39	0.55
1:E:565:GLN:NE2	1:E:1213:PHE:CA	2.69	0.55
1:F:844:GLN:HE22	2:M:79:LYS:HE3	1.71	0.55
1:G:845:TYR:HB3	1:G:858:ALA:HB3	1.89	0.55
3:R:15:ARG:HD2	3:R:19:GLU:OE2	2.07	0.55
3:R:8:LEU:HD23	3:R:8:LEU:C	2.27	0.55
1:F:170:ASP:OD1	1:F:171:HIS:N	2.39	0.55
1:D:1086:GLY:CA	2:K:39:LYS:NZ	2.66	0.55
2:N:60:GLY:N	2:N:63:THR:OG1	2.34	0.55
3:P:8:LEU:C	3:P:8:LEU:HD23	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ALA:HA	1:B:904:GLN:HG2	1.89	0.55
1:D:845:TYR:HB3	1:D:858:ALA:HB3	1.89	0.55
1:D:884:TRP:CD1	1:D:884:TRP:N	2.73	0.55
1:F:524:HIS:HB2	1:F:646:THR:CG2	2.32	0.55
1:A:482:TYR:HH	1:A:490:HIS:HE2	1.47	0.54
1:E:143:LEU:C	1:E:145:GLY:H	2.09	0.54
1:F:565:GLN:NE2	1:F:1213:PHE:CA	2.69	0.54
1:A:550:LEU:HD21	1:A:607:SER:CB	2.35	0.54
1:B:1219:ASN:HB2	1:B:1237:ASN:HB3	1.89	0.54
1:B:716:LEU:HB3	1:B:728:TRP:HB2	1.87	0.54
1:E:170:ASP:OD1	1:E:171:HIS:N	2.39	0.54
1:G:1023:ASP:OD1	1:G:1046:THR:OG1	2.24	0.54
1:G:265:ARG:HH11	1:G:371:SER:HG	1.52	0.54
1:E:844:GLN:HE22	2:L:79:LYS:HE3	1.71	0.54
1:C:1219:ASN:HB2	1:C:1237:ASN:HB3	1.89	0.54
1:F:550:LEU:HD21	1:F:607:SER:CB	2.35	0.54
1:F:884:TRP:CD1	1:F:884:TRP:N	2.73	0.54
3:Q:8:LEU:HD23	3:Q:8:LEU:C	2.27	0.54
1:B:482:TYR:OH	1:B:490:HIS:NE2	2.35	0.54
1:C:727:LEU:HB3	1:C:737:ASN:HB2	1.90	0.54
1:D:1087:THR:N	2:K:39:LYS:HZ3	2.06	0.54
1:D:800:ILE:H	1:D:818:LYS:HE2	1.73	0.54
1:E:217:PRO:HG3	1:E:226:ARG:HH12	1.71	0.54
1:E:617:ALA:HA	1:E:904:GLN:HG2	1.89	0.54
1:A:143:LEU:C	1:A:145:GLY:H	2.09	0.54
1:A:217:PRO:HG3	1:A:226:ARG:HH12	1.71	0.54
1:D:1023:ASP:OD1	1:D:1046:THR:OG1	2.24	0.54
1:D:727:LEU:HB3	1:D:737:ASN:HB2	1.90	0.54
1:F:800:ILE:H	1:F:818:LYS:HE2	1.73	0.54
1:G:143:LEU:C	1:G:145:GLY:H	2.09	0.54
1:A:219:ASN:HD21	1:G:201:ASN:HD21	1.54	0.54
1:B:800:ILE:H	1:B:818:LYS:HE2	1.73	0.54
1:E:884:TRP:CZ3	2:L:79:LYS:CA	2.74	0.54
3:O:15:ARG:HD2	3:O:19:GLU:OE2	2.07	0.54
1:B:217:PRO:HG3	1:B:226:ARG:HH12	1.72	0.54
1:B:727:LEU:HB3	1:B:737:ASN:HB2	1.90	0.54
1:C:143:LEU:C	1:C:145:GLY:H	2.09	0.54
1:C:800:ILE:H	1:C:818:LYS:HE2	1.73	0.54
1:D:558:GLN:HA	1:D:559:PRO:C	2.28	0.54
1:D:612:ARG:NH2	1:D:903:ASP:O	2.41	0.54
1:E:727:LEU:HB3	1:E:737:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:612:ARG:NH2	1:F:903:ASP:O	2.41	0.54
1:F:845:TYR:HB3	1:F:858:ALA:HB3	1.89	0.54
2:I:40:THR:HA	2:I:59:TRP:HE1	1.73	0.54
1:E:1086:GLY:CA	2:L:39:LYS:NZ	2.66	0.54
1:A:1219:ASN:HB2	1:A:1237:ASN:HB3	1.89	0.54
1:A:800:ILE:H	1:A:818:LYS:HE2	1.73	0.54
1:C:265:ARG:NH1	1:C:371:SER:OG	2.37	0.54
1:D:30:ILE:CG2	3:Q:10:ARG:CB	2.80	0.54
1:A:265:ARG:HH11	1:A:371:SER:HG	1.55	0.54
1:E:558:GLN:HA	1:E:559:PRO:C	2.28	0.54
1:F:558:GLN:HA	1:F:559:PRO:C	2.28	0.54
1:G:482:TYR:HH	1:G:490:HIS:HE2	1.52	0.54
1:G:550:LEU:HD21	1:G:607:SER:CB	2.35	0.54
2:L:40:THR:HA	2:L:59:TRP:HE1	1.73	0.54
1:A:558:GLN:HA	1:A:559:PRO:C	2.28	0.54
1:A:617:ALA:HA	1:A:904:GLN:HG2	1.89	0.54
1:A:864:VAL:CG2	1:A:885:VAL:HG21	2.38	0.54
1:B:336:ASN:HB2	1:C:431:LYS:HE3	1.90	0.54
1:D:1219:ASN:HB2	1:D:1237:ASN:HB3	1.89	0.54
1:F:987:ILE:HD11	1:F:1018:LEU:HD22	1.90	0.54
1:F:1219:ASN:HB2	1:F:1237:ASN:HB3	1.89	0.54
1:F:265:ARG:HH11	1:F:371:SER:HG	1.55	0.54
1:G:217:PRO:HG3	1:G:226:ARG:HH12	1.72	0.54
1:G:612:ARG:NH2	1:G:903:ASP:O	2.41	0.54
3:Q:15:ARG:HD2	3:Q:19:GLU:OE2	2.07	0.54
1:B:13:ARG:O	1:B:17:GLU:HG3	2.09	0.53
1:B:558:GLN:HA	1:B:559:PRO:C	2.28	0.53
1:B:612:ARG:NH2	1:B:903:ASP:O	2.41	0.53
1:C:558:GLN:HA	1:C:559:PRO:C	2.28	0.53
1:F:727:LEU:HB3	1:F:737:ASN:HB2	1.90	0.53
1:D:358:SER:HB3	1:E:274:MET:HE3	1.89	0.53
1:D:524:HIS:HB2	1:D:646:THR:CG2	2.32	0.53
1:E:987:ILE:HD11	1:E:1018:LEU:HD22	1.90	0.53
1:E:845:TYR:HB3	1:E:858:ALA:HB3	1.89	0.53
1:F:266:ASP:OD1	1:F:267:LYS:N	2.41	0.53
1:G:800:ILE:H	1:G:818:LYS:HE2	1.73	0.53
3:O:8:LEU:C	3:O:8:LEU:HD23	2.27	0.53
1:A:266:ASP:OD1	1:A:267:LYS:N	2.41	0.53
1:C:1061:TRP:CE2	1:C:1090:SER:HA	2.43	0.53
1:C:266:ASP:OD1	1:C:267:LYS:N	2.42	0.53
1:E:1023:ASP:OD1	1:E:1046:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASP:OD1	1:E:267:LYS:N	2.42	0.53
1:E:612:ARG:NH2	1:E:903:ASP:O	2.41	0.53
1:F:1023:ASP:OD1	1:F:1046:THR:OG1	2.24	0.53
2:K:40:THR:HA	2:K:59:TRP:HE1	1.73	0.53
2:N:40:THR:HA	2:N:59:TRP:HE1	1.73	0.53
1:C:864:VAL:CG2	1:C:885:VAL:HG21	2.38	0.53
1:D:1061:TRP:CE2	1:D:1090:SER:HA	2.43	0.53
1:D:13:ARG:O	1:D:17:GLU:HG3	2.09	0.53
1:E:1061:TRP:CE2	1:E:1090:SER:HA	2.43	0.53
1:E:698:HIS:CE1	1:E:726:LYS:HD2	2.44	0.53
1:E:864:VAL:CG2	1:E:885:VAL:HG21	2.38	0.53
1:F:358:SER:OG	1:G:274:MET:HG2	2.09	0.53
1:G:266:ASP:OD1	1:G:267:LYS:N	2.41	0.53
1:G:558:GLN:HA	1:G:559:PRO:C	2.28	0.53
1:G:864:VAL:CG2	1:G:885:VAL:HG21	2.38	0.53
1:G:987:ILE:HD11	1:G:1018:LEU:HD22	1.91	0.53
1:A:884:TRP:N	1:A:884:TRP:CD1	2.73	0.53
1:A:612:ARG:NH2	1:A:903:ASP:O	2.41	0.53
1:B:1061:TRP:CE2	1:B:1090:SER:HA	2.43	0.53
1:B:267:LYS:HZ1	1:B:419:VAL:HG12	1.74	0.53
1:E:13:ARG:O	1:E:17:GLU:HG3	2.09	0.53
1:E:800:ILE:H	1:E:818:LYS:HE2	1.73	0.53
1:F:617:ALA:HA	1:F:904:GLN:HG2	1.89	0.53
1:B:584:ALA:HB1	1:B:594:TYR:CD2	2.44	0.53
1:B:884:TRP:CD1	1:B:884:TRP:N	2.73	0.53
1:C:612:ARG:NH2	1:C:903:ASP:O	2.41	0.53
1:D:1149:GLY:HA3	1:D:1178:GLY:HA2	1.91	0.53
1:E:1149:GLY:HA3	1:E:1178:GLY:HA2	1.91	0.53
2:M:40:THR:HA	2:M:59:TRP:HE1	1.73	0.53
1:A:1087:THR:N	2:H:39:LYS:HZ3	2.06	0.53
1:A:698:HIS:CE1	1:A:726:LYS:HD2	2.44	0.53
1:B:463:GLN:OE1	1:B:466:ARG:NH2	2.28	0.53
1:C:884:TRP:N	1:C:884:TRP:CD1	2.73	0.53
1:D:987:ILE:HD11	1:D:1018:LEU:HD22	1.90	0.53
1:D:864:VAL:CG2	1:D:885:VAL:HG21	2.38	0.53
1:G:1149:GLY:HA3	1:G:1178:GLY:HA2	1.91	0.53
1:G:727:LEU:HB3	1:G:737:ASN:HB2	1.90	0.53
1:A:1086:GLY:CA	2:H:39:LYS:NZ	2.66	0.53
2:I:67:TYR:OH	2:I:80:MET:SD	2.57	0.53
2:J:40:THR:HA	2:J:59:TRP:HE1	1.73	0.53
1:A:1149:GLY:HA3	1:A:1178:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:HB2	1:B:431:LYS:HE3	1.90	0.53
1:B:266:ASP:OD1	1:B:267:LYS:N	2.41	0.53
1:B:864:VAL:CG2	1:B:885:VAL:HG21	2.38	0.53
1:F:864:VAL:CG2	1:F:885:VAL:HG21	2.38	0.53
1:G:524:HIS:HB2	1:G:646:THR:CG2	2.32	0.53
1:A:267:LYS:HZ1	1:A:419:VAL:HG12	1.74	0.53
1:A:727:LEU:HB3	1:A:737:ASN:HB2	1.90	0.53
1:C:267:LYS:HZ1	1:C:419:VAL:HG12	1.74	0.53
1:D:584:ALA:HB1	1:D:594:TYR:CD2	2.44	0.53
1:F:698:HIS:CE1	1:F:726:LYS:HD2	2.44	0.53
1:G:1219:ASN:HB2	1:G:1237:ASN:HB3	1.90	0.53
1:G:698:HIS:CE1	1:G:726:LYS:HD2	2.44	0.53
1:G:617:ALA:HA	1:G:904:GLN:HG2	1.89	0.53
1:C:524:HIS:HB2	1:C:646:THR:CG2	2.32	0.53
1:C:584:ALA:HB1	1:C:594:TYR:CD2	2.44	0.53
1:D:698:HIS:CE1	1:D:726:LYS:HD2	2.44	0.53
1:F:1061:TRP:CE2	1:F:1090:SER:HA	2.43	0.53
1:F:1149:GLY:HA3	1:F:1178:GLY:HA2	1.91	0.53
1:F:1191:MET:SD	1:F:1209:SER:OG	2.63	0.53
1:F:631:ALA:HB1	1:F:639:LEU:HD11	1.91	0.53
2:H:40:THR:HA	2:H:59:TRP:HE1	1.73	0.53
1:D:266:ASP:OD1	1:D:267:LYS:N	2.41	0.52
1:D:267:LYS:HZ1	1:D:419:VAL:HG12	1.74	0.52
1:E:1219:ASN:HB2	1:E:1237:ASN:HB3	1.89	0.52
1:E:844:GLN:HE22	2:L:79:LYS:HZ2	1.56	0.52
1:G:13:ARG:O	1:G:17:GLU:HG3	2.08	0.52
1:A:274:MET:HE2	1:G:358:SER:HB3	1.91	0.52
1:G:884:TRP:CD1	1:G:884:TRP:N	2.73	0.52
1:A:1061:TRP:CE2	1:A:1090:SER:HA	2.43	0.52
1:A:844:GLN:HE22	2:H:79:LYS:HZ2	1.56	0.52
1:C:1149:GLY:HA3	1:C:1178:GLY:HA2	1.91	0.52
1:D:609:LEU:HD23	1:D:908:LEU:HD13	1.91	0.52
1:E:336:ASN:HB2	1:F:431:LYS:HE3	1.91	0.52
1:F:1087:THR:N	2:M:39:LYS:HZ3	2.07	0.52
1:G:584:ALA:HB1	1:G:594:TYR:CD2	2.44	0.52
1:A:987:ILE:HD11	1:A:1018:LEU:HD22	1.90	0.52
1:B:1126:HIS:CE1	1:B:1129:CYS:H	2.28	0.52
1:B:1149:GLY:HA3	1:B:1178:GLY:HA2	1.91	0.52
1:B:326:LEU:HD13	1:B:353:ILE:HG22	1.92	0.52
1:C:698:HIS:CE1	1:C:726:LYS:HD2	2.44	0.52
1:E:631:ALA:HB1	1:E:639:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1061:TRP:CE2	1:G:1090:SER:HA	2.43	0.52
1:G:945:ARG:HD2	1:G:961:GLU:HB2	1.92	0.52
2:K:67:TYR:OH	2:K:80:MET:SD	2.57	0.52
1:A:365:ASP:OD1	1:A:444:PHE:CE1	2.63	0.52
1:B:1087:THR:N	2:I:39:LYS:HZ3	2.07	0.52
1:C:265:ARG:HH11	1:C:371:SER:HG	1.57	0.52
1:E:267:LYS:HZ1	1:E:419:VAL:HG12	1.74	0.52
1:E:609:LEU:HD23	1:E:908:LEU:HD13	1.91	0.52
1:G:365:ASP:OD1	1:G:444:PHE:CE1	2.63	0.52
3:P:50:SER:HB3	3:Q:45:ARG:NH1	2.24	0.52
1:A:584:ALA:HB1	1:A:594:TYR:CD2	2.44	0.52
1:C:336:ASN:HB2	1:D:431:LYS:HE3	1.91	0.52
1:D:326:LEU:HD13	1:D:353:ILE:HG22	1.92	0.52
1:F:945:ARG:HD2	1:F:961:GLU:HB2	1.92	0.52
1:F:358:SER:HB3	1:G:274:MET:HE2	1.92	0.52
2:M:60:GLY:N	2:M:63:THR:OG1	2.34	0.52
1:A:945:ARG:HD2	1:A:961:GLU:HB2	1.92	0.52
1:C:326:LEU:HD13	1:C:353:ILE:HG22	1.92	0.52
1:E:326:LEU:HD13	1:E:353:ILE:HG22	1.92	0.52
1:E:584:ALA:HB1	1:E:594:TYR:CD2	2.44	0.52
1:G:631:ALA:HB1	1:G:639:LEU:HD11	1.91	0.52
2:H:67:TYR:OH	2:H:80:MET:SD	2.57	0.52
1:F:1086:GLY:CA	2:M:39:LYS:NZ	2.66	0.52
1:G:844:GLN:NE2	2:N:79:LYS:NZ	2.58	0.52
1:B:987:ILE:HD11	1:B:1018:LEU:HD22	1.90	0.52
1:C:987:ILE:HD11	1:C:1018:LEU:HD22	1.90	0.52
1:D:37:ILE:HG12	3:Q:10:ARG:CD	2.40	0.52
1:D:725:LEU:HB2	1:D:739:MET:HB2	1.92	0.52
1:F:365:ASP:OD1	1:F:444:PHE:CE1	2.63	0.52
1:A:882:LEU:HD12	1:A:1176:HIS:NE2	2.25	0.52
1:A:326:LEU:HD13	1:A:353:ILE:HG22	1.92	0.52
1:A:609:LEU:HD23	1:A:908:LEU:HD13	1.91	0.52
1:B:550:LEU:HD21	1:B:607:SER:CB	2.35	0.52
1:C:1126:HIS:CE1	1:C:1129:CYS:H	2.28	0.52
1:D:14:GLU:HB2	1:E:31:SER:OG	2.09	0.52
1:D:864:VAL:HG23	1:D:885:VAL:HG21	1.92	0.52
1:E:945:ARG:HD2	1:E:961:GLU:HB2	1.92	0.52
2:N:67:TYR:OH	2:N:80:MET:SD	2.57	0.52
1:A:1126:HIS:CE1	1:A:1129:CYS:H	2.28	0.52
1:B:365:ASP:OD1	1:B:444:PHE:CE1	2.63	0.52
1:E:365:ASP:OD1	1:E:444:PHE:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:LYS:HZ1	1:F:419:VAL:HG12	1.75	0.52
1:F:326:LEU:HD13	1:F:353:ILE:HG22	1.92	0.52
1:A:265:ARG:NH2	4:A:1301:DTP:O2G	2.31	0.52
1:A:530:ARG:HD2	1:A:545:GLN:HE22	1.75	0.52
1:B:698:HIS:CE1	1:B:726:LYS:HD2	2.44	0.52
1:B:945:ARG:HD2	1:B:961:GLU:HB2	1.92	0.52
1:C:864:VAL:HG23	1:C:885:VAL:HG21	1.92	0.52
1:D:1126:HIS:CE1	1:D:1129:CYS:H	2.28	0.52
1:D:882:LEU:HD12	1:D:1176:HIS:NE2	2.25	0.52
1:D:844:GLN:NE2	2:K:79:LYS:NZ	2.57	0.52
1:E:864:VAL:HG23	1:E:885:VAL:HG21	1.92	0.52
1:F:584:ALA:HB1	1:F:594:TYR:CD2	2.44	0.52
1:A:416:GLN:HE21	1:G:334:PHE:HE1	1.57	0.52
1:G:609:LEU:HD23	1:G:908:LEU:HD13	1.91	0.52
1:B:844:GLN:NE2	2:I:79:LYS:NZ	2.57	0.51
1:C:609:LEU:HD23	1:C:908:LEU:HD13	1.91	0.51
1:E:600:LYS:HZ1	1:E:1213:PHE:HZ	1.58	0.51
1:E:550:LEU:HD21	1:E:607:SER:CB	2.35	0.51
1:G:265:ARG:NH1	1:G:371:SER:OG	2.37	0.51
1:E:725:LEU:HB2	1:E:739:MET:HB2	1.92	0.51
1:F:882:LEU:HD12	1:F:1176:HIS:NE2	2.25	0.51
1:G:267:LYS:HZ1	1:G:419:VAL:HG12	1.74	0.51
1:A:844:GLN:NE2	2:H:79:LYS:NZ	2.58	0.51
2:J:60:GLY:N	2:J:63:THR:OG1	2.34	0.51
1:C:550:LEU:HD21	1:C:607:SER:CB	2.35	0.51
1:C:725:LEU:HB2	1:C:739:MET:HB2	1.92	0.51
1:F:337:ARG:NH1	1:G:409:GLU:OE2	2.44	0.51
1:G:326:LEU:HD13	1:G:353:ILE:HG22	1.92	0.51
1:B:400:LEU:HB3	1:B:404:TRP:CZ3	2.46	0.51
1:C:334:PHE:HE1	1:D:416:GLN:HE21	1.57	0.51
1:C:400:LEU:HB3	1:C:404:TRP:CZ3	2.46	0.51
1:D:365:ASP:OD1	1:D:444:PHE:CE1	2.63	0.51
1:D:530:ARG:HD2	1:D:545:GLN:HE22	1.75	0.51
1:D:550:LEU:HD21	1:D:607:SER:CB	2.35	0.51
1:D:631:ALA:HB1	1:D:639:LEU:HD11	1.91	0.51
1:E:530:ARG:HD2	1:E:545:GLN:HE22	1.76	0.51
1:F:482:TYR:OH	1:F:490:HIS:NE2	2.35	0.51
1:F:692:VAL:HG12	1:F:693:HIS:ND1	2.26	0.51
1:F:884:TRP:CZ3	2:M:79:LYS:CA	2.74	0.51
1:F:609:LEU:HD23	1:F:908:LEU:HD13	1.91	0.51
1:G:864:VAL:HG23	1:G:885:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASN:C	1:A:592:MET:N	2.64	0.51
1:A:692:VAL:HG12	1:A:693:HIS:ND1	2.25	0.51
1:A:725:LEU:HB2	1:A:739:MET:HB2	1.92	0.51
1:B:609:LEU:HD23	1:B:908:LEU:HD13	1.91	0.51
1:D:1191:MET:SD	1:D:1209:SER:OG	2.63	0.51
1:E:882:LEU:HD12	1:E:1176:HIS:NE2	2.25	0.51
1:F:844:GLN:NE2	2:M:79:LYS:NZ	2.57	0.51
2:K:60:GLY:N	2:K:63:THR:OG1	2.34	0.51
3:P:50:SER:HB3	3:Q:45:ARG:HH12	1.74	0.51
1:B:692:VAL:HG12	1:B:693:HIS:ND1	2.26	0.51
1:C:692:VAL:HG12	1:C:693:HIS:ND1	2.26	0.51
1:F:1126:HIS:CE1	1:F:1129:CYS:H	2.28	0.51
1:F:530:ARG:HD2	1:F:545:GLN:HE22	1.75	0.51
1:E:1086:GLY:HA2	2:L:39:LYS:HE2	1.92	0.51
1:C:365:ASP:OD1	1:C:444:PHE:CE1	2.63	0.51
1:D:590:ASN:C	1:D:592:MET:N	2.64	0.51
1:F:590:ASN:C	1:F:592:MET:N	2.64	0.51
1:G:1086:GLY:HA2	2:N:39:LYS:HE2	1.92	0.51
1:G:1126:HIS:CE1	1:G:1129:CYS:H	2.28	0.51
2:L:60:GLY:N	2:L:63:THR:OG1	2.34	0.51
1:G:1086:GLY:CA	2:N:39:LYS:NZ	2.66	0.51
1:A:400:LEU:HB3	1:A:404:TRP:CZ3	2.46	0.51
1:A:631:ALA:HB1	1:A:639:LEU:HD11	1.91	0.51
1:B:265:ARG:HH11	1:B:371:SER:HG	1.54	0.51
1:B:725:LEU:HB2	1:B:739:MET:HB2	1.92	0.51
1:B:864:VAL:HG23	1:B:885:VAL:HG21	1.92	0.51
1:C:945:ARG:HD2	1:C:961:GLU:HB2	1.92	0.51
1:D:336:ASN:HB2	1:E:431:LYS:HE3	1.93	0.51
1:D:400:LEU:HB3	1:D:404:TRP:CZ3	2.46	0.51
1:F:265:ARG:NH1	1:F:371:SER:OG	2.37	0.51
1:G:590:ASN:C	1:G:592:MET:N	2.64	0.51
2:H:60:GLY:N	2:H:63:THR:OG1	2.34	0.51
2:H:94:LEU:HD21	5:H:500:HEC:HMB1	1.93	0.51
2:M:94:LEU:HD21	5:M:500:HEC:HMB1	1.93	0.51
1:B:590:ASN:C	1:B:592:MET:N	2.64	0.51
1:C:530:ARG:HD2	1:C:545:GLN:HE22	1.76	0.51
1:E:1126:HIS:CE1	1:E:1129:CYS:H	2.28	0.51
1:G:152:ILE:HD11	1:G:263:THR:HG22	1.92	0.51
2:I:94:LEU:HD21	5:I:500:HEC:HMB1	1.93	0.51
2:N:94:LEU:HD21	5:N:500:HEC:HMB1	1.93	0.51
3:P:32:ARG:HD2	3:P:76:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:HIS:ND1	1:B:1024:ASP:OD2	2.44	0.51
1:B:530:ARG:HD2	1:B:545:GLN:HE22	1.76	0.51
1:C:562:ASN:HB2	1:C:565:GLN:HG2	1.93	0.51
1:F:725:LEU:HB2	1:F:739:MET:HB2	1.92	0.51
1:G:882:LEU:HD12	1:G:1176:HIS:NE2	2.25	0.51
1:F:334:PHE:HE1	1:G:416:GLN:HE21	1.58	0.51
1:G:530:ARG:HD2	1:G:545:GLN:HE22	1.76	0.51
1:G:725:LEU:HB2	1:G:739:MET:HB2	1.92	0.51
1:A:152:ILE:HD11	1:A:263:THR:HG22	1.92	0.50
1:A:864:VAL:HG23	1:A:885:VAL:HG21	1.92	0.50
1:B:608:ARG:HD2	1:B:910:GLU:HB2	1.94	0.50
1:C:844:GLN:NE2	2:J:79:LYS:NZ	2.57	0.50
1:D:562:ASN:HB2	1:D:565:GLN:HG2	1.94	0.50
1:D:945:ARG:HD2	1:D:961:GLU:HB2	1.92	0.50
1:E:692:VAL:HG12	1:E:693:HIS:ND1	2.26	0.50
1:F:864:VAL:HG23	1:F:885:VAL:HG21	1.92	0.50
2:I:60:GLY:N	2:I:63:THR:OG1	2.34	0.50
3:O:32:ARG:HD2	3:O:76:CYS:SG	2.51	0.50
1:B:700:GLU:HG3	1:B:721:SER:HB2	1.94	0.50
1:C:1002:HIS:ND1	1:C:1024:ASP:OD2	2.45	0.50
1:D:1002:HIS:ND1	1:D:1024:ASP:OD2	2.44	0.50
1:E:400:LEU:HB3	1:E:404:TRP:CZ3	2.46	0.50
1:F:1002:HIS:ND1	1:F:1024:ASP:OD2	2.44	0.50
1:F:862:TYR:HB3	1:F:884:TRP:CA	2.42	0.50
1:A:1002:HIS:ND1	1:A:1024:ASP:OD2	2.44	0.50
1:A:334:PHE:HE1	1:B:416:GLN:HE21	1.58	0.50
1:A:608:ARG:HD2	1:A:910:GLU:HB2	1.94	0.50
1:B:344:GLN:OE1	1:B:349:GLN:NE2	2.44	0.50
1:B:562:ASN:HB2	1:B:565:GLN:HG2	1.94	0.50
1:C:1086:GLY:HA2	2:J:39:LYS:HE2	1.92	0.50
1:G:819:ASN:ND2	1:G:840:HIS:O	2.45	0.50
1:C:348:LYS:NZ	1:C:443:ASP:OD1	2.45	0.50
1:G:1002:HIS:ND1	1:G:1024:ASP:OD2	2.44	0.50
1:G:692:VAL:HG12	1:G:693:HIS:ND1	2.26	0.50
2:L:94:LEU:HD21	5:L:500:HEC:HMB1	1.93	0.50
3:P:15:ARG:HD2	3:P:19:GLU:OE2	2.07	0.50
1:A:482:TYR:OH	1:A:490:HIS:NE2	2.35	0.50
1:A:762:SER:OG	1:A:764:ASP:OD1	2.26	0.50
1:B:631:ALA:HB1	1:B:639:LEU:HD11	1.91	0.50
1:E:562:ASN:HB2	1:E:565:GLN:HG2	1.94	0.50
1:E:862:TYR:HB3	1:E:884:TRP:CA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ILE:HD11	1:F:263:THR:HG22	1.92	0.50
1:A:431:LYS:HE3	1:G:336:ASN:HB2	1.92	0.50
1:G:400:LEU:HB3	1:G:404:TRP:CZ3	2.46	0.50
3:Q:52:ARG:HD2	3:R:38:HIS:ND1	2.22	0.50
1:B:152:ILE:HD11	1:B:263:THR:HG22	1.92	0.50
1:B:348:LYS:NZ	1:B:443:ASP:OD1	2.45	0.50
1:C:882:LEU:HD12	1:C:1176:HIS:NE2	2.25	0.50
1:D:348:LYS:NZ	1:D:443:ASP:OD1	2.45	0.50
1:D:265:ARG:NH1	1:D:371:SER:OG	2.37	0.50
1:E:463:GLN:OE1	1:E:466:ARG:NH2	2.28	0.50
1:F:562:ASN:HB2	1:F:565:GLN:HG2	1.93	0.50
1:F:819:ASN:ND2	1:F:840:HIS:O	2.45	0.50
1:G:646:THR:HG23	1:G:648:GLU:HG3	1.94	0.50
1:A:700:GLU:HG3	1:A:721:SER:HB2	1.94	0.50
1:A:819:ASN:ND2	1:A:840:HIS:O	2.45	0.50
1:C:631:ALA:HB1	1:C:639:LEU:HD11	1.91	0.50
1:C:700:GLU:HG3	1:C:721:SER:HB2	1.94	0.50
1:D:692:VAL:HG12	1:D:693:HIS:ND1	2.26	0.50
1:F:862:TYR:OH	1:F:1237:ASN:O	2.30	0.50
3:R:32:ARG:HD2	3:R:76:CYS:SG	2.51	0.50
1:C:152:ILE:HD11	1:C:263:THR:HG22	1.92	0.50
1:C:825:ASP:HB2	1:C:832:LEU:HD22	1.93	0.50
1:D:1222:LYS:HB3	1:D:1224:HIS:HE1	1.77	0.50
1:E:1002:HIS:ND1	1:E:1024:ASP:OD2	2.44	0.50
1:F:400:LEU:HB3	1:F:404:TRP:CZ3	2.46	0.50
1:D:1086:GLY:HA2	2:K:39:LYS:HE2	1.92	0.50
1:A:298:PHE:HD2	1:A:328:GLY:HA3	1.77	0.50
1:A:562:ASN:HB2	1:A:565:GLN:HG2	1.93	0.50
1:B:825:ASP:HB2	1:B:832:LEU:HD22	1.93	0.50
1:C:608:ARG:HD2	1:C:910:GLU:HB2	1.94	0.50
1:C:819:ASN:ND2	1:C:840:HIS:O	2.45	0.50
1:C:358:SER:HB3	1:D:274:MET:HE2	1.93	0.50
1:D:819:ASN:ND2	1:D:840:HIS:O	2.45	0.50
1:E:348:LYS:NZ	1:E:443:ASP:OD1	2.45	0.50
1:E:862:TYR:OH	1:E:1237:ASN:O	2.30	0.50
1:G:348:LYS:NZ	1:G:443:ASP:OD1	2.45	0.50
1:A:1222:LYS:HB3	1:A:1224:HIS:HE1	1.77	0.49
1:A:365:ASP:OD1	1:A:444:PHE:HE1	1.95	0.49
1:A:646:THR:HG23	1:A:648:GLU:HG3	1.94	0.49
1:B:819:ASN:ND2	1:B:840:HIS:O	2.45	0.49
1:D:152:ILE:HD11	1:D:263:THR:HG22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ASP:OD1	1:D:444:PHE:HE1	1.95	0.49
1:F:646:THR:HG23	1:F:648:GLU:HG3	1.94	0.49
1:G:862:TYR:OH	1:G:1237:ASN:O	2.30	0.49
1:G:298:PHE:HD2	1:G:328:GLY:HA3	1.77	0.49
1:G:862:TYR:HB3	1:G:884:TRP:CA	2.42	0.49
2:I:41:GLY:HA2	2:I:48:TYR:CE1	2.47	0.49
2:J:41:GLY:HA2	2:J:48:TYR:CE1	2.47	0.49
3:Q:16:LEU:O	3:Q:20:LEU:HB2	2.12	0.49
1:B:1222:LYS:HB3	1:B:1224:HIS:HE1	1.77	0.49
1:E:819:ASN:ND2	1:E:840:HIS:O	2.45	0.49
1:E:884:TRP:CE3	2:L:81:ILE:HD11	2.48	0.49
1:F:1222:LYS:HB3	1:F:1224:HIS:HE1	1.77	0.49
1:F:298:PHE:HD2	1:F:328:GLY:HA3	1.77	0.49
1:F:463:GLN:OE1	1:F:466:ARG:NH2	2.28	0.49
1:G:562:ASN:HB2	1:G:565:GLN:HG2	1.94	0.49
1:A:1086:GLY:HA2	2:H:39:LYS:HE2	1.92	0.49
2:H:41:GLY:HA2	2:H:48:TYR:CE1	2.47	0.49
1:E:1086:GLY:CA	2:L:39:LYS:HZ1	2.20	0.49
3:R:16:LEU:O	3:R:20:LEU:HB2	2.12	0.49
1:C:365:ASP:OD1	1:C:444:PHE:HE1	1.96	0.49
1:C:862:TYR:HB3	1:C:884:TRP:CA	2.42	0.49
1:D:762:SER:OG	1:D:764:ASP:OD1	2.26	0.49
1:F:600:LYS:HZ1	1:F:1213:PHE:HZ	1.60	0.49
1:G:1020:SER:HB2	1:G:1028:GLN:HE21	1.77	0.49
2:J:94:LEU:HD21	5:J:500:HEC:HMB1	1.93	0.49
1:C:884:TRP:CE3	2:J:81:ILE:HD11	2.48	0.49
2:K:41:GLY:HA2	2:K:48:TYR:CE1	2.47	0.49
1:F:884:TRP:CE3	2:M:81:ILE:HD11	2.47	0.49
1:A:331:LEU:HD13	1:A:338:TRP:CH2	2.48	0.49
1:A:265:ARG:NH1	1:A:371:SER:OG	2.37	0.49
1:C:1222:LYS:HB3	1:C:1224:HIS:HE1	1.77	0.49
1:D:825:ASP:HB2	1:D:832:LEU:HD22	1.93	0.49
1:E:152:ILE:HD11	1:E:263:THR:HG22	1.92	0.49
1:F:365:ASP:OD1	1:F:444:PHE:HE1	1.96	0.49
1:F:700:GLU:HG3	1:F:721:SER:HB2	1.94	0.49
2:N:41:GLY:HA2	2:N:48:TYR:CE1	2.47	0.49
3:Q:32:ARG:HD2	3:Q:76:CYS:SG	2.52	0.49
1:A:825:ASP:HB2	1:A:832:LEU:HD22	1.93	0.49
1:B:298:PHE:HD2	1:B:328:GLY:HA3	1.77	0.49
1:B:885:VAL:HG12	1:B:887:GLY:N	2.28	0.49
1:D:862:TYR:OH	1:D:1237:ASN:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:THR:HG23	1:D:648:GLU:HG3	1.94	0.49
1:D:700:GLU:HG3	1:D:721:SER:HB2	1.94	0.49
1:E:700:GLU:HG3	1:E:721:SER:HB2	1.94	0.49
1:B:1086:GLY:HA2	2:I:39:LYS:HE2	1.92	0.49
2:I:40:THR:HG22	2:I:59:TRP:CE2	2.48	0.49
1:D:884:TRP:CE3	2:K:81:ILE:HD11	2.47	0.49
1:B:118:GLY:O	1:B:184:TRP:HB2	2.13	0.49
1:B:862:TYR:HB3	1:B:884:TRP:CA	2.42	0.49
1:D:334:PHE:HE1	1:E:416:GLN:HE21	1.60	0.49
1:E:590:ASN:C	1:E:592:MET:N	2.64	0.49
1:E:885:VAL:HG12	1:E:887:GLY:N	2.28	0.49
1:F:118:GLY:O	1:F:184:TRP:HB2	2.13	0.49
1:F:348:LYS:NZ	1:F:443:ASP:OD1	2.45	0.49
1:F:825:ASP:HB2	1:F:832:LEU:HD22	1.93	0.49
1:G:608:ARG:HD2	1:G:910:GLU:HB2	1.94	0.49
1:D:31:SER:HA	3:Q:11:ARG:HA	1.95	0.49
1:A:862:TYR:HB3	1:A:884:TRP:CA	2.42	0.49
1:B:334:PHE:HE1	1:C:416:GLN:HE21	1.60	0.49
1:D:118:GLY:O	1:D:184:TRP:HB2	2.13	0.49
1:D:565:GLN:NE2	1:D:1213:PHE:HA	2.28	0.49
1:E:365:ASP:OD1	1:E:444:PHE:HE1	1.95	0.49
1:E:265:ARG:NH1	1:E:371:SER:OG	2.37	0.49
1:F:608:ARG:HD2	1:F:910:GLU:HB2	1.94	0.49
1:G:1222:LYS:HB3	1:G:1224:HIS:HE1	1.76	0.49
1:G:825:ASP:HB2	1:G:832:LEU:HD22	1.93	0.49
1:B:884:TRP:CE3	2:I:81:ILE:HD11	2.48	0.49
1:E:844:GLN:NE2	2:L:79:LYS:NZ	2.57	0.49
1:A:862:TYR:OH	1:A:1237:ASN:O	2.30	0.49
1:C:1020:SER:HB2	1:C:1028:GLN:HE21	1.77	0.49
1:C:118:GLY:O	1:C:184:TRP:HB2	2.13	0.49
1:C:885:VAL:HG12	1:C:887:GLY:N	2.28	0.49
1:D:1020:SER:HB2	1:D:1028:GLN:HE21	1.77	0.49
1:E:331:LEU:HD13	1:E:338:TRP:CH2	2.48	0.49
1:E:825:ASP:HB2	1:E:832:LEU:HD22	1.93	0.49
2:L:41:GLY:HA2	2:L:48:TYR:CE1	2.47	0.49
2:M:40:THR:HG22	2:M:59:TRP:CE2	2.48	0.49
3:O:16:LEU:O	3:O:20:LEU:HB2	2.12	0.49
1:B:365:ASP:OD1	1:B:444:PHE:HE1	1.96	0.49
1:B:929:VAL:HB	1:B:936:MET:HB2	1.95	0.49
1:D:569:CYS:CB	1:D:600:LYS:HZ3	2.25	0.49
1:D:862:TYR:HB3	1:D:884:TRP:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:PHE:HD2	1:E:328:GLY:HA3	1.77	0.49
1:E:608:ARG:HD2	1:E:910:GLU:HB2	1.94	0.49
1:F:565:GLN:NE2	1:F:1213:PHE:HA	2.28	0.49
1:F:331:LEU:HD13	1:F:338:TRP:CH2	2.47	0.49
2:H:40:THR:HG22	2:H:59:TRP:CE2	2.48	0.49
2:J:40:THR:HG22	2:J:59:TRP:CE2	2.48	0.49
2:K:94:LEU:HD21	5:K:500:HEC:HMB1	1.93	0.49
2:L:40:THR:HG22	2:L:59:TRP:CE2	2.48	0.49
1:A:885:VAL:HG12	1:A:887:GLY:N	2.28	0.49
1:B:1203:ASN:OD1	1:B:1204:VAL:N	2.46	0.49
1:B:265:ARG:NH1	1:B:371:SER:OG	2.37	0.49
1:C:331:LEU:HD13	1:C:338:TRP:CH2	2.47	0.49
1:C:646:THR:HG23	1:C:648:GLU:HG3	1.94	0.49
1:F:1086:GLY:HA2	2:M:39:LYS:HE2	1.92	0.49
1:G:700:GLU:HG3	1:G:721:SER:HB2	1.94	0.49
1:B:646:THR:HG23	1:B:648:GLU:HG3	1.94	0.48
1:C:565:GLN:NE2	1:C:1213:PHE:HA	2.28	0.48
1:D:1026:GLU:HG3	1:D:1041:ARG:HG2	1.95	0.48
1:D:1203:ASN:OD1	1:D:1204:VAL:N	2.46	0.48
1:D:608:ARG:HD2	1:D:910:GLU:HB2	1.94	0.48
1:E:1203:ASN:OD1	1:E:1204:VAL:N	2.46	0.48
1:E:646:THR:HG23	1:E:648:GLU:HG3	1.94	0.48
1:G:118:GLY:O	1:G:184:TRP:HB2	2.13	0.48
1:G:565:GLN:NE2	1:G:1213:PHE:HA	2.28	0.48
1:G:884:TRP:CE3	2:N:81:ILE:HD11	2.47	0.48
1:A:565:GLN:NE2	1:A:1213:PHE:HA	2.28	0.48
1:A:884:TRP:CE3	2:H:81:ILE:HD11	2.47	0.48
1:B:565:GLN:NE2	1:B:1213:PHE:HA	2.28	0.48
1:B:862:TYR:OH	1:B:1237:ASN:O	2.30	0.48
1:D:113:VAL:HG11	1:D:174:LEU:HD21	1.95	0.48
1:D:885:VAL:HG12	1:D:887:GLY:N	2.28	0.48
1:E:1026:GLU:HG3	1:E:1041:ARG:HG2	1.95	0.48
1:E:1222:LYS:HB3	1:E:1224:HIS:HE1	1.77	0.48
1:E:265:ARG:HH11	1:E:371:SER:HG	1.58	0.48
1:E:568:LEU:HD13	1:E:595:LEU:O	2.13	0.48
1:F:752:SER:HB2	1:F:753:PRO:HD2	1.95	0.48
1:G:1026:GLU:HG3	1:G:1041:ARG:HG2	1.95	0.48
1:G:1203:ASN:OD1	1:G:1204:VAL:N	2.46	0.48
2:K:40:THR:HG22	2:K:59:TRP:CE2	2.48	0.48
2:M:41:GLY:HA2	2:M:48:TYR:CE1	2.47	0.48
3:P:16:LEU:O	3:P:20:LEU:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLY:O	1:A:184:TRP:HB2	2.13	0.48
1:A:568:LEU:HD13	1:A:595:LEU:O	2.13	0.48
1:A:929:VAL:HB	1:A:936:MET:HB2	1.95	0.48
1:E:1020:SER:HB2	1:E:1028:GLN:HE21	1.77	0.48
1:E:113:VAL:HG11	1:E:174:LEU:HD21	1.95	0.48
1:F:885:VAL:HG12	1:F:887:GLY:N	2.28	0.48
1:G:752:SER:HB2	1:G:753:PRO:HD2	1.95	0.48
1:A:1026:GLU:HG3	1:A:1041:ARG:HG2	1.95	0.48
1:A:196:LEU:HG	1:A:200:GLN:HE22	1.78	0.48
1:B:1198:TYR:HA	1:B:1215:THR:HB	1.96	0.48
1:D:568:LEU:HD13	1:D:595:LEU:O	2.13	0.48
1:E:565:GLN:NE2	1:E:1213:PHE:HA	2.28	0.48
1:E:230:LEU:O	1:E:234:LYS:N	2.41	0.48
1:F:1026:GLU:HG3	1:F:1041:ARG:HG2	1.95	0.48
1:F:344:GLN:OE1	1:F:349:GLN:NE2	2.44	0.48
1:G:550:LEU:HD23	1:G:607:SER:HB2	1.91	0.48
1:B:1191:MET:SD	1:B:1209:SER:OG	2.63	0.48
1:B:331:LEU:HD13	1:B:338:TRP:CH2	2.48	0.48
1:C:1026:GLU:HG3	1:C:1041:ARG:HG2	1.95	0.48
1:C:1198:TYR:HA	1:C:1215:THR:HB	1.96	0.48
1:C:862:TYR:OH	1:C:1237:ASN:O	2.30	0.48
1:C:113:VAL:HG11	1:C:174:LEU:HD21	1.95	0.48
1:C:929:VAL:HB	1:C:936:MET:HB2	1.95	0.48
1:D:1198:TYR:HA	1:D:1215:THR:HB	1.96	0.48
1:G:331:LEU:HD13	1:G:338:TRP:CH2	2.48	0.48
1:G:885:VAL:HG12	1:G:887:GLY:N	2.28	0.48
2:N:40:THR:HG22	2:N:59:TRP:CE2	2.48	0.48
1:B:1020:SER:HB2	1:B:1028:GLN:HE21	1.77	0.48
1:C:298:PHE:HD2	1:C:328:GLY:HA3	1.77	0.48
1:D:298:PHE:HD2	1:D:328:GLY:HA3	1.77	0.48
1:F:196:LEU:HG	1:F:200:GLN:HE22	1.78	0.48
1:A:1203:ASN:OD1	1:A:1204:VAL:N	2.46	0.48
1:A:113:VAL:HG11	1:A:174:LEU:HD21	1.95	0.48
1:B:113:VAL:HG11	1:B:174:LEU:HD21	1.95	0.48
1:B:752:SER:HB2	1:B:753:PRO:HD2	1.95	0.48
1:D:331:LEU:HD13	1:D:338:TRP:CH2	2.48	0.48
1:D:752:SER:HB2	1:D:753:PRO:HD2	1.95	0.48
1:E:1198:TYR:HA	1:E:1215:THR:HB	1.96	0.48
1:F:1203:ASN:OD1	1:F:1204:VAL:N	2.46	0.48
1:C:170:ASP:OD2	1:C:172:SER:OG	2.32	0.48
1:D:326:LEU:HD23	1:D:326:LEU:HA	1.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:HIS:HA	1:E:500:LEU:HB3	1.96	0.48
1:F:1020:SER:HB2	1:F:1028:GLN:HE21	1.77	0.48
1:F:113:VAL:HG11	1:F:174:LEU:HD21	1.95	0.48
1:F:497:HIS:HA	1:F:500:LEU:HB3	1.96	0.48
1:G:541:SER:O	1:G:545:GLN:HG3	2.14	0.48
1:G:929:VAL:HB	1:G:936:MET:HB2	1.95	0.48
1:A:1198:TYR:HA	1:A:1215:THR:HB	1.96	0.48
1:B:1026:GLU:HG3	1:B:1041:ARG:HG2	1.95	0.48
1:B:497:HIS:HA	1:B:500:LEU:HB3	1.95	0.48
1:B:882:LEU:HD12	1:B:1176:HIS:NE2	2.25	0.48
1:C:158:CYS:SG	1:C:159:GLY:N	2.87	0.48
1:D:14:GLU:OE1	1:E:31:SER:CB	2.62	0.48
1:D:929:VAL:HB	1:D:936:MET:HB2	1.95	0.48
1:E:170:ASP:OD2	1:E:172:SER:OG	2.32	0.48
1:E:118:GLY:O	1:E:184:TRP:HB2	2.13	0.48
1:G:113:VAL:HG11	1:G:174:LEU:HD21	1.95	0.48
1:G:196:LEU:HG	1:G:200:GLN:HE22	1.78	0.48
1:G:568:LEU:HD13	1:G:595:LEU:O	2.13	0.48
1:G:762:SER:OG	1:G:764:ASP:OD1	2.26	0.48
1:A:330:LEU:HD13	1:A:341:TYR:OH	2.14	0.48
1:B:196:LEU:HG	1:B:200:GLN:HE22	1.78	0.48
1:C:541:SER:O	1:C:545:GLN:HG3	2.14	0.48
1:C:568:LEU:HD13	1:C:595:LEU:O	2.13	0.48
1:C:590:ASN:C	1:C:592:MET:N	2.64	0.48
1:D:541:SER:O	1:D:545:GLN:HG3	2.14	0.48
1:D:550:LEU:HD23	1:D:607:SER:HB2	1.91	0.48
1:E:158:CYS:SG	1:E:159:GLY:N	2.87	0.48
1:E:196:LEU:HG	1:E:200:GLN:HE22	1.78	0.48
1:E:929:VAL:HB	1:E:936:MET:HB2	1.95	0.48
1:F:158:CYS:SG	1:F:159:GLY:N	2.87	0.48
1:F:568:LEU:HD13	1:F:595:LEU:O	2.13	0.48
1:F:550:LEU:HD23	1:F:607:SER:HB2	1.91	0.48
1:B:569:CYS:HB3	1:B:600:LYS:HZ3	1.79	0.47
1:D:330:LEU:HD13	1:D:341:TYR:OH	2.14	0.47
1:E:752:SER:HB2	1:E:753:PRO:HD2	1.95	0.47
1:G:365:ASP:OD1	1:G:444:PHE:HE1	1.95	0.47
1:A:344:GLN:OE1	1:A:349:GLN:NE2	2.44	0.47
1:A:752:SER:HB2	1:A:753:PRO:HD2	1.95	0.47
1:B:568:LEU:HD13	1:B:595:LEU:O	2.13	0.47
1:C:330:LEU:HD13	1:C:341:TYR:OH	2.14	0.47
1:C:600:LYS:HZ1	1:C:1213:PHE:HZ	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:SER:HB2	1:A:1028:GLN:HE21	1.77	0.47
1:A:348:LYS:NZ	1:A:443:ASP:OD1	2.45	0.47
1:A:541:SER:O	1:A:545:GLN:HG3	2.14	0.47
1:C:1203:ASN:OD1	1:C:1204:VAL:N	2.46	0.47
1:C:497:HIS:HA	1:C:500:LEU:HB3	1.96	0.47
1:D:344:GLN:OE1	1:D:349:GLN:NE2	2.44	0.47
1:F:1198:TYR:HA	1:F:1215:THR:HB	1.96	0.47
1:F:330:LEU:HD13	1:F:341:TYR:OH	2.14	0.47
1:F:844:GLN:HE22	2:M:79:LYS:HZ2	1.61	0.47
1:B:821:ILE:HB	1:B:835:ILE:HB	1.97	0.47
1:C:344:GLN:OE1	1:C:349:GLN:NE2	2.44	0.47
1:D:196:LEU:HG	1:D:200:GLN:HE22	1.78	0.47
1:E:1131:ARG:H	1:E:1146:ASP:HA	1.80	0.47
1:G:158:CYS:SG	1:G:159:GLY:N	2.87	0.47
1:A:109:TYR:CE1	1:G:4:LYS:CD	2.58	0.47
1:A:106:ILE:HA	1:A:110:VAL:HG21	1.97	0.47
1:B:170:ASP:OD2	1:B:172:SER:OG	2.32	0.47
1:C:752:SER:HB2	1:C:753:PRO:HD2	1.95	0.47
1:C:821:ILE:HB	1:C:835:ILE:HB	1.97	0.47
1:E:330:LEU:HD13	1:E:341:TYR:OH	2.14	0.47
1:F:541:SER:O	1:F:545:GLN:HG3	2.14	0.47
1:B:230:LEU:O	1:B:234:LYS:N	2.41	0.47
1:C:1131:ARG:H	1:C:1146:ASP:HA	1.80	0.47
1:E:160:LYS:HB3	4:E:1301:DTP:O1B	2.15	0.47
1:D:14:GLU:HB2	1:E:31:SER:HG	1.80	0.47
1:G:600:LYS:HZ1	1:G:1213:PHE:HZ	1.63	0.47
2:K:39:LYS:HB2	2:K:42:GLN:HG3	1.97	0.47
2:L:39:LYS:HB2	2:L:42:GLN:HG3	1.97	0.47
1:B:1221:LYS:HE3	1:B:1222:LYS:HE3	1.97	0.47
1:B:330:LEU:HD13	1:B:341:TYR:OH	2.14	0.47
1:A:337:ARG:NH1	1:B:409:GLU:OE2	2.48	0.47
1:D:497:HIS:HA	1:D:500:LEU:HB3	1.96	0.47
1:D:821:ILE:HB	1:D:835:ILE:HB	1.97	0.47
1:E:344:GLN:OE1	1:E:349:GLN:NE2	2.44	0.47
1:E:541:SER:O	1:E:545:GLN:HG3	2.14	0.47
1:F:106:ILE:HA	1:F:110:VAL:HG21	1.97	0.47
1:F:1131:ARG:H	1:F:1146:ASP:HA	1.80	0.47
1:G:497:HIS:HA	1:G:500:LEU:HB3	1.96	0.47
1:A:600:LYS:HZ1	1:A:1213:PHE:HZ	1.63	0.47
1:A:230:LEU:O	1:A:234:LYS:N	2.41	0.47
1:A:497:HIS:HA	1:A:500:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD23	1:A:607:SER:HB2	1.91	0.47
1:B:158:CYS:SG	1:B:159:GLY:N	2.87	0.47
1:D:1131:ARG:H	1:D:1146:ASP:HA	1.80	0.47
1:F:160:LYS:HB3	4:F:1301:DTP:O1B	2.15	0.47
1:G:106:ILE:HA	1:G:110:VAL:HG21	1.97	0.47
1:G:1198:TYR:HA	1:G:1215:THR:HB	1.96	0.47
2:I:39:LYS:HB2	2:I:42:GLN:HG3	1.97	0.47
1:A:1221:LYS:HE3	1:A:1222:LYS:HE3	1.97	0.47
1:A:158:CYS:SG	1:A:159:GLY:N	2.87	0.47
1:A:170:ASP:OD2	1:A:172:SER:OG	2.32	0.47
1:B:541:SER:O	1:B:545:GLN:HG3	2.14	0.47
1:C:196:LEU:HG	1:C:200:GLN:HE22	1.78	0.47
1:B:337:ARG:NH1	1:C:409:GLU:OE2	2.48	0.47
1:D:158:CYS:SG	1:D:159:GLY:N	2.87	0.47
1:G:170:ASP:OD2	1:G:172:SER:OG	2.32	0.47
1:A:821:ILE:HB	1:A:835:ILE:HB	1.97	0.47
1:B:106:ILE:HA	1:B:110:VAL:HG21	1.97	0.47
1:B:1222:LYS:HB3	1:B:1224:HIS:CE1	2.50	0.47
1:D:170:ASP:OD2	1:D:172:SER:OG	2.32	0.47
1:D:230:LEU:O	1:D:234:LYS:N	2.41	0.47
1:E:266:ASP:CG	1:E:268:SER:HG	2.18	0.47
1:F:929:VAL:HB	1:F:936:MET:HB2	1.95	0.47
1:A:1131:ARG:H	1:A:1146:ASP:HA	1.80	0.47
1:A:1222:LYS:HB3	1:A:1224:HIS:CE1	2.50	0.47
1:B:570:GLU:HB2	1:B:577:TYR:HB2	1.97	0.47
1:C:1222:LYS:HB3	1:C:1224:HIS:CE1	2.50	0.47
1:D:1222:LYS:HB3	1:D:1224:HIS:CE1	2.50	0.47
1:E:1222:LYS:HB3	1:E:1224:HIS:CE1	2.50	0.47
1:D:337:ARG:NH1	1:E:409:GLU:OE2	2.48	0.47
2:J:39:LYS:HB2	2:J:42:GLN:HG3	1.97	0.47
1:A:570:GLU:HB2	1:A:577:TYR:HB2	1.97	0.46
1:C:230:LEU:O	1:C:234:LYS:N	2.41	0.46
1:C:1221:LYS:HE3	1:C:1222:LYS:HE3	1.97	0.46
1:C:612:ARG:HG3	1:C:904:GLN:O	2.16	0.46
1:D:160:LYS:HB3	4:D:1301:DTP:O1B	2.15	0.46
1:E:152:ILE:HG22	1:E:280:VAL:HB	1.97	0.46
1:G:330:LEU:HD13	1:G:341:TYR:OH	2.14	0.46
2:H:39:LYS:HB2	2:H:42:GLN:HG3	1.97	0.46
1:B:160:LYS:HB3	4:B:1301:DTP:O1B	2.15	0.46
1:C:337:ARG:NH1	1:D:409:GLU:OE2	2.49	0.46
1:E:1221:LYS:HE3	1:E:1222:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:HIS:CB	1:E:646:THR:HG21	2.36	0.46
1:E:612:ARG:HG3	1:E:904:GLN:O	2.16	0.46
1:G:1222:LYS:HB3	1:G:1224:HIS:CE1	2.50	0.46
2:I:70:ASN:HD22	2:I:73:LYS:HB2	1.81	0.46
2:M:39:LYS:HB2	2:M:42:GLN:HG3	1.97	0.46
1:A:160:LYS:HB3	4:A:1301:DTP:O1B	2.15	0.46
1:B:862:TYR:HB3	1:B:884:TRP:N	2.31	0.46
1:E:106:ILE:HA	1:E:110:VAL:HG21	1.97	0.46
1:E:862:TYR:HB3	1:E:884:TRP:N	2.31	0.46
1:F:152:ILE:HG22	1:F:280:VAL:HB	1.97	0.46
1:G:1131:ARG:H	1:G:1146:ASP:HA	1.80	0.46
2:L:70:ASN:HD22	2:L:73:LYS:HB2	1.81	0.46
1:A:472:THR:O	1:A:473:LEU:HD12	2.16	0.46
1:A:888:VAL:HG12	1:A:899:THR:HA	1.98	0.46
1:C:524:HIS:CB	1:C:646:THR:HG21	2.36	0.46
1:D:152:ILE:HG22	1:D:280:VAL:HB	1.97	0.46
1:D:862:TYR:HB3	1:D:884:TRP:N	2.31	0.46
1:E:472:THR:O	1:E:473:LEU:HD12	2.16	0.46
1:E:821:ILE:HB	1:E:835:ILE:HB	1.97	0.46
1:E:337:ARG:NH1	1:F:409:GLU:OE2	2.48	0.46
1:G:160:LYS:HB3	4:G:1301:DTP:O1B	2.15	0.46
1:C:950:ASN:OD1	1:C:951:GLY:N	2.49	0.46
1:D:265:ARG:HH11	1:D:371:SER:HG	1.57	0.46
1:D:950:ASN:OD1	1:D:951:GLY:N	2.49	0.46
1:G:821:ILE:HB	1:G:835:ILE:HB	1.97	0.46
1:G:888:VAL:HG12	1:G:899:THR:HA	1.98	0.46
2:H:10:PHE:HA	2:H:14:CYS:HB2	1.98	0.46
1:C:570:GLU:HB2	1:C:577:TYR:HB2	1.97	0.46
1:C:862:TYR:HB3	1:C:884:TRP:N	2.31	0.46
1:F:1221:LYS:HE3	1:F:1222:LYS:HE3	1.97	0.46
1:F:170:ASP:OD2	1:F:172:SER:OG	2.32	0.46
1:G:1011:PHE:HE1	1:G:1018:LEU:HD13	1.81	0.46
1:G:152:ILE:HG22	1:G:280:VAL:HB	1.97	0.46
2:N:39:LYS:HB2	2:N:42:GLN:HG3	1.97	0.46
1:A:1011:PHE:HE1	1:A:1018:LEU:HD13	1.81	0.46
1:A:643:LYS:HD3	1:A:646:THR:HG22	1.98	0.46
1:B:888:VAL:HG12	1:B:899:THR:HA	1.98	0.46
1:B:950:ASN:OD1	1:B:951:GLY:N	2.49	0.46
1:D:1011:PHE:HE1	1:D:1018:LEU:HD13	1.81	0.46
1:G:1191:MET:SD	1:G:1209:SER:OG	2.63	0.46
1:B:472:THR:O	1:B:473:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LYS:HD3	1:B:646:THR:HG22	1.98	0.46
1:D:106:ILE:HA	1:D:110:VAL:HG21	1.97	0.46
1:E:950:ASN:OD1	1:E:951:GLY:N	2.49	0.46
1:F:1222:LYS:HB3	1:F:1224:HIS:CE1	2.50	0.46
1:F:570:GLU:HB2	1:F:577:TYR:HB2	1.97	0.46
1:F:821:ILE:HB	1:F:835:ILE:HB	1.97	0.46
1:G:570:GLU:HB2	1:G:577:TYR:HB2	1.97	0.46
1:G:862:TYR:HB3	1:G:884:TRP:N	2.31	0.46
2:M:10:PHE:HA	2:M:14:CYS:HB2	1.98	0.46
2:M:70:ASN:HD22	2:M:73:LYS:HB2	1.81	0.46
2:N:10:PHE:HA	2:N:14:CYS:HB2	1.98	0.46
3:R:90:ARG:NH2	3:R:90:ARG:HG2	2.31	0.46
1:A:612:ARG:HG3	1:A:904:GLN:O	2.16	0.46
1:B:152:ILE:HG22	1:B:280:VAL:HB	1.97	0.46
1:F:1215:THR:HG21	1:F:1220:LEU:HD21	1.98	0.46
1:F:950:ASN:OD1	1:F:951:GLY:N	2.49	0.46
1:G:1215:THR:HG21	1:G:1220:LEU:HD21	1.98	0.46
2:H:70:ASN:HD22	2:H:73:LYS:HB2	1.81	0.46
1:A:1215:THR:HG21	1:A:1220:LEU:HD21	1.98	0.45
1:A:950:ASN:OD1	1:A:951:GLY:N	2.49	0.45
1:B:1215:THR:HG21	1:B:1220:LEU:HD21	1.99	0.45
1:C:1215:THR:HG21	1:C:1220:LEU:HD21	1.98	0.45
1:C:160:LYS:HB3	4:C:1301:DTP:O1B	2.15	0.45
1:C:472:THR:O	1:C:473:LEU:HD12	2.16	0.45
1:D:1221:LYS:HE3	1:D:1222:LYS:HE3	1.97	0.45
1:E:1011:PHE:HE1	1:E:1018:LEU:HD13	1.81	0.45
1:E:550:LEU:HD23	1:E:607:SER:HB2	1.91	0.45
1:F:862:TYR:HB3	1:F:884:TRP:N	2.31	0.45
1:G:472:THR:O	1:G:473:LEU:HD12	2.16	0.45
1:C:1011:PHE:HE1	1:C:1018:LEU:HD13	1.81	0.45
1:C:106:ILE:HA	1:C:110:VAL:HG21	1.97	0.45
1:C:844:GLN:HE22	2:J:79:LYS:HZ2	1.62	0.45
1:D:472:THR:O	1:D:473:LEU:HD12	2.16	0.45
1:D:570:GLU:HB2	1:D:577:TYR:HB2	1.97	0.45
1:G:1221:LYS:HE3	1:G:1222:LYS:HE3	1.97	0.45
2:J:68:LEU:HB3	2:J:85:ILE:HD12	1.98	0.45
2:K:68:LEU:HB3	2:K:85:ILE:HD12	1.98	0.45
3:O:90:ARG:NH2	3:O:90:ARG:HG2	2.31	0.45
3:Q:90:ARG:HG2	3:Q:90:ARG:NH2	2.31	0.45
1:A:298:PHE:CD2	1:A:328:GLY:HA3	2.52	0.45
1:A:461:ILE:HD11	1:A:491:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ILE:HG22	1:C:280:VAL:HB	1.97	0.45
1:B:48:THR:CG2	1:D:45:ASN:OD1	2.64	0.45
1:F:1011:PHE:HE1	1:F:1018:LEU:HD13	1.81	0.45
2:I:10:PHE:HA	2:I:14:CYS:HB2	1.98	0.45
1:A:862:TYR:HB3	1:A:884:TRP:N	2.31	0.45
1:D:1215:THR:HG21	1:D:1220:LEU:HD21	1.98	0.45
1:E:1215:THR:HG21	1:E:1220:LEU:HD21	1.99	0.45
1:F:612:ARG:HG3	1:F:904:GLN:O	2.16	0.45
1:G:612:ARG:HG3	1:G:904:GLN:O	2.16	0.45
2:H:68:LEU:HB3	2:H:85:ILE:HD12	1.98	0.45
1:A:1150:GLU:HB2	1:A:1167:PRO:HG2	1.99	0.45
1:B:461:ILE:HD11	1:B:491:MET:HA	1.99	0.45
1:E:334:PHE:HE1	1:F:416:GLN:HE21	1.63	0.45
1:E:570:GLU:HB2	1:E:577:TYR:HB2	1.97	0.45
1:F:1150:GLU:HB2	1:F:1167:PRO:HG2	1.99	0.45
1:F:472:THR:O	1:F:473:LEU:HD12	2.16	0.45
1:G:1150:GLU:HB2	1:G:1167:PRO:HG2	1.99	0.45
1:G:950:ASN:OD1	1:G:951:GLY:N	2.49	0.45
2:J:70:ASN:HD22	2:J:73:LYS:HB2	1.81	0.45
2:L:10:PHE:HA	2:L:14:CYS:HB2	1.98	0.45
1:A:152:ILE:HG22	1:A:280:VAL:HB	1.97	0.45
1:B:1131:ARG:H	1:B:1146:ASP:HA	1.80	0.45
1:B:1150:GLU:HB2	1:B:1167:PRO:HG2	1.99	0.45
1:C:1191:MET:SD	1:C:1209:SER:OG	2.63	0.45
1:C:643:LYS:HD3	1:C:646:THR:HG22	1.98	0.45
1:D:612:ARG:HG3	1:D:904:GLN:O	2.16	0.45
1:F:461:ILE:HD11	1:F:491:MET:HA	1.99	0.45
1:G:461:ILE:HD11	1:G:491:MET:HA	1.99	0.45
1:B:298:PHE:CD2	1:B:328:GLY:HA3	2.52	0.45
1:B:821:ILE:HD11	1:B:857:VAL:HG21	1.99	0.45
1:B:612:ARG:HG3	1:B:904:GLN:O	2.16	0.45
1:C:888:VAL:HG12	1:C:899:THR:HA	1.98	0.45
1:E:821:ILE:HD11	1:E:857:VAL:HG21	1.99	0.45
1:F:888:VAL:HG12	1:F:899:THR:HA	1.98	0.45
2:K:10:PHE:HA	2:K:14:CYS:HB2	1.98	0.45
1:C:216:LEU:HA	1:C:217:PRO:HD2	1.84	0.45
1:C:821:ILE:HD11	1:C:857:VAL:HG21	1.99	0.45
1:D:868:ASN:OD1	1:D:869:THR:N	2.50	0.45
1:F:326:LEU:HA	1:F:326:LEU:HD23	1.44	0.45
1:F:821:ILE:HD11	1:F:857:VAL:HG21	1.99	0.45
1:A:868:ASN:OD1	1:A:869:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:ASN:OD1	1:B:869:THR:N	2.50	0.45
1:E:1150:GLU:HB2	1:E:1167:PRO:HG2	1.99	0.45
1:E:326:LEU:HD23	1:E:326:LEU:HA	1.44	0.45
1:F:868:ASN:OD1	1:F:869:THR:N	2.50	0.45
1:G:298:PHE:CD2	1:G:328:GLY:HA3	2.52	0.45
2:J:10:PHE:HA	2:J:14:CYS:HB2	1.98	0.45
2:K:70:ASN:HD22	2:K:73:LYS:HB2	1.81	0.45
2:N:68:LEU:HB3	2:N:85:ILE:HD12	1.98	0.45
3:P:90:ARG:HG2	3:P:90:ARG:NH2	2.31	0.45
1:A:480:CYS:SG	1:A:481:MET:N	2.90	0.45
1:B:1011:PHE:HE1	1:B:1018:LEU:HD13	1.81	0.45
1:C:1150:GLU:HB2	1:C:1167:PRO:HG2	1.99	0.45
1:E:390:GLN:HB2	1:E:393:VAL:HG21	1.99	0.45
1:E:461:ILE:HD11	1:E:491:MET:HA	1.99	0.45
1:F:762:SER:OG	1:F:764:ASP:OD1	2.26	0.45
1:A:409:GLU:OE2	1:G:337:ARG:NH1	2.49	0.45
1:G:643:LYS:HD3	1:G:646:THR:HG22	1.98	0.45
1:G:868:ASN:OD1	1:G:869:THR:N	2.50	0.45
2:N:70:ASN:HD22	2:N:73:LYS:HB2	1.81	0.45
1:B:600:LYS:HA	1:B:603:ILE:HG13	2.00	0.44
1:D:821:ILE:HD11	1:D:857:VAL:HG21	1.99	0.44
1:E:643:LYS:HD3	1:E:646:THR:HG22	1.98	0.44
2:I:72:LYS:NZ	2:I:78:THR:O	2.51	0.44
3:Q:41:GLU:HA	3:Q:44:GLN:HE21	1.83	0.44
1:A:821:ILE:HD11	1:A:857:VAL:HG21	1.99	0.44
1:C:868:ASN:OD1	1:C:869:THR:N	2.50	0.44
1:D:1150:GLU:HB2	1:D:1167:PRO:HG2	1.99	0.44
1:D:357:SER:OG	1:D:358:SER:N	2.50	0.44
1:D:888:VAL:HG12	1:D:899:THR:HA	1.98	0.44
1:E:480:CYS:SG	1:E:481:MET:N	2.90	0.44
1:F:230:LEU:O	1:F:234:LYS:N	2.41	0.44
1:F:643:LYS:HD3	1:F:646:THR:HG22	1.98	0.44
1:G:266:ASP:CG	1:G:268:SER:HG	2.19	0.44
2:L:68:LEU:HB3	2:L:85:ILE:HD12	1.98	0.44
1:G:1087:THR:N	2:N:39:LYS:HZ3	2.15	0.44
3:O:45:ARG:HG2	3:O:45:ARG:O	2.17	0.44
1:A:569:CYS:HB3	1:A:600:LYS:HZ3	1.82	0.44
1:B:357:SER:OG	1:B:358:SER:N	2.50	0.44
1:B:480:CYS:SG	1:B:481:MET:N	2.90	0.44
1:C:480:CYS:SG	1:C:481:MET:N	2.90	0.44
1:C:600:LYS:HA	1:C:603:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:PHE:CD2	1:D:328:GLY:HA3	2.52	0.44
1:D:643:LYS:HD3	1:D:646:THR:HG22	1.98	0.44
1:E:888:VAL:HG12	1:E:899:THR:HA	1.98	0.44
1:G:346:GLN:C	1:G:348:LYS:N	2.71	0.44
2:L:67:TYR:OH	2:L:80:MET:SD	2.57	0.44
2:M:68:LEU:HB3	2:M:85:ILE:HD12	1.98	0.44
2:M:72:LYS:NZ	2:M:78:THR:O	2.51	0.44
1:A:600:LYS:HA	1:A:603:ILE:HG13	2.00	0.44
1:C:461:ILE:HD11	1:C:491:MET:HA	1.99	0.44
1:D:342:LEU:O	1:D:346:GLN:CG	2.66	0.44
1:D:480:CYS:SG	1:D:481:MET:N	2.90	0.44
1:E:1191:MET:SD	1:E:1209:SER:OG	2.63	0.44
1:E:530:ARG:NH1	1:E:545:GLN:OE1	2.51	0.44
1:F:342:LEU:O	1:F:346:GLN:CG	2.66	0.44
2:J:72:LYS:NZ	2:J:78:THR:O	2.51	0.44
3:R:10:ARG:HG2	3:R:10:ARG:H	1.60	0.44
1:A:357:SER:OG	1:A:358:SER:N	2.50	0.44
1:C:342:LEU:O	1:C:346:GLN:CG	2.66	0.44
1:D:390:GLN:HB2	1:D:393:VAL:HG21	1.99	0.44
1:E:357:SER:OG	1:E:358:SER:N	2.50	0.44
1:F:390:GLN:HB2	1:F:393:VAL:HG21	1.99	0.44
1:F:600:LYS:HA	1:F:603:ILE:HG13	2.00	0.44
1:G:342:LEU:O	1:G:346:GLN:CG	2.66	0.44
1:G:600:LYS:HA	1:G:603:ILE:HG13	2.00	0.44
1:G:695:TYR:HE1	1:G:733:LYS:HD2	1.83	0.44
1:G:821:ILE:HD11	1:G:857:VAL:HG21	1.99	0.44
2:I:68:LEU:HB3	2:I:85:ILE:HD12	1.98	0.44
2:J:3:VAL:O	2:J:97:TYR:HB2	2.18	0.44
2:N:3:VAL:O	2:N:97:TYR:HB2	2.18	0.44
1:B:390:GLN:HB2	1:B:393:VAL:HG21	1.99	0.44
1:B:550:LEU:HD23	1:B:607:SER:HB2	1.91	0.44
1:C:695:TYR:HE1	1:C:733:LYS:HD2	1.82	0.44
1:E:600:LYS:HA	1:E:603:ILE:HG13	2.00	0.44
1:E:868:ASN:OD1	1:E:869:THR:N	2.50	0.44
1:G:230:LEU:O	1:G:234:LYS:N	2.41	0.44
1:G:530:ARG:NH1	1:G:545:GLN:OE1	2.51	0.44
1:G:795:GLU:O	1:G:795:GLU:HG3	2.18	0.44
1:A:530:ARG:NH1	1:A:545:GLN:OE1	2.51	0.44
1:B:695:TYR:HE1	1:B:733:LYS:HD2	1.83	0.44
1:C:1135:PHE:CE1	1:C:1142:LEU:HD13	2.53	0.44
1:C:298:PHE:CD2	1:C:328:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:GLU:O	1:C:795:GLU:HG3	2.18	0.44
1:D:461:ILE:HD11	1:D:491:MET:HA	1.99	0.44
1:D:600:LYS:HA	1:D:603:ILE:HG13	2.00	0.44
1:D:685:ASN:HB3	1:D:688:THR:HB	1.99	0.44
1:F:298:PHE:CD2	1:F:328:GLY:HA3	2.52	0.44
1:G:344:GLN:OE1	1:G:349:GLN:NE2	2.44	0.44
1:G:390:GLN:HB2	1:G:393:VAL:HG21	1.99	0.44
2:K:3:VAL:O	2:K:97:TYR:HB2	2.18	0.44
2:L:3:VAL:O	2:L:97:TYR:HB2	2.18	0.44
2:M:70:ASN:ND2	2:M:73:LYS:HB2	2.33	0.44
1:A:342:LEU:O	1:A:346:GLN:CG	2.66	0.44
1:A:346:GLN:C	1:A:348:LYS:N	2.71	0.44
1:A:685:ASN:HB3	1:A:688:THR:HB	1.99	0.44
1:B:1135:PHE:CE1	1:B:1142:LEU:HD13	2.53	0.44
1:B:600:LYS:HZ1	1:B:1213:PHE:HZ	1.65	0.44
1:B:346:GLN:C	1:B:348:LYS:N	2.71	0.44
1:B:391:LYS:H	1:B:391:LYS:HG2	1.62	0.44
1:C:357:SER:OG	1:C:358:SER:N	2.50	0.44
1:D:524:HIS:N	1:D:646:THR:OG1	2.51	0.44
2:K:72:LYS:NZ	2:K:78:THR:O	2.51	0.44
2:N:70:ASN:ND2	2:N:73:LYS:HB2	2.33	0.44
1:A:695:TYR:OH	1:A:732:GLN:O	2.31	0.44
1:B:685:ASN:HB3	1:B:688:THR:HB	1.99	0.44
1:C:346:GLN:C	1:C:348:LYS:N	2.71	0.44
1:C:530:ARG:NH1	1:C:545:GLN:OE1	2.51	0.44
1:C:847:ASP:OD1	1:C:848:PHE:N	2.51	0.44
1:D:530:ARG:NH1	1:D:545:GLN:OE1	2.51	0.44
1:D:695:TYR:HE1	1:D:733:LYS:HD2	1.83	0.44
1:D:847:ASP:OD1	1:D:848:PHE:N	2.51	0.44
1:E:685:ASN:HB3	1:E:688:THR:HB	2.00	0.44
1:G:480:CYS:SG	1:G:481:MET:N	2.90	0.44
2:H:72:LYS:NZ	2:H:78:THR:O	2.51	0.44
3:O:41:GLU:HA	3:O:44:GLN:HE21	1.83	0.44
1:A:795:GLU:O	1:A:795:GLU:HG3	2.18	0.43
1:B:326:LEU:HA	1:B:326:LEU:HD23	1.44	0.43
1:B:524:HIS:N	1:B:646:THR:OG1	2.51	0.43
1:C:390:GLN:HB2	1:C:393:VAL:HG21	1.99	0.43
1:E:342:LEU:O	1:E:346:GLN:CG	2.66	0.43
1:E:695:TYR:HE1	1:E:733:LYS:HD2	1.83	0.43
1:E:795:GLU:O	1:E:795:GLU:HG3	2.18	0.43
1:F:524:HIS:N	1:F:646:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:795:GLU:HG3	1:F:795:GLU:O	2.18	0.43
1:G:685:ASN:HB3	1:G:688:THR:HB	1.99	0.43
2:L:18:HIS:CE1	2:L:29:GLY:HA3	2.53	0.43
2:L:72:LYS:NZ	2:L:78:THR:O	2.51	0.43
2:N:18:HIS:CE1	2:N:29:GLY:HA3	2.53	0.43
1:B:224:LYS:HE3	1:B:255:ASP:O	2.18	0.43
1:B:342:LEU:O	1:B:346:GLN:CG	2.66	0.43
1:B:530:ARG:NH1	1:B:545:GLN:OE1	2.51	0.43
1:B:795:GLU:O	1:B:795:GLU:HG3	2.18	0.43
1:C:334:PHE:HD2	1:C:337:ARG:HH11	1.66	0.43
1:E:298:PHE:CD2	1:E:328:GLY:HA3	2.52	0.43
1:E:891:SER:OG	1:E:896:SER:O	2.34	0.43
1:F:480:CYS:SG	1:F:481:MET:N	2.90	0.43
1:G:224:LYS:HE3	1:G:255:ASP:O	2.18	0.43
1:G:357:SER:OG	1:G:358:SER:N	2.50	0.43
1:G:524:HIS:N	1:G:646:THR:OG1	2.51	0.43
2:H:18:HIS:CE1	2:H:29:GLY:HA3	2.53	0.43
2:J:70:ASN:ND2	2:J:73:LYS:HB2	2.33	0.43
1:F:884:TRP:HH2	2:M:78:THR:C	2.22	0.43
1:A:1135:PHE:CE1	1:A:1142:LEU:HD13	2.53	0.43
1:A:524:HIS:N	1:A:646:THR:OG1	2.51	0.43
1:A:695:TYR:HE1	1:A:733:LYS:HD2	1.83	0.43
1:A:847:ASP:OD1	1:A:848:PHE:N	2.51	0.43
1:B:428:ARG:HG2	1:B:433:PHE:CE1	2.54	0.43
1:E:524:HIS:N	1:E:646:THR:OG1	2.51	0.43
1:F:357:SER:OG	1:F:358:SER:N	2.50	0.43
1:G:268:SER:O	1:G:271:ASP:N	2.51	0.43
1:G:844:GLN:HE22	2:N:79:LYS:HZ2	1.63	0.43
1:G:884:TRP:HH2	2:N:78:THR:C	2.22	0.43
2:N:72:LYS:NZ	2:N:78:THR:O	2.51	0.43
3:R:41:GLU:HA	3:R:44:GLN:HE21	1.83	0.43
1:A:386:LEU:HD23	1:A:386:LEU:O	2.19	0.43
1:A:390:GLN:HB2	1:A:393:VAL:HG21	1.99	0.43
1:A:965:SER:H	1:A:980:ASP:HA	1.84	0.43
1:B:937:VAL:HB	1:B:949:ILE:HB	2.00	0.43
1:C:685:ASN:HB3	1:C:688:THR:HB	2.00	0.43
1:C:937:VAL:HB	1:C:949:ILE:HB	2.00	0.43
1:C:965:SER:H	1:C:980:ASP:HA	1.84	0.43
1:D:582:LEU:O	1:D:586:GLN:HG3	2.19	0.43
1:F:530:ARG:NH1	1:F:545:GLN:OE1	2.51	0.43
1:G:386:LEU:HD23	1:G:386:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:569:CYS:HB3	1:G:600:LYS:HZ3	1.83	0.43
2:H:70:ASN:ND2	2:H:73:LYS:HB2	2.33	0.43
2:M:26:HIS:O	2:M:27:LYS:HD2	2.19	0.43
1:A:224:LYS:HE3	1:A:255:ASP:O	2.18	0.43
1:B:334:PHE:HD2	1:B:337:ARG:HH11	1.66	0.43
1:B:582:LEU:O	1:B:586:GLN:HG3	2.19	0.43
1:E:1135:PHE:CE1	1:E:1142:LEU:HD13	2.53	0.43
1:E:762:SER:OG	1:E:764:ASP:OD1	2.26	0.43
1:F:965:SER:H	1:F:980:ASP:HA	1.84	0.43
1:G:1218:THR:H	1:G:1237:ASN:ND2	2.17	0.43
2:J:18:HIS:CE1	2:J:29:GLY:HA3	2.53	0.43
2:N:26:HIS:O	2:N:27:LYS:HD2	2.19	0.43
1:A:266:ASP:CG	1:A:268:SER:H	2.20	0.43
1:A:346:GLN:O	1:A:348:LYS:N	2.52	0.43
1:C:428:ARG:HG2	1:C:433:PHE:CE1	2.54	0.43
1:C:524:HIS:N	1:C:646:THR:OG1	2.51	0.43
1:D:224:LYS:HE3	1:D:255:ASP:O	2.18	0.43
1:D:386:LEU:O	1:D:386:LEU:HD23	2.19	0.43
1:D:937:VAL:HB	1:D:949:ILE:HB	2.00	0.43
1:E:1166:ALA:HA	1:E:1167:PRO:HD2	1.93	0.43
1:E:224:LYS:HE3	1:E:255:ASP:O	2.18	0.43
1:E:346:GLN:C	1:E:348:LYS:N	2.71	0.43
1:E:428:ARG:HG2	1:E:433:PHE:CE1	2.54	0.43
1:F:346:GLN:C	1:F:348:LYS:N	2.71	0.43
1:A:884:TRP:HH2	2:H:78:THR:C	2.22	0.43
2:I:26:HIS:O	2:I:27:LYS:HD2	2.19	0.43
2:J:26:HIS:O	2:J:27:LYS:HD2	2.19	0.43
1:C:884:TRP:HH2	2:J:78:THR:O	2.02	0.43
1:E:884:TRP:HH2	2:L:78:THR:C	2.22	0.43
2:M:18:HIS:CE1	2:M:29:GLY:HA3	2.53	0.43
2:N:82:PHE:HE2	2:N:85:ILE:HG13	1.84	0.43
1:A:379:ILE:O	1:A:382:TYR:N	2.52	0.43
1:B:346:GLN:O	1:B:348:LYS:N	2.52	0.43
1:B:386:LEU:O	1:B:386:LEU:HD23	2.19	0.43
1:D:965:SER:H	1:D:980:ASP:HA	1.84	0.43
1:E:1100:PHE:HB3	1:E:1111:ILE:HD11	2.00	0.43
1:E:268:SER:O	1:E:271:ASP:N	2.51	0.43
1:F:224:LYS:HE3	1:F:255:ASP:O	2.18	0.43
1:F:386:LEU:O	1:F:386:LEU:HD23	2.19	0.43
1:F:685:ASN:HB3	1:F:688:THR:HB	1.99	0.43
1:F:695:TYR:HE1	1:F:733:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:847:ASP:OD1	1:F:848:PHE:N	2.51	0.43
1:G:266:ASP:CG	1:G:268:SER:H	2.20	0.43
1:G:379:ILE:O	1:G:382:TYR:N	2.52	0.43
2:H:3:VAL:O	2:H:97:TYR:HB2	2.18	0.43
2:I:18:HIS:CE1	2:I:29:GLY:HA3	2.53	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.44	0.43
1:C:379:ILE:O	1:C:382:TYR:N	2.52	0.43
1:D:428:ARG:HG2	1:D:433:PHE:CE1	2.54	0.43
1:F:582:LEU:O	1:F:586:GLN:HG3	2.19	0.43
1:F:937:VAL:HB	1:F:949:ILE:HB	2.00	0.43
1:G:847:ASP:OD1	1:G:848:PHE:N	2.51	0.43
2:I:70:ASN:ND2	2:I:73:LYS:HB2	2.33	0.43
2:I:3:VAL:O	2:I:97:TYR:HB2	2.18	0.43
2:K:26:HIS:O	2:K:27:LYS:HD2	2.19	0.43
2:L:41:GLY:HA2	2:L:48:TYR:CZ	2.54	0.43
1:A:524:HIS:CB	1:A:646:THR:HG21	2.36	0.43
1:B:1100:PHE:HB3	1:B:1111:ILE:HD11	2.00	0.43
1:B:379:ILE:O	1:B:382:TYR:N	2.52	0.43
1:B:767:LEU:HD21	1:B:801:VAL:HG11	2.01	0.43
1:C:224:LYS:HE3	1:C:255:ASP:O	2.18	0.43
1:C:346:GLN:O	1:C:348:LYS:N	2.52	0.43
1:D:1100:PHE:HB3	1:D:1111:ILE:HD11	2.00	0.43
1:D:725:LEU:HD11	1:D:742:HIS:CD2	2.54	0.43
1:D:884:TRP:HH2	2:K:78:THR:C	2.22	0.43
1:E:725:LEU:HD11	1:E:742:HIS:CD2	2.54	0.43
1:E:847:ASP:OD1	1:E:848:PHE:N	2.51	0.43
1:E:965:SER:H	1:E:980:ASP:HA	1.84	0.43
1:F:379:ILE:O	1:F:382:TYR:N	2.52	0.43
1:G:428:ARG:HG2	1:G:433:PHE:CE1	2.54	0.43
2:H:41:GLY:HA2	2:H:48:TYR:CZ	2.54	0.43
2:H:82:PHE:HE2	2:H:85:ILE:HG13	1.84	0.43
2:K:18:HIS:CE1	2:K:29:GLY:HA3	2.53	0.43
2:K:70:ASN:ND2	2:K:73:LYS:HB2	2.33	0.43
2:M:3:VAL:O	2:M:97:TYR:HB2	2.18	0.43
1:B:965:SER:H	1:B:980:ASP:HA	1.84	0.43
1:C:582:LEU:O	1:C:586:GLN:HG3	2.19	0.43
1:C:767:LEU:HD21	1:C:801:VAL:HG11	2.01	0.43
1:D:1135:PHE:CE1	1:D:1142:LEU:HD13	2.53	0.43
1:D:334:PHE:HD2	1:D:337:ARG:HH11	1.66	0.43
1:D:795:GLU:O	1:D:795:GLU:HG3	2.18	0.43
1:E:1218:THR:H	1:E:1237:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1100:PHE:HB3	1:F:1111:ILE:HD11	2.00	0.43
1:F:346:GLN:O	1:F:348:LYS:N	2.52	0.43
1:G:1050:PHE:CD1	1:G:1058:LEU:HD11	2.54	0.43
1:F:201:ASN:ND2	1:G:219:ASN:HD21	2.14	0.43
1:G:346:GLN:O	1:G:348:LYS:N	2.52	0.43
2:H:67:TYR:HD1	2:H:74:TYR:HB3	1.84	0.43
1:B:884:TRP:HH2	2:I:78:THR:C	2.22	0.43
2:L:26:HIS:O	2:L:27:LYS:HD2	2.19	0.43
2:L:70:ASN:ND2	2:L:73:LYS:HB2	2.33	0.43
2:L:82:PHE:HE2	2:L:85:ILE:HG13	1.84	0.43
3:P:41:GLU:HA	3:P:44:GLN:HE21	1.83	0.43
1:C:676:SER:OG	1:C:678:ASP:OD1	2.37	0.42
1:C:884:TRP:HH2	2:J:78:THR:C	2.22	0.42
1:D:767:LEU:HD21	1:D:801:VAL:HG11	2.01	0.42
1:E:658:ASP:HB3	1:E:677:VAL:HB	2.00	0.42
1:F:1135:PHE:CE1	1:F:1142:LEU:HD13	2.53	0.42
1:G:658:ASP:HB3	1:G:677:VAL:HB	2.00	0.42
1:G:937:VAL:HB	1:G:949:ILE:HB	2.00	0.42
2:I:82:PHE:HE2	2:I:85:ILE:HG13	1.84	0.42
2:N:41:GLY:HA2	2:N:48:TYR:CZ	2.54	0.42
3:P:90:ARG:HH21	3:P:90:ARG:HG2	1.84	0.42
1:A:1050:PHE:CD1	1:A:1058:LEU:HD11	2.54	0.42
1:A:658:ASP:HB3	1:A:677:VAL:HB	2.00	0.42
1:B:266:ASP:CG	1:B:268:SER:H	2.20	0.42
1:C:1100:PHE:HB3	1:C:1111:ILE:HD11	2.00	0.42
1:C:550:LEU:HD23	1:C:607:SER:HB2	1.91	0.42
1:D:658:ASP:HB3	1:D:677:VAL:HB	2.00	0.42
1:E:767:LEU:HD21	1:E:801:VAL:HG11	2.01	0.42
1:F:808:ALA:HB2	1:F:850:PRO:HA	2.01	0.42
1:G:1135:PHE:CE1	1:G:1142:LEU:HD13	2.53	0.42
2:M:82:PHE:HE2	2:M:85:ILE:HG13	1.84	0.42
3:R:90:ARG:HH21	3:R:90:ARG:HG2	1.85	0.42
1:A:511:LYS:HB2	1:A:563:ILE:HG13	2.02	0.42
1:A:767:LEU:HD21	1:A:801:VAL:HG11	2.01	0.42
1:B:1218:THR:H	1:B:1237:ASN:ND2	2.17	0.42
1:B:658:ASP:HB3	1:B:677:VAL:HB	2.00	0.42
1:D:524:HIS:CB	1:D:646:THR:HG21	2.36	0.42
1:F:266:ASP:CG	1:F:268:SER:H	2.20	0.42
1:G:808:ALA:HB2	1:G:850:PRO:HA	2.02	0.42
2:J:14:CYS:SG	5:J:500:HEC:HBB3	2.59	0.42
2:J:82:PHE:HE2	2:J:85:ILE:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:CYS:SG	5:N:500:HEC:HBB3	2.59	0.42
3:O:90:ARG:HH21	3:O:90:ARG:HG2	1.85	0.42
1:A:1100:PHE:HB3	1:A:1111:ILE:HD11	2.00	0.42
1:A:1218:THR:H	1:A:1237:ASN:ND2	2.17	0.42
1:A:428:ARG:HG2	1:A:433:PHE:CE1	2.54	0.42
1:A:937:VAL:HB	1:A:949:ILE:HB	2.00	0.42
1:D:346:GLN:C	1:D:348:LYS:N	2.71	0.42
1:E:379:ILE:O	1:E:382:TYR:N	2.52	0.42
1:E:937:VAL:HB	1:E:949:ILE:HB	2.00	0.42
1:F:658:ASP:HB3	1:F:677:VAL:HB	2.00	0.42
1:F:725:LEU:HD11	1:F:742:HIS:CD2	2.54	0.42
1:F:767:LEU:HD21	1:F:801:VAL:HG11	2.01	0.42
2:J:67:TYR:HD1	2:J:74:TYR:HB3	1.84	0.42
2:K:14:CYS:SG	5:K:500:HEC:HBB3	2.59	0.42
3:O:34:LEU:HA	3:O:34:LEU:HD12	1.93	0.42
3:Q:90:ARG:HG2	3:Q:90:ARG:HH21	1.84	0.42
1:B:511:LYS:HB2	1:B:563:ILE:HG13	2.02	0.42
1:B:847:ASP:OD1	1:B:848:PHE:N	2.51	0.42
1:B:989:GLU:HG2	1:B:991:VAL:H	1.85	0.42
1:C:1135:PHE:HE1	1:C:1142:LEU:HD13	1.85	0.42
1:C:725:LEU:HD11	1:C:742:HIS:CD2	2.54	0.42
1:D:1218:THR:H	1:D:1237:ASN:ND2	2.17	0.42
1:D:676:SER:OG	1:D:678:ASP:OD1	2.37	0.42
1:E:346:GLN:O	1:E:348:LYS:N	2.52	0.42
1:E:808:ALA:HB2	1:E:850:PRO:HA	2.01	0.42
1:G:145:GLY:HA2	1:G:259:GLN:HE21	1.85	0.42
2:H:26:HIS:O	2:H:27:LYS:HD2	2.19	0.42
2:I:14:CYS:SG	5:I:500:HEC:HBB3	2.59	0.42
2:K:41:GLY:HA2	2:K:48:TYR:CZ	2.54	0.42
3:R:7:ARG:HA	3:R:10:ARG:HG3	2.02	0.42
1:A:808:ALA:HB2	1:A:850:PRO:HA	2.01	0.42
1:C:658:ASP:HB3	1:C:677:VAL:HB	2.00	0.42
1:D:452:GLN:N	1:D:452:GLN:OE1	2.53	0.42
1:D:14:GLU:CB	1:E:31:SER:HG	2.33	0.42
1:E:386:LEU:HD23	1:E:386:LEU:O	2.19	0.42
1:E:582:LEU:O	1:E:586:GLN:HG3	2.19	0.42
1:F:1050:PHE:CD1	1:F:1058:LEU:HD11	2.54	0.42
1:F:334:PHE:HD2	1:F:337:ARG:HH11	1.66	0.42
2:H:40:THR:HG23	2:H:57:ILE:HG13	2.02	0.42
2:K:82:PHE:HE2	2:K:85:ILE:HG13	1.84	0.42
2:N:67:TYR:HD1	2:N:74:TYR:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:HA	1:A:321:PRO:HD3	1.87	0.42
1:B:1032:TRP:C	1:B:1034:LEU:H	2.23	0.42
1:C:1050:PHE:CD1	1:C:1058:LEU:HD11	2.54	0.42
1:C:386:LEU:O	1:C:386:LEU:HD23	2.19	0.42
1:C:400:LEU:HB3	1:C:404:TRP:HZ3	1.84	0.42
1:G:10:LEU:CD2	1:G:13:ARG:NH2	2.83	0.42
1:G:320:SER:HA	1:G:321:PRO:HD3	1.87	0.42
1:G:511:LYS:HB2	1:G:563:ILE:HG13	2.02	0.42
1:G:582:LEU:O	1:G:586:GLN:HG3	2.19	0.42
2:I:94:LEU:O	2:I:98:LEU:HG	2.20	0.42
2:J:41:GLY:HA2	2:J:48:TYR:CZ	2.54	0.42
1:D:884:TRP:HH2	2:K:78:THR:O	2.02	0.42
2:M:41:GLY:HA2	2:M:48:TYR:CZ	2.54	0.42
1:B:1050:PHE:CD1	1:B:1058:LEU:HD11	2.54	0.42
1:B:1135:PHE:HE1	1:B:1142:LEU:HD13	1.85	0.42
1:B:265:ARG:O	1:B:265:ARG:HG3	2.20	0.42
1:B:320:SER:HA	1:B:321:PRO:HD3	1.87	0.42
1:C:1218:THR:H	1:C:1237:ASN:ND2	2.17	0.42
1:C:145:GLY:HA2	1:C:259:GLN:HE21	1.85	0.42
1:C:266:ASP:CG	1:C:268:SER:H	2.20	0.42
1:D:10:LEU:CD2	1:D:13:ARG:NH2	2.83	0.42
1:D:265:ARG:O	1:D:265:ARG:HG3	2.20	0.42
1:D:379:ILE:O	1:D:382:TYR:N	2.52	0.42
1:F:1218:THR:H	1:F:1237:ASN:ND2	2.17	0.42
1:G:1135:PHE:HE1	1:G:1142:LEU:HD13	1.85	0.42
1:G:400:LEU:HB3	1:G:404:TRP:HZ3	1.85	0.42
1:G:767:LEU:HD21	1:G:801:VAL:HG11	2.01	0.42
2:H:14:CYS:SG	5:H:500:HEC:HBB3	2.59	0.42
2:L:14:CYS:SG	5:L:500:HEC:HBB3	2.59	0.42
2:N:40:THR:HG23	2:N:57:ILE:HG13	2.02	0.42
3:O:7:ARG:HA	3:O:10:ARG:HG3	2.02	0.42
1:A:265:ARG:O	1:A:265:ARG:HG3	2.20	0.42
1:B:268:SER:O	1:B:271:ASP:N	2.51	0.42
1:D:346:GLN:O	1:D:348:LYS:N	2.52	0.42
1:E:1050:PHE:CD1	1:E:1058:LEU:HD11	2.54	0.42
1:E:452:GLN:OE1	1:E:452:GLN:N	2.53	0.42
1:F:428:ARG:HG2	1:F:433:PHE:CE1	2.54	0.42
1:G:452:GLN:N	1:G:452:GLN:OE1	2.53	0.42
2:H:94:LEU:O	2:H:98:LEU:HG	2.20	0.42
2:M:40:THR:HG23	2:M:57:ILE:HG13	2.02	0.42
2:M:67:TYR:HD1	2:M:74:TYR:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:TRP:C	1:A:1034:LEU:H	2.23	0.42
1:A:582:LEU:O	1:A:586:GLN:HG3	2.19	0.42
1:A:864:VAL:HB	1:A:878:CYS:HB2	2.02	0.42
1:B:10:LEU:CD2	1:B:13:ARG:NH2	2.83	0.42
1:B:452:GLN:OE1	1:B:452:GLN:N	2.53	0.42
1:C:265:ARG:O	1:C:265:ARG:HG3	2.20	0.42
1:C:268:SER:O	1:C:271:ASP:N	2.51	0.42
1:C:452:GLN:OE1	1:C:452:GLN:N	2.53	0.42
1:C:864:VAL:HB	1:C:878:CYS:HB2	2.02	0.42
1:D:864:VAL:HB	1:D:878:CYS:HB2	2.02	0.42
1:D:989:GLU:HG2	1:D:991:VAL:H	1.85	0.42
1:E:265:ARG:O	1:E:265:ARG:HG3	2.20	0.42
1:E:266:ASP:CG	1:E:268:SER:H	2.20	0.42
1:F:989:GLU:HG2	1:F:991:VAL:H	1.85	0.42
1:G:334:PHE:HD2	1:G:337:ARG:HH11	1.66	0.42
1:G:676:SER:OG	1:G:678:ASP:OD1	2.37	0.42
1:G:725:LEU:HD11	1:G:742:HIS:CD2	2.54	0.42
1:G:965:SER:H	1:G:980:ASP:HA	1.84	0.42
2:J:94:LEU:O	2:J:98:LEU:HG	2.20	0.42
2:L:67:TYR:HD1	2:L:74:TYR:HB3	1.84	0.42
2:M:14:CYS:SG	5:M:500:HEC:HBB3	2.59	0.42
1:A:452:GLN:N	1:A:452:GLN:OE1	2.53	0.41
1:A:989:GLU:HG2	1:A:991:VAL:H	1.85	0.41
1:F:947:GLN:HG2	1:F:958:TYR:HD1	1.85	0.41
1:A:862:TYR:HB3	1:A:883:SER:C	2.41	0.41
1:B:456:LEU:O	1:B:459:LYS:HB3	2.20	0.41
1:D:1050:PHE:CD1	1:D:1058:LEU:HD11	2.54	0.41
1:D:266:ASP:CG	1:D:268:SER:H	2.20	0.41
1:F:369:SER:O	1:F:373:GLU:HG2	2.21	0.41
1:F:511:LYS:HB2	1:F:563:ILE:HG13	2.01	0.41
1:F:864:VAL:HB	1:F:878:CYS:HB2	2.02	0.41
2:K:67:TYR:HD1	2:K:74:TYR:HB3	1.84	0.41
2:K:94:LEU:O	2:K:98:LEU:HG	2.20	0.41
2:L:94:LEU:O	2:L:98:LEU:HG	2.20	0.41
1:A:1191:MET:SD	1:A:1209:SER:OG	2.63	0.41
1:A:145:GLY:HA2	1:A:259:GLN:HE21	1.85	0.41
1:C:269:VAL:C	1:C:271:ASP:H	2.24	0.41
1:G:1100:PHE:HB3	1:G:1111:ILE:HD11	2.00	0.41
1:G:282:VAL:O	1:G:282:VAL:HG12	2.21	0.41
1:G:947:GLN:HG2	1:G:958:TYR:HD1	1.85	0.41
2:I:41:GLY:HA2	2:I:48:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:PHE:HD2	1:A:337:ARG:HH11	1.66	0.41
1:B:725:LEU:HD11	1:B:742:HIS:CD2	2.54	0.41
1:B:862:TYR:HB3	1:B:883:SER:C	2.41	0.41
1:C:511:LYS:HB2	1:C:563:ILE:HG13	2.02	0.41
1:D:342:LEU:O	1:D:346:GLN:HG3	2.21	0.41
1:D:456:LEU:O	1:D:459:LYS:HB3	2.21	0.41
1:D:808:ALA:HB2	1:D:850:PRO:HA	2.02	0.41
1:D:885:VAL:HG13	1:D:900:SER:O	2.21	0.41
1:E:1135:PHE:HE1	1:E:1142:LEU:HD13	1.85	0.41
1:E:282:VAL:HG12	1:E:282:VAL:O	2.20	0.41
1:F:265:ARG:O	1:F:265:ARG:HG3	2.20	0.41
1:F:337:ARG:O	1:F:340:TYR:N	2.54	0.41
1:G:265:ARG:O	1:G:265:ARG:HG3	2.20	0.41
1:G:369:SER:O	1:G:373:GLU:HG2	2.20	0.41
2:I:40:THR:HG23	2:I:57:ILE:HG13	2.02	0.41
2:K:40:THR:HG23	2:K:57:ILE:HG13	2.02	0.41
1:A:676:SER:OG	1:A:678:ASP:OD1	2.37	0.41
1:B:808:ALA:HB2	1:B:850:PRO:HA	2.01	0.41
1:C:456:LEU:O	1:C:459:LYS:HB3	2.21	0.41
1:C:808:ALA:HB2	1:C:850:PRO:HA	2.01	0.41
1:D:268:SER:O	1:D:271:ASP:N	2.51	0.41
1:E:369:SER:O	1:E:373:GLU:HG2	2.20	0.41
1:E:474:SER:HA	1:E:475:PRO:HD2	1.91	0.41
1:F:452:GLN:OE1	1:F:452:GLN:N	2.53	0.41
2:N:94:LEU:O	2:N:98:LEU:HG	2.20	0.41
1:D:30:ILE:HG21	3:Q:10:ARG:HB3	1.93	0.41
3:Q:7:ARG:HA	3:Q:10:ARG:HG3	2.02	0.41
1:C:369:SER:O	1:C:373:GLU:HG2	2.20	0.41
1:D:400:LEU:HB3	1:D:404:TRP:HZ3	1.84	0.41
1:D:947:GLN:HG2	1:D:958:TYR:HD1	1.85	0.41
1:E:337:ARG:O	1:E:340:TYR:N	2.54	0.41
1:F:268:SER:O	1:F:271:ASP:N	2.51	0.41
1:F:282:VAL:HG12	1:F:282:VAL:O	2.20	0.41
1:F:456:LEU:O	1:F:459:LYS:HB3	2.21	0.41
1:F:884:TRP:HH2	2:M:79:LYS:N	2.18	0.41
1:G:337:ARG:O	1:G:340:TYR:N	2.54	0.41
1:G:989:GLU:HG2	1:G:991:VAL:H	1.85	0.41
1:A:884:TRP:HH2	2:H:78:THR:O	2.02	0.41
2:J:40:THR:HG23	2:J:57:ILE:HG13	2.02	0.41
2:L:40:THR:HG23	2:L:57:ILE:HG13	2.02	0.41
1:F:884:TRP:HH2	2:M:78:THR:O	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:94:LEU:O	2:M:98:LEU:HG	2.20	0.41
1:A:342:LEU:O	1:A:346:GLN:HG3	2.21	0.41
1:A:947:GLN:HG2	1:A:958:TYR:HD1	1.85	0.41
1:B:282:VAL:HG12	1:B:282:VAL:O	2.21	0.41
1:C:700:GLU:HB2	1:C:720:SER:HB2	2.03	0.41
1:D:216:LEU:HA	1:D:217:PRO:HD2	1.84	0.41
1:D:282:VAL:O	1:D:282:VAL:HG12	2.20	0.41
1:G:342:LEU:O	1:G:346:GLN:HG3	2.21	0.41
1:G:862:TYR:HB3	1:G:883:SER:C	2.41	0.41
1:A:1135:PHE:HE1	1:A:1142:LEU:HD13	1.85	0.41
1:A:725:LEU:HD11	1:A:742:HIS:CD2	2.54	0.41
1:B:145:GLY:HA2	1:B:259:GLN:HE21	1.85	0.41
1:B:569:CYS:CB	1:B:600:LYS:HZ3	2.33	0.41
1:B:885:VAL:HG13	1:B:900:SER:O	2.21	0.41
1:C:153:HIS:HA	1:C:264:THR:O	2.21	0.41
1:C:584:ALA:CA	1:C:594:TYR:CE2	2.98	0.41
1:C:762:SER:OG	1:C:764:ASP:OD1	2.26	0.41
1:D:196:LEU:O	1:D:199:LEU:HB2	2.21	0.41
1:E:1032:TRP:C	1:E:1034:LEU:H	2.23	0.41
1:E:334:PHE:HD2	1:E:337:ARG:HH11	1.66	0.41
1:E:864:VAL:HB	1:E:878:CYS:HB2	2.02	0.41
1:F:322:LEU:HD23	1:F:364:LEU:HD13	2.03	0.41
1:F:676:SER:OG	1:F:678:ASP:OD1	2.37	0.41
1:F:885:VAL:HG13	1:F:900:SER:O	2.21	0.41
1:G:864:VAL:HB	1:G:878:CYS:HB2	2.02	0.41
2:I:30:PRO:HB3	2:I:46:PHE:CD2	2.56	0.41
2:K:30:PRO:HB3	2:K:46:PHE:CD2	2.56	0.41
2:M:55:LYS:HG2	2:M:75:ILE:HG12	2.03	0.41
1:A:400:LEU:HB3	1:A:404:TRP:HZ3	1.84	0.41
1:B:369:SER:O	1:B:373:GLU:HG2	2.21	0.41
1:B:400:LEU:HB3	1:B:404:TRP:HZ3	1.84	0.41
1:B:700:GLU:HB2	1:B:720:SER:HB2	2.03	0.41
1:C:196:LEU:O	1:C:199:LEU:HB2	2.21	0.41
1:C:282:VAL:O	1:C:282:VAL:HG12	2.21	0.41
1:C:342:LEU:O	1:C:346:GLN:HG3	2.21	0.41
1:C:862:TYR:HB3	1:C:883:SER:C	2.41	0.41
1:D:1032:TRP:C	1:D:1034:LEU:H	2.23	0.41
1:D:369:SER:O	1:D:373:GLU:HG2	2.21	0.41
1:E:530:ARG:HD2	1:E:545:GLN:NE2	2.36	0.41
1:E:884:TRP:HH2	2:L:78:THR:O	2.02	0.41
1:F:1141:LEU:HG	1:F:1155:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ARG:HD3	1:G:256:SER:HB3	2.03	0.41
1:G:326:LEU:HA	1:G:326:LEU:HD23	1.44	0.41
2:I:67:TYR:HD1	2:I:74:TYR:HB3	1.84	0.41
2:L:55:LYS:HG2	2:L:75:ILE:HG12	2.03	0.41
1:B:864:VAL:HB	1:B:878:CYS:HB2	2.02	0.41
1:D:530:ARG:HD2	1:D:545:GLN:NE2	2.36	0.41
1:E:10:LEU:CD2	1:E:13:ARG:NH2	2.83	0.41
1:E:565:GLN:OE1	1:E:1212:THR:HB	2.21	0.41
1:E:322:LEU:HD23	1:E:364:LEU:HD13	2.03	0.41
1:E:456:LEU:O	1:E:459:LYS:HB3	2.21	0.41
1:E:511:LYS:HB2	1:E:563:ILE:HG13	2.02	0.41
1:F:565:GLN:OE1	1:F:1212:THR:HB	2.21	0.41
1:F:862:TYR:HB3	1:F:883:SER:C	2.41	0.41
1:G:565:GLN:OE1	1:G:1212:THR:HB	2.21	0.41
1:G:456:LEU:O	1:G:459:LYS:HB3	2.21	0.41
2:L:30:PRO:HB3	2:L:46:PHE:CD2	2.56	0.41
5:M:500:HEC:HMC1	5:M:500:HEC:CBC	2.51	0.41
1:A:153:HIS:HA	1:A:264:THR:O	2.21	0.41
1:B:337:ARG:O	1:B:340:TYR:N	2.54	0.41
1:B:342:LEU:O	1:B:346:GLN:HG3	2.21	0.41
1:B:676:SER:OG	1:B:678:ASP:OD1	2.37	0.41
1:C:569:CYS:HB3	1:C:600:LYS:HZ3	1.85	0.41
1:D:474:SER:HA	1:D:475:PRO:HD2	1.91	0.41
1:D:511:LYS:HB2	1:D:563:ILE:HG13	2.02	0.41
1:D:700:GLU:HB2	1:D:720:SER:HB2	2.03	0.41
1:E:342:LEU:O	1:E:346:GLN:HG3	2.21	0.41
1:E:676:SER:OG	1:E:678:ASP:OD1	2.37	0.41
1:E:947:GLN:HG2	1:E:958:TYR:HD1	1.85	0.41
1:F:1032:TRP:C	1:F:1034:LEU:H	2.23	0.41
1:F:153:HIS:HA	1:F:264:THR:O	2.21	0.41
1:F:400:LEU:HB3	1:F:404:TRP:HZ3	1.85	0.41
2:J:30:PRO:HB3	2:J:46:PHE:CD2	2.56	0.41
5:N:500:HEC:CBC	5:N:500:HEC:HMC1	2.51	0.41
1:A:1155:ASN:HB3	1:A:1162:LEU:HB2	2.04	0.40
1:B:269:VAL:C	1:B:271:ASP:H	2.24	0.40
1:B:351:LYS:NZ	1:B:365:ASP:OD2	2.54	0.40
1:C:1141:LEU:HG	1:C:1155:ASN:HA	2.03	0.40
1:C:322:LEU:HD23	1:C:364:LEU:HD13	2.03	0.40
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.44	0.40
1:C:885:VAL:HG13	1:C:900:SER:O	2.21	0.40
1:D:1141:LEU:HG	1:D:1155:ASN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1166:ALA:HA	1:D:1167:PRO:HD2	1.93	0.40
1:D:37:ILE:HG12	3:Q:10:ARG:HD2	2.03	0.40
1:D:862:TYR:HB3	1:D:883:SER:C	2.41	0.40
1:E:153:HIS:HA	1:E:264:THR:O	2.21	0.40
1:E:885:VAL:HG13	1:E:900:SER:O	2.21	0.40
1:F:1155:ASN:HB3	1:F:1162:LEU:HB2	2.04	0.40
1:F:631:ALA:H	1:F:665:PHE:HZ	1.69	0.40
1:G:1141:LEU:HG	1:G:1155:ASN:HA	2.03	0.40
1:G:1155:ASN:HB3	1:G:1162:LEU:HB2	2.04	0.40
1:G:322:LEU:HD23	1:G:364:LEU:HD13	2.03	0.40
2:N:55:LYS:HG2	2:N:75:ILE:HG12	2.03	0.40
3:R:14:LEU:HA	3:R:14:LEU:HD13	1.97	0.40
1:A:228:ARG:HD3	1:A:256:SER:HB3	2.03	0.40
1:A:282:VAL:HG12	1:A:282:VAL:O	2.21	0.40
1:A:289:GLU:OE2	1:A:303:LYS:NZ	2.43	0.40
1:D:1135:PHE:HE1	1:D:1142:LEU:HD13	1.85	0.40
1:D:565:GLN:OE1	1:D:1212:THR:HB	2.21	0.40
1:D:153:HIS:HA	1:D:264:THR:O	2.21	0.40
1:E:1155:ASN:HB3	1:E:1162:LEU:HB2	2.04	0.40
1:E:196:LEU:O	1:E:199:LEU:HB2	2.21	0.40
1:E:862:TYR:HB3	1:E:883:SER:C	2.41	0.40
1:F:530:ARG:HD2	1:F:545:GLN:NE2	2.36	0.40
1:F:584:ALA:CA	1:F:594:TYR:CE2	2.98	0.40
1:G:196:LEU:O	1:G:199:LEU:HB2	2.21	0.40
2:H:30:PRO:HB3	2:H:46:PHE:CD2	2.56	0.40
5:H:500:HEC:HMC1	5:H:500:HEC:CBC	2.51	0.40
5:I:500:HEC:CBC	5:I:500:HEC:HMC1	2.51	0.40
5:J:500:HEC:CBC	5:J:500:HEC:HMC1	2.51	0.40
3:P:34:LEU:HD12	3:P:34:LEU:HA	1.93	0.40
1:A:885:VAL:HG13	1:A:900:SER:O	2.21	0.40
1:B:884:TRP:HH2	2:I:79:LYS:N	2.18	0.40
1:B:947:GLN:HG2	1:B:958:TYR:HD1	1.85	0.40
1:C:1032:TRP:C	1:C:1034:LEU:H	2.23	0.40
1:C:947:GLN:HG2	1:C:958:TYR:HD1	1.85	0.40
1:E:351:LYS:NZ	1:E:365:ASP:OD2	2.54	0.40
1:E:7:ASN:CG	1:F:236:PRO:CG	2.81	0.40
1:E:989:GLU:HG2	1:E:991:VAL:H	1.85	0.40
1:G:153:HIS:HA	1:G:264:THR:O	2.21	0.40
1:G:631:ALA:H	1:G:665:PHE:HZ	1.69	0.40
2:K:55:LYS:HG2	2:K:75:ILE:HG12	2.03	0.40
5:L:500:HEC:CBC	5:L:500:HEC:HMC1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:14:LEU:HD13	3:Q:14:LEU:HA	1.98	0.40
1:A:1141:LEU:HG	1:A:1155:ASN:HA	2.03	0.40
1:A:196:LEU:O	1:A:199:LEU:HB2	2.21	0.40
1:B:1146:ASP:HB2	1:B:1150:GLU:HG2	2.04	0.40
1:B:228:ARG:HD3	1:B:256:SER:HB3	2.03	0.40
1:B:266:ASP:CG	1:B:268:SER:HG	2.23	0.40
1:C:337:ARG:O	1:C:340:TYR:N	2.54	0.40
1:C:351:LYS:NZ	1:C:365:ASP:OD2	2.54	0.40
1:C:884:TRP:HH2	2:J:79:LYS:N	2.18	0.40
1:C:989:GLU:HG2	1:C:991:VAL:H	1.85	0.40
1:D:597:TRP:CD2	1:D:600:LYS:HE3	2.57	0.40
1:E:631:ALA:H	1:E:665:PHE:HZ	1.69	0.40
1:F:289:GLU:OE2	1:F:303:LYS:NZ	2.43	0.40
2:H:55:LYS:HG2	2:H:75:ILE:HG12	2.03	0.40
2:H:39:LYS:HD2	2:H:56:GLY:O	2.22	0.40
2:I:71:PRO:CD	2:I:84:GLY:HA2	2.52	0.40
2:J:55:LYS:HG2	2:J:75:ILE:HG12	2.03	0.40
2:M:39:LYS:HD2	2:M:56:GLY:O	2.22	0.40
1:A:217:PRO:HG3	1:A:226:ARG:NH1	2.36	0.40
1:A:369:SER:O	1:A:373:GLU:HG2	2.21	0.40
1:A:597:TRP:CD2	1:A:600:LYS:HE3	2.57	0.40
1:B:322:LEU:HD23	1:B:364:LEU:HD13	2.02	0.40
1:D:145:GLY:HA2	1:D:259:GLN:HE21	1.85	0.40
1:E:400:LEU:HB3	1:E:404:TRP:HZ3	1.84	0.40
2:I:55:LYS:HG2	2:I:75:ILE:HG12	2.03	0.40
5:K:500:HEC:CBC	5:K:500:HEC:HMC1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	32	73
1	B	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	32	73
1	C	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	32	73
1	D	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	32	73
1	E	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	32	73
1	F	1135/1248 (91%)	1045 (92%)	84 (7%)	6 (0%)	32	73
1	G	1228/1248 (98%)	1138 (93%)	84 (7%)	6 (0%)	32	73
2	H	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	I	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	J	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	K	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	L	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	M	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	N	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
3	O	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	P	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	Q	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
3	R	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
All	All	9403/9844 (96%)	8741 (93%)	620 (7%)	42 (0%)	42	76

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	ILE
1	B	1073	ILE
1	C	1073	ILE
1	D	1073	ILE
1	E	1073	ILE
1	F	1073	ILE
1	G	1073	ILE
1	A	591	GLY
1	B	591	GLY
1	C	591	GLY
1	D	591	GLY
1	E	591	GLY
1	F	591	GLY
1	G	591	GLY

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Mol	Chain	Res	Type
1	A	347	ASN
1	B	347	ASN
1	C	347	ASN
1	D	347	ASN
1	E	347	ASN
1	F	347	ASN
1	G	347	ASN
1	A	266	ASP
1	B	266	ASP
1	C	266	ASP
1	D	266	ASP
1	E	266	ASP
1	F	266	ASP
1	G	266	ASP
1	A	613	PRO
1	B	613	PRO
1	C	613	PRO
1	D	613	PRO
1	E	613	PRO
1	F	613	PRO
1	G	613	PRO
1	A	1205	VAL
1	B	1205	VAL
1	C	1205	VAL
1	D	1205	VAL
1	E	1205	VAL
1	F	1205	VAL
1	G	1205	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1022/1119 (91%)	1019 (100%)	3 (0%)	94	96
1	B	1106/1119 (99%)	1101 (100%)	5 (0%)	91	96
1	C	1022/1119 (91%)	1019 (100%)	3 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	1106/1119 (99%)	1101 (100%)	5 (0%)	91	96
1	E	1106/1119 (99%)	1101 (100%)	5 (0%)	91	96
1	F	1022/1119 (91%)	1019 (100%)	3 (0%)	94	96
1	G	1106/1119 (99%)	1101 (100%)	5 (0%)	91	96
2	H	84/84 (100%)	84 (100%)	0	100	100
2	I	84/84 (100%)	84 (100%)	0	100	100
2	J	84/84 (100%)	84 (100%)	0	100	100
2	K	84/84 (100%)	84 (100%)	0	100	100
2	L	84/84 (100%)	84 (100%)	0	100	100
2	M	84/84 (100%)	84 (100%)	0	100	100
2	N	84/84 (100%)	84 (100%)	0	100	100
3	O	84/84 (100%)	77 (92%)	7 (8%)	13	47
3	P	84/84 (100%)	77 (92%)	7 (8%)	13	47
3	Q	84/84 (100%)	77 (92%)	7 (8%)	13	47
3	R	84/84 (100%)	77 (92%)	7 (8%)	13	47
All	All	8414/8757 (96%)	8357 (99%)	57 (1%)	87	94

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	LYS
1	A	392	ASP
1	A	884	TRP
1	B	58	LYS
1	B	81	LYS
1	B	391	LYS
1	B	392	ASP
1	B	884	TRP
1	C	391	LYS
1	C	392	ASP
1	C	884	TRP
1	D	58	LYS
1	D	81	LYS
1	D	391	LYS
1	D	392	ASP
1	D	884	TRP
1	E	58	LYS

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Mol	Chain	Res	Type
1	E	81	LYS
1	E	391	LYS
1	E	392	ASP
1	E	884	TRP
1	F	391	LYS
1	F	392	ASP
1	F	884	TRP
1	G	58	LYS
1	G	81	LYS
1	G	391	LYS
1	G	392	ASP
1	G	884	TRP
3	O	10	ARG
3	O	14	LEU
3	O	20	LEU
3	O	34	LEU
3	O	87	SER
3	O	92	ASN
3	O	93	ARG
3	P	10	ARG
3	P	14	LEU
3	P	20	LEU
3	P	34	LEU
3	P	87	SER
3	P	92	ASN
3	P	93	ARG
3	Q	10	ARG
3	Q	14	LEU
3	Q	20	LEU
3	Q	34	LEU
3	Q	87	SER
3	Q	92	ASN
3	Q	93	ARG
3	R	10	ARG
3	R	14	LEU
3	R	20	LEU
3	R	34	LEU
3	R	87	SER
3	R	92	ASN
3	R	93	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	201	ASN
1	A	214	GLN
1	A	602	ASN
1	A	703	ASN
1	A	712	HIS
1	A	713	HIS
1	A	782	ASN
1	A	819	ASN
1	A	844	GLN
1	A	924	GLN
1	A	992	ASN
1	A	1076	ASN
1	A	1126	HIS
1	B	11	GLN
1	B	45	ASN
1	B	51	GLN
1	B	201	ASN
1	B	214	GLN
1	B	602	ASN
1	B	703	ASN
1	B	712	HIS
1	B	713	HIS
1	B	782	ASN
1	B	819	ASN
1	B	844	GLN
1	B	924	GLN
1	B	992	ASN
1	B	1076	ASN
1	B	1126	HIS
1	C	121	GLN
1	C	201	ASN
1	C	214	GLN
1	C	416	GLN
1	C	602	ASN
1	C	703	ASN
1	C	712	HIS
1	C	713	HIS
1	C	782	ASN
1	C	819	ASN
1	C	844	GLN
1	C	924	GLN
1	C	992	ASN

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Mol	Chain	Res	Type
1	C	1076	ASN
1	C	1126	HIS
1	D	11	GLN
1	D	51	GLN
1	D	201	ASN
1	D	214	GLN
1	D	416	GLN
1	D	602	ASN
1	D	703	ASN
1	D	712	HIS
1	D	713	HIS
1	D	782	ASN
1	D	819	ASN
1	D	844	GLN
1	D	924	GLN
1	D	992	ASN
1	D	1076	ASN
1	D	1126	HIS
1	E	11	GLN
1	E	45	ASN
1	E	51	GLN
1	E	201	ASN
1	E	214	GLN
1	E	602	ASN
1	E	703	ASN
1	E	712	HIS
1	E	713	HIS
1	E	782	ASN
1	E	819	ASN
1	E	844	GLN
1	E	924	GLN
1	E	992	ASN
1	E	1076	ASN
1	E	1126	HIS
1	F	201	ASN
1	F	214	GLN
1	F	416	GLN
1	F	602	ASN
1	F	703	ASN
1	F	712	HIS
1	F	713	HIS
1	F	782	ASN

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Mol	Chain	Res	Type
1	F	819	ASN
1	F	844	GLN
1	F	924	GLN
1	F	992	ASN
1	F	1076	ASN
1	F	1126	HIS
1	G	11	GLN
1	G	45	ASN
1	G	51	GLN
1	G	121	GLN
1	G	201	ASN
1	G	214	GLN
1	G	416	GLN
1	G	602	ASN
1	G	703	ASN
1	G	712	HIS
1	G	713	HIS
1	G	782	ASN
1	G	819	ASN
1	G	844	GLN
1	G	924	GLN
1	G	992	ASN
1	G	1076	ASN
1	G	1126	HIS
2	H	70	ASN
2	I	70	ASN
2	K	70	ASN
2	M	70	ASN
2	N	70	ASN
3	O	44	GLN
3	O	92	ASN
3	P	44	GLN
3	P	92	ASN
3	Q	44	GLN
3	Q	92	ASN
3	R	38	HIS
3	R	44	GLN
3	R	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

14 ligands are modelled in this entry.

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$
4	DTP	A	1301	-	26,32,32	3.24	7 (26%)	26,50,50	2.79	3 (11%)
4	DTP	B	1301	-	26,32,32	3.23	7 (26%)	26,50,50	2.78	3 (11%)
4	DTP	C	1301	-	26,32,32	3.23	7 (26%)	26,50,50	2.78	3 (11%)
4	DTP	D	1301	-	26,32,32	3.24	7 (26%)	26,50,50	2.79	3 (11%)
4	DTP	E	1301	-	26,32,32	3.24	7 (26%)	26,50,50	2.79	3 (11%)
4	DTP	F	1301	-	26,32,32	3.24	7 (26%)	26,50,50	2.78	3 (11%)
4	DTP	G	1301	-	26,32,32	3.24	7 (26%)	26,50,50	2.79	3 (11%)
5	HEC	H	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.81	3 (18%)
5	HEC	I	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.81	3 (18%)
5	HEC	J	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.81	3 (18%)
5	HEC	K	500	-	28,50,50	2.32	5 (17%)	16,82,82	1.82	3 (18%)
5	HEC	L	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.81	3 (18%)
5	HEC	M	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.81	3 (18%)
5	HEC	N	500	-	28,50,50	2.31	5 (17%)	16,82,82	1.82	3 (18%)

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
4	DTP	A	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	B	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	C	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	D	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	E	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	F	1301	-	-	0/18/34/34	0/3/3/3
4	DTP	G	1301	-	-	0/18/34/34	0/3/3/3
5	HEC	H	500	-	-	0/6/54/54	0/0/8/8
5	HEC	I	500	-	-	0/6/54/54	0/0/8/8
5	HEC	J	500	-	-	0/6/54/54	0/0/8/8
5	HEC	K	500	-	-	0/6/54/54	0/0/8/8
5	HEC	L	500	-	-	0/6/54/54	0/0/8/8
5	HEC	M	500	-	-	0/6/54/54	0/0/8/8
5	HEC	N	500	-	-	0/6/54/54	0/0/8/8

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1301	DTP	C2'-C3'	-11.81	1.21	1.52
4	G	1301	DTP	C2'-C3'	-11.80	1.21	1.52
4	F	1301	DTP	C2'-C3'	-11.80	1.21	1.52
4	A	1301	DTP	C2'-C3'	-11.79	1.21	1.52
4	E	1301	DTP	C2'-C3'	-11.78	1.21	1.52
4	C	1301	DTP	C2'-C3'	-11.78	1.21	1.52
4	B	1301	DTP	C2'-C3'	-11.76	1.21	1.52
4	G	1301	DTP	O4'-C4'	-8.14	1.26	1.45
4	D	1301	DTP	O4'-C4'	-8.13	1.26	1.45
4	F	1301	DTP	O4'-C4'	-8.13	1.26	1.45
4	A	1301	DTP	O4'-C4'	-8.13	1.26	1.45
4	E	1301	DTP	O4'-C4'	-8.13	1.26	1.45
4	C	1301	DTP	O4'-C4'	-8.13	1.26	1.45
4	B	1301	DTP	O4'-C4'	-8.11	1.26	1.45
5	K	500	HEC	C3B-C2B	-5.49	1.35	1.40
5	N	500	HEC	C3B-C2B	-5.46	1.35	1.40
5	J	500	HEC	C3B-C2B	-5.45	1.35	1.40
5	L	500	HEC	C3B-C2B	-5.45	1.35	1.40
5	I	500	HEC	C3B-C2B	-5.44	1.35	1.40
5	M	500	HEC	C3B-C2B	-5.44	1.35	1.40
5	H	500	HEC	C3B-C2B	-5.42	1.35	1.40
5	J	500	HEC	C3C-C2C	-5.12	1.35	1.40
5	I	500	HEC	C3C-C2C	-5.12	1.35	1.40
5	K	500	HEC	C3C-C2C	-5.11	1.35	1.40
5	H	500	HEC	C3C-C2C	-5.11	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	500	HEC	C3C-C2C	-5.09	1.35	1.40
5	N	500	HEC	C3C-C2C	-5.09	1.35	1.40
5	M	500	HEC	C3C-C2C	-5.08	1.35	1.40
5	N	500	HEC	CBB-CAB	-3.88	1.34	1.49
5	H	500	HEC	CBB-CAB	-3.86	1.34	1.49
5	M	500	HEC	CBB-CAB	-3.86	1.34	1.49
5	L	500	HEC	CBB-CAB	-3.86	1.34	1.49
5	J	500	HEC	CBB-CAB	-3.86	1.34	1.49
5	K	500	HEC	CBB-CAB	-3.85	1.34	1.49
5	I	500	HEC	CBB-CAB	-3.85	1.34	1.49
5	H	500	HEC	CBC-CAC	-3.81	1.34	1.49
5	J	500	HEC	CBC-CAC	-3.81	1.34	1.49
5	N	500	HEC	CBC-CAC	-3.80	1.34	1.49
5	L	500	HEC	CBC-CAC	-3.79	1.34	1.49
5	K	500	HEC	CBC-CAC	-3.79	1.34	1.49
5	I	500	HEC	CBC-CAC	-3.79	1.34	1.49
5	M	500	HEC	CBC-CAC	-3.79	1.34	1.49
4	C	1301	DTP	C5-C4	-2.82	1.34	1.40
4	A	1301	DTP	C5-C4	-2.80	1.34	1.40
4	F	1301	DTP	C5-C4	-2.80	1.34	1.40
4	B	1301	DTP	C5-C4	-2.80	1.34	1.40
4	D	1301	DTP	C5-C4	-2.79	1.34	1.40
4	E	1301	DTP	C5-C4	-2.79	1.34	1.40
4	G	1301	DTP	C5-C4	-2.79	1.34	1.40
4	F	1301	DTP	C2-N3	2.31	1.36	1.32
4	B	1301	DTP	C2-N3	2.33	1.36	1.32
4	A	1301	DTP	C2-N3	2.34	1.36	1.32
4	C	1301	DTP	C2-N3	2.34	1.36	1.32
4	E	1301	DTP	C2-N3	2.35	1.36	1.32
4	D	1301	DTP	C2-N3	2.36	1.36	1.32
4	G	1301	DTP	C2-N3	2.39	1.36	1.32
4	E	1301	DTP	O3'-C3'	2.59	1.49	1.43
4	D	1301	DTP	O3'-C3'	2.60	1.49	1.43
4	B	1301	DTP	O3'-C3'	2.60	1.49	1.43
4	A	1301	DTP	O3'-C3'	2.62	1.49	1.43
4	C	1301	DTP	O3'-C3'	2.62	1.49	1.43
4	F	1301	DTP	O3'-C3'	2.64	1.49	1.43
4	G	1301	DTP	O3'-C3'	2.66	1.49	1.43
4	B	1301	DTP	O4'-C1'	3.25	1.49	1.42
4	F	1301	DTP	O4'-C1'	3.25	1.49	1.42
4	C	1301	DTP	O4'-C1'	3.26	1.49	1.42
4	G	1301	DTP	O4'-C1'	3.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	DTP	O4'-C1'	3.28	1.49	1.42
4	D	1301	DTP	O4'-C1'	3.29	1.49	1.42
4	E	1301	DTP	O4'-C1'	3.30	1.49	1.42
4	F	1301	DTP	C3'-C4'	3.98	1.64	1.53
4	A	1301	DTP	C3'-C4'	3.99	1.64	1.53
4	B	1301	DTP	C3'-C4'	3.99	1.64	1.53
4	C	1301	DTP	C3'-C4'	3.99	1.64	1.53
4	G	1301	DTP	C3'-C4'	3.99	1.64	1.53
4	E	1301	DTP	C3'-C4'	4.01	1.64	1.53
4	D	1301	DTP	C3'-C4'	4.02	1.64	1.53
5	N	500	HEC	C3D-C2D	5.43	1.53	1.37
5	M	500	HEC	C3D-C2D	5.45	1.53	1.37
5	L	500	HEC	C3D-C2D	5.46	1.53	1.37
5	J	500	HEC	C3D-C2D	5.46	1.53	1.37
5	H	500	HEC	C3D-C2D	5.47	1.53	1.37
5	I	500	HEC	C3D-C2D	5.47	1.53	1.37
5	K	500	HEC	C3D-C2D	5.48	1.53	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1301	DTP	N3-C2-N1	-10.17	120.00	128.86
4	G	1301	DTP	N3-C2-N1	-10.16	120.01	128.86
4	E	1301	DTP	N3-C2-N1	-10.16	120.01	128.86
4	C	1301	DTP	N3-C2-N1	-10.12	120.04	128.86
4	A	1301	DTP	N3-C2-N1	-10.12	120.04	128.86
4	B	1301	DTP	N3-C2-N1	-10.09	120.07	128.86
4	F	1301	DTP	N3-C2-N1	-10.05	120.10	128.86
4	D	1301	DTP	N6-C6-N1	-6.32	106.23	118.77
4	G	1301	DTP	N6-C6-N1	-6.32	106.24	118.77
4	E	1301	DTP	N6-C6-N1	-6.32	106.24	118.77
4	F	1301	DTP	N6-C6-N1	-6.32	106.24	118.77
4	B	1301	DTP	N6-C6-N1	-6.31	106.25	118.77
4	A	1301	DTP	N6-C6-N1	-6.31	106.25	118.77
4	C	1301	DTP	N6-C6-N1	-6.30	106.28	118.77
5	K	500	HEC	CMB-C2B-C1B	-3.96	122.38	128.46
5	I	500	HEC	CMB-C2B-C1B	-3.93	122.42	128.46
5	N	500	HEC	CMB-C2B-C1B	-3.93	122.43	128.46
5	J	500	HEC	CMB-C2B-C1B	-3.93	122.43	128.46
5	M	500	HEC	CMB-C2B-C1B	-3.93	122.43	128.46
5	L	500	HEC	CMB-C2B-C1B	-3.92	122.43	128.46
5	H	500	HEC	CMB-C2B-C1B	-3.92	122.44	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	500	HEC	CMC-C2C-C1C	-3.39	123.26	128.46
5	J	500	HEC	CMC-C2C-C1C	-3.37	123.28	128.46
5	M	500	HEC	CMC-C2C-C1C	-3.37	123.28	128.46
5	I	500	HEC	CMC-C2C-C1C	-3.37	123.28	128.46
5	L	500	HEC	CMC-C2C-C1C	-3.37	123.29	128.46
5	H	500	HEC	CMC-C2C-C1C	-3.36	123.29	128.46
5	K	500	HEC	CMC-C2C-C1C	-3.35	123.31	128.46
5	K	500	HEC	CAD-CBD-CGD	-2.03	109.19	112.66
5	H	500	HEC	CAD-CBD-CGD	-2.03	109.19	112.66
5	N	500	HEC	CAD-CBD-CGD	-2.03	109.19	112.66
5	L	500	HEC	CAD-CBD-CGD	-2.02	109.20	112.66
5	M	500	HEC	CAD-CBD-CGD	-2.02	109.21	112.66
5	J	500	HEC	CAD-CBD-CGD	-2.01	109.22	112.66
5	I	500	HEC	CAD-CBD-CGD	-2.01	109.23	112.66
4	G	1301	DTP	C5-C6-N6	6.60	133.92	120.47
4	D	1301	DTP	C5-C6-N6	6.60	133.93	120.47
4	C	1301	DTP	C5-C6-N6	6.61	133.94	120.47
4	A	1301	DTP	C5-C6-N6	6.62	133.97	120.47
4	B	1301	DTP	C5-C6-N6	6.63	133.98	120.47
4	F	1301	DTP	C5-C6-N6	6.63	133.98	120.47
4	E	1301	DTP	C5-C6-N6	6.65	134.02	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	3	0
4	B	1301	DTP	3	0
4	C	1301	DTP	3	0
4	D	1301	DTP	3	0
4	E	1301	DTP	3	0
4	F	1301	DTP	3	0
4	G	1301	DTP	3	0
5	H	500	HEC	4	0
5	I	500	HEC	4	0
5	J	500	HEC	4	0
5	K	500	HEC	4	0
5	L	500	HEC	4	0
5	M	500	HEC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	500	HEC	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.